Supporting Information file

Carbon Di-carbene Allotrope as a Zero-Dimensional Carbon Platform for Small-Molecule Activation and Nitrogen-to-Ammonia Conversion

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Supporting Information file

S1.1 CDCA-Singlet

%chk=cdca.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd/Def2TZVP

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300
C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000

S1.2CDCA-Triplet

%chk=t-nbo-cdca.chk
%nprocshared=6
%mem=6GB
#p opt freq rowb97xd/def2tzvp

title card

0 3

C	3.62262800	-0.67438000	0.01007700
C	3.00695200	-1.72787100	0.04940200
C	3.62220900	0.67414800	-0.00988900
C	1.85421700	-2.42718700	0.05012200
C	3.00731400	1.72808300	-0.04931600
C	0.64420900	-2.57267900	0.05758300
C	1.85421600	2.42685400	-0.05015600
C	-0.66665200	-2.25387800	0.01662100
C	0.64428700	2.57290500	-0.05768000
C	-1.73178100	-1.67109600	-0.02586900
C	-0.66652700	2.25381700	-0.01676200

C	-2.68701500	-0.67952200	-0.16825000
C	-1.73175700	1.67120200	0.02547100
C	-2.68690200	0.67957500	0.16810500
C	-4.04286500	-0.40264400	-0.60178100
C	-4.04253300	0.40267300	0.60232200

S1.3 CDCA – CO

%chk=cdca-co.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300
C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
O	-4.94490341	-0.84295081	-1.49802607
C	-5.01505624	0.87223713	1.57921281

S1.4 CDCA – NO

%chk=cdca-no.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd/lanl2dz

title card

0 2

C	4.33938800	-0.67898800	0.04886600
C	3.69799000	-1.75991800	0.16149800
C	4.34289200	0.65204000	-0.06877800

C	2.55195000	-2.44220400	0.22353500
C	3.71309500	1.74032900	-0.17516400
C	1.30268300	-2.59086000	0.24087200
C	2.57131900	2.43075700	-0.22767900
C	0.00732200	-2.26450500	0.19716500
C	1.32386000	2.59412700	-0.23403200
C	-1.09199400	-1.67273200	0.10476000
C	0.02599200	2.27915700	-0.17849300
C	-2.03388900	-0.69980600	-0.08492900
C	-1.07824900	1.69829900	-0.07582900
C	-2.02614700	0.73369600	0.12472700
C	-3.46215400	-0.46947100	-0.51657200
C	-3.45272000	0.51597200	0.57179600
N	-4.64541468	0.14828419	0.21706594
O	-4.20257582	0.36903864	-0.72126122

S1.5 CDCA – CO_2

%chk=cdca-co2.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300
C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
O	-4.94490341	-0.84295081	-1.49802607
C	-5.01505624	0.87223713	1.57921281
O	-5.81111857	1.24977618	2.47772246

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S1.6 CDCA – NO_2

%chk=cdca-no2.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 2

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300
C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
O	-4.94490341	-0.84295081	-1.49802607
N	-4.98310999	0.85708637	1.54315533
O	-4.49549974	1.35544304	2.72920024

S1.7 CDCA – H_2O

%chk=cdca-h2o.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300

C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
O	-4.94490341	-0.84295081	-1.49802607
H	-4.60473017	-1.19163028	-2.32525324
H	-4.80541293	0.77281214	1.34259008

S1.8 CDCA – SO_2

%chk=cdca-so2.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300
C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
O	-4.94490341	-0.84295081	-1.49802607
S	-5.09128442	0.90838895	1.66525094
O	-4.22402011	1.46123257	2.98096997

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S1.9 CDCA – SO_3

%chk=cdca-so3.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300
C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
O	-4.94490341	-0.84295081	-1.49802607
S	-5.18851489	0.95450127	1.77499419
O	-6.83683566	0.85060158	1.52772210
O	-4.59663444	1.55942613	3.21466202

S1.10 CDCA – N_2 Type-a

%chk=cdca-n2-a.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300

C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
N	-4.97425878	-0.85690778	-1.53113838
N	-5.72279478	-1.30645956	-2.32352330

S1.11 CDCA – N_2 Type-b

%chk=cdca-n2-b.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	3.67177500	-0.66746800	0.01221400
C	3.03520800	-1.75658800	0.04517200
C	3.66925000	0.66854300	-0.01135100
C	1.89227700	-2.44681700	0.05319200
C	3.03458600	1.75871400	-0.04399100
C	0.64369300	-2.60207300	0.05369300
C	1.88966900	2.44586400	-0.05351300
C	-0.65304600	-2.27941400	0.02653300
C	0.64146100	2.60353200	-0.05465200
C	-1.75482700	-1.68766700	-0.02951400
C	-0.65508100	2.27946200	-0.02800600
C	-2.70061800	-0.70813700	-0.15495500
C	-1.75690700	1.68773700	0.02789600
C	-2.70095800	0.70704700	0.15520200
C	-4.12795100	-0.45453200	-0.57651900
C	-4.12853200	0.45179600	0.57860000
N	-4.97425878	-0.85690778	-1.53113838
N	-4.95635105	0.84439573	1.51295273

S1.12 CDCA – N(NH_2)

%chk=cdca-n2-b-h2.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

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title card

0 1

C	4.41321400	0.67386800	-0.00063200
C	3.74239400	1.69531500	-0.00207300
C	4.41328900	-0.67389300	0.00083400
C	2.53503200	2.29160400	-0.00303800
C	3.74234900	-1.69526300	0.00218100
C	1.31687800	2.34061300	-0.00326200
C	2.53503900	-2.29164500	0.00302100
C	0.01565300	1.98966300	-0.00247500
C	1.31688100	-2.34059800	0.00309800
C	-1.06870400	1.44414400	-0.00124900
C	0.01564900	-1.98968700	0.00221700
C	-2.24548500	0.69116500	-0.00033300
C	-1.06870200	-1.44415400	0.00112800
C	-2.24548900	-0.69118600	0.00030300
C	-3.48786000	1.40415000	0.00012800
C	-3.48785700	-1.40416500	-0.00010400
N	-4.47521800	1.98954800	0.01084800
N	-4.47530800	-1.98948700	-0.01062900
H	-4.48422003	2.95927984	-0.23315841
H	-5.32635642	1.52978790	0.26419369

S1.13 CDCA - $(NH_2)_2$

%chk=cdca-n2-b-2h2.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	4.41321400	0.67386800	-0.00063200
C	3.74239400	1.69531500	-0.00207300
C	4.41328900	-0.67389300	0.00083400
C	2.53503200	2.29160400	-0.00303800
C	3.74234900	-1.69526300	0.00218100
C	1.31687800	2.34061300	-0.00326200
C	2.53503900	-2.29164500	0.00302100
C	0.01565300	1.98966300	-0.00247500
C	1.31688100	-2.34059800	0.00309800
C	-1.06870400	1.44414400	-0.00124900
C	0.01564900	-1.98968700	0.00221700
C	-2.24548500	0.69116500	-0.00033300
C	-1.06870200	-1.44415400	0.00112800

C	-2.24548900	-0.69118600	0.00030300
C	-3.48786000	1.40415000	0.00012800
C	-3.48785700	-1.40416500	-0.00010400
N	-4.47521800	1.98954800	0.01084800
N	-4.47530800	-1.98948700	-0.01062900
H	-4.48422003	2.95927984	-0.23315841
H	-5.32635642	1.52978790	0.26419369
H	-4.48420396	-2.95945764	0.23243031
H	-5.32660397	-1.52940436	-0.26285734

S1.14 CDCA – (NH_2)(NH_3)

%chk=cdca-n2-b-3h2.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1

C	4.41321400	0.67386800	-0.00063200
C	3.74239400	1.69531500	-0.00207300
C	4.41328900	-0.67389300	0.00083400
C	2.53503200	2.29160400	-0.00303800
C	3.74234900	-1.69526300	0.00218100
C	1.31687800	2.34061300	-0.00326200
C	2.53503900	-2.29164500	0.00302100
C	0.01565300	1.98966300	-0.00247500
C	1.31688100	-2.34059800	0.00309800
C	-1.06870400	1.44414400	-0.00124900
C	0.01564900	-1.98968700	0.00221700
C	-2.24548500	0.69116500	-0.00033300
C	-1.06870200	-1.44415400	0.00112800
C	-2.24548900	-0.69118600	0.00030300
C	-3.48786000	1.40415000	0.00012800
C	-3.48785700	-1.40416500	-0.00010400
N	-4.47521800	1.98954800	0.01084800
N	-4.47530800	-1.98948700	-0.01062900
H	-4.43760861	2.71911777	-0.67202350
H	-5.23158252	1.37137968	-0.20311611
H	-4.48420396	-2.95945764	0.23243031
H	-5.32660397	-1.52940436	-0.26285734
H	-4.61660340	2.38811815	0.91702238
H	-3.94520161	0.62566485	-0.57406667

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S1.15 CDCA – $(NH_3)_2$

```
%chk=cdca-n2-b-4h2.chk
%nprocshared=6
%mem=6GB
#p opt freq wb97xd def2tzvp

title card

0 1
 C              4.41321400    0.67386800   -0.00063200
 C              3.74239400    1.69531500   -0.00207300
 C              4.41328900   -0.67389300    0.00083400
 C              2.53503200    2.29160400   -0.00303800
 C              3.74234900   -1.69526300    0.00218100
 C              1.31687800    2.34061300   -0.00326200
 C              2.53503900   -2.29164500    0.00302100
 C              0.01565300    1.98966300   -0.00247500
 C              1.31688100   -2.34059800    0.00309800
 C             -1.06870400    1.44414400   -0.00124900
 C              0.01564900   -1.98968700    0.00221700
 C             -2.24548500    0.69116500   -0.00033300
 C             -1.06870200   -1.44415400    0.00112800
 C             -2.24548900   -0.69118600    0.00030300
 C             -3.48786000    1.40415000    0.00012800
 C             -3.48785700   -1.40416500   -0.00010400
 N             -4.47521800    1.98954800    0.01084800
 N             -4.47530800   -1.98948700   -0.01062900
 H             -4.43760861    2.71911777   -0.67202350
 H             -5.23158252    1.37137968   -0.20311611
 H             -4.43722887   -2.71973145    0.67149490
 H             -5.23145132   -1.37146415    0.20453382
 H             -4.61660340    2.38811815    0.91702238
 H             -3.94520161    0.62566485   -0.57406667
 H             -3.94612990   -0.62384523    0.57084872
 H             -4.61743581   -2.38715328   -0.91708430
```

S1. 16 CP2K input file (300K)

```
&GLOBAL
  PROJECT carbon16_300K
  RUN_TYPE MD
  PRINT_LEVEL LOW
&END GLOBAL

&FORCE_EVAL
  METHOD Quickstep
```

Supporting Information file

```
 &DFT
  BASIS_SET_FILE_NAME BASIS_MOLOPT
  POTENTIAL_FILE_NAME GTH_POTENTIALS
  &MGRID
   CUTOFF 400
   REL_CUTOFF 60
   NGRIDS 4
  &END MGRID
  &QS
   METHOD GPW
   EPS_DEFAULT 1.0E-12
   EXTRAPOLATION ASPC
   EXTRAPOLATION_ORDER 3
  &END QS
  &SCF
   SCF_GUESS ATOMIC
   EPS_SCF 1.0E-6
   MAX_SCF 50
   &OT
    PRECONDITIONER FULL_SINGLE_INVERSE
    MINIMIZER DIIS
   &END OT
   &OUTER_SCF
    EPS_SCF 1.0E-6
    MAX_SCF 20
   &END OUTER_SCF
  &END SCF
  &XC
   &XC_FUNCTIONAL PBE
   &END XC_FUNCTIONAL
   &VDW_POTENTIAL
    POTENTIAL_TYPE PAIR_POTENTIAL
    &PAIR_POTENTIAL
     TYPE DFTD3
     PARAMETER_FILE_NAME dftd3.dat
     REFERENCE_FUNCTIONAL PBE
     R_CUTOFF 15.0
    &END PAIR_POTENTIAL
   &END VDW_POTENTIAL
  &END XC
  &POISSON
   PERIODIC NONE
   PSOLVER MT              ! Martyna-Tuckerman for isolated system
  &END POISSON
 &END DFT

 &SUBSYS
  &CELL
```

```
      ABC 20.0 20.0 20.0        ! large enough box for the molecule
      PERIODIC NONE
    &END CELL
    &COORD
C              3.67177500   -0.66746800    0.01221400
C              3.03520800   -1.75658800    0.04517200
C              3.66925000    0.66854300   -0.01135100
C              1.89227700   -2.44681700    0.05319200
C              3.03458600    1.75871400   -0.04399100
C              0.64369300   -2.60207300    0.05369300
C              1.88966900    2.44586400   -0.05351300
C             -0.65304600   -2.27941400    0.02653300
C              0.64146100    2.60353200   -0.05465200
C             -1.75482700   -1.68766700   -0.02951400
C             -0.65508100    2.27946200   -0.02800600
C             -2.70061800   -0.70813700   -0.15495500
C             -1.75690700    1.68773700    0.02789600
C             -2.70095800    0.70704700    0.15520200
C             -4.12795100   -0.45453200   -0.57651900
C             -4.12853200    0.45179600    0.57860000
    &END COORD
    &KIND C
      BASIS_SET DZVP-MOLOPT-SR-GTH
      POTENTIAL GTH-PBE-q4
    &END KIND
  &END SUBSYS
&END FORCE_EVAL

&MOTION
  &MD
    ENSEMBLE NVT
    TEMPERATURE 300.0
    TIMESTEP 0.5              ! fs; safe for pure carbon
    STEPS 320                 ! 0.16 ps; increase for longer sampling
    &THERMOSTAT
      TYPE CSVR
      &CSVR
        TIMECON 50.0          ! fs; use ~50 for quick equilibration
      &END CSVR
    &END THERMOSTAT
  &END MD

  &PRINT
    &TRAJECTORY
      FORMAT XYZ
      &EACH
        MD 10                 ! write every 5 fs
      &END EACH
```

```
   &END TRAJECTORY
   &VELOCITIES OFF
   &FORCES OFF
   &RESTART
    &EACH
      MD 500
    &END EACH
   &END RESTART
   &RESTART_HISTORY
    &EACH
      MD 1000
    &END EACH
   &END RESTART_HISTORY
  &END PRINT
&END MOTION
```

S2.1 CDCA: Singlet

```
 Entering Gaussian System, Link 0=g16
 Input=cdca.gjf
 Output=cdca.log
 Initial command:
            /home/user/gauss16/g16/l1.exe            "/home/user/paper/rahul/grun/Gau-3362053.inp"
-scrdir="/home/user/paper/rahul/grun/"
 Entering Link 1 = /home/user/gauss16/g16/l1.exe PID=   3362055.

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Gaussian 16, Revision C.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone,
G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich,
J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian,
J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young,
F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone,
T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega,
G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda,
J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai,
T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta,
F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin,
V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar,
J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi,
J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas,
J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

Supporting Information file

```
 ******************************************
 Gaussian 16:  ES64L-G16RevC.01  3-Jul-2019
               21-Aug-2026
 ******************************************
 %chk=cdca.chk
 %nprocshared=6
 Will use up to    6 processors via shared memory.
 %mem=6GB
 ----------------------------
 #p opt freq wb97xd/Def2TZVP
 ----------------------------
 1/18=20,19=15,26=3,38=1/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=44,7=101,11=2,25=1,30=1,71=1,74=-58/1,2,3;
 4//1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7//1,2,3,16;
 1/18=20,19=15,26=3/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=44,7=101,11=2,25=1,30=1,71=1,74=-58/1,2,3;
 4/5=5,16=3,69=1/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
 1/18=20,19=15,26=3/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 Leave Link     1 at Fri Aug 21 17:46:48 2026, MaxMem=    805306368 cpu:                  0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l101.exe)
 ----------
 title card
 ----------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                  3.67178  -0.66747   0.01221
 C                  3.03521  -1.75659   0.04517
 C                  3.66925   0.66854  -0.01135
 C                  1.89228  -2.44682   0.05319
 C                  3.03459   1.75871  -0.04399
 C                  0.64369  -2.60207   0.05369
 C                  1.88967   2.44586  -0.05351
 C                 -0.65305  -2.27941   0.02653
 C                  0.64146   2.60353  -0.05465
 C                 -1.75483  -1.68767  -0.02951
```

C -0.65508 2.27946 -0.02801
C -2.70062 -0.70814 -0.15496
C -1.75691 1.68774 0.0279
C -2.70096 0.70705 0.1552
C -4.12795 -0.45453 -0.57652
C -4.12853 0.4518 0.5786

ITRead= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MicOpt= -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
NAtoms= 16 NQM= 16 NQMF= 0 NMMI= 0 NMMIF= 0
NMic= 0 NMicF= 0.
Isotopes and Nuclear Properties:
(Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic moments (NMagM)
in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10
IAtWgt= 12 12 12 12 12 12 12 12 12 12
AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000
12.0000000 12.0000000 12.0000000 12.0000000
NucSpn= 0 0 0 0 0 0 0 0 0 0
AtZEff= -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -
0.0000000 -0.0000000 -0.0000000
NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
0.0000000 0.0000000 0.0000000
NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
0.0000000 0.0000000 0.0000000
AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000
6.0000000 6.0000000 6.0000000

Atom 11 12 13 14 15 16
IAtWgt= 12 12 12 12 12 12
AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000
NucSpn= 0 0 0 0 0 0
AtZEff= -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000
NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000
Leave Link 101 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 1.7 elap:
0.3
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !
--- ---

Supporting Information file

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.2619	estimate D2E/DX2
R2	R(1,3)	1.3362	estimate D2E/DX2
R3	R(2,4)	1.3352	estimate D2E/DX2
R4	R(3,5)	1.2619	estimate D2E/DX2
R5	R(4,6)	1.2582	estimate D2E/DX2
R6	R(5,7)	1.3353	estimate D2E/DX2
R7	R(6,8)	1.3366	estimate D2E/DX2
R8	R(7,9)	1.2581	estimate D2E/DX2
R9	R(8,10)	1.2519	estimate D2E/DX2
R10	R(9,11)	1.3367	estimate D2E/DX2
R11	R(10,12)	1.3674	estimate D2E/DX2
R12	R(11,13)	1.2519	estimate D2E/DX2
R13	R(12,14)	1.4488	estimate D2E/DX2
R14	R(12,15)	1.5097	estimate D2E/DX2
R15	R(13,14)	1.3672	estimate D2E/DX2
R16	R(14,16)	1.5108	estimate D2E/DX2
R17	R(15,16)	1.4682	estimate D2E/DX2
A1	A(2,1,3)	149.59	estimate D2E/DX2
A2	A(1,2,4)	151.4146	estimate D2E/DX2
A3	A(1,3,5)	149.9053	estimate D2E/DX2
A4	A(2,4,6)	155.9579	estimate D2E/DX2
A5	A(3,5,7)	151.1622	estimate D2E/DX2
A6	A(4,6,8)	158.9071	estimate D2E/DX2
A7	A(5,7,9)	156.2257	estimate D2E/DX2
A8	A(7,9,11)	158.7351	estimate D2E/DX2
A9	A(8,10,12)	162.0748	estimate D2E/DX2
A10	A(10,12,14)	132.8646	estimate D2E/DX2
A11	A(10,12,15)	143.1181	estimate D2E/DX2
A12	A(14,12,15)	84.0	estimate D2E/DX2
A13	A(11,13,14)	161.9754	estimate D2E/DX2
A14	A(12,14,13)	132.889	estimate D2E/DX2
A15	A(12,14,16)	83.9833	estimate D2E/DX2
A16	A(13,14,16)	143.1088	estimate D2E/DX2
A17	A(12,15,16)	83.3609	estimate D2E/DX2
A18	A(14,16,15)	83.306	estimate D2E/DX2
A19	L(6,8,10,7,-1)	165.7176	estimate D2E/DX2
A20	L(9,11,13,4,-1)	165.7795	estimate D2E/DX2
A21	L(6,8,10,7,-2)	178.8531	estimate D2E/DX2
A22	L(9,11,13,4,-2)	178.8388	estimate D2E/DX2
D1	D(3,1,2,4)	2.5816	estimate D2E/DX2
D2	D(2,1,3,5)	-2.4473	estimate D2E/DX2
D3	D(1,2,4,6)	-1.7812	estimate D2E/DX2
D4	D(1,3,5,7)	2.3877	estimate D2E/DX2
D5	D(2,4,6,8)	2.5026	estimate D2E/DX2
D6	D(3,5,7,9)	-1.5325	estimate D2E/DX2
D7	D(4,6,10,12)	4.8617	estimate D2E/DX2

Supporting Information file

```
! D8    D(5,7,9,11)           2.3885         estimate D2E/DX2              !
! D9    D(7,9,13,14)          5.0483         estimate D2E/DX2              !
! D10   D(8,10,12,14)        -30.2344         estimate D2E/DX2              !
! D11   D(8,10,12,15)        151.8784         estimate D2E/DX2              !
! D12   D(10,12,14,13)        38.8549         estimate D2E/DX2              !
! D13   D(10,12,14,16)      -142.4823         estimate D2E/DX2              !
! D14   D(15,12,14,13)      -142.4199         estimate D2E/DX2              !
! D15   D(15,12,14,16)        36.2428         estimate D2E/DX2              !
! D16   D(10,12,15,16)       140.9213         estimate D2E/DX2              !
! D17   D(14,12,15,16)       -37.5217         estimate D2E/DX2              !
! D18   D(11,13,14,12)       -30.5456         estimate D2E/DX2              !
! D19   D(11,13,14,16)       151.6702         estimate D2E/DX2              !
! D20   D(12,14,16,15)       -37.4983         estimate D2E/DX2              !
! D21   D(13,14,16,15)       140.8695         estimate D2E/DX2              !
! D22   D(12,15,16,14)        35.7931         estimate D2E/DX2              !
 ---------------------------------------------------------------------------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06 EigMax=2.50D+02 EigMin=1.00D-
04
 Number of steps in this run=     71 maximum allowed number of steps=    100.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link  103 at Fri Aug 21 17:46:48 2026, MaxMem=    805306368 cpu:                0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l202.exe)
                      Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.671775   -0.667468    0.012214
     2          6           0        3.035208   -1.756588    0.045172
     3          6           0        3.669250    0.668543   -0.011351
     4          6           0        1.892277   -2.446817    0.053192
     5          6           0        3.034586    1.758714   -0.043991
     6          6           0        0.643693   -2.602073    0.053693
     7          6           0        1.889669    2.445864   -0.053513
     8          6           0       -0.653046   -2.279414    0.026533
     9          6           0        0.641461    2.603532   -0.054652
    10          6           0       -1.754827   -1.687667   -0.029514
    11          6           0       -0.655081    2.279462   -0.028006
    12          6           0       -2.700618   -0.708137   -0.154955
    13          6           0       -1.756907    1.687737    0.027896
    14          6           0       -2.700958    0.707047    0.155202
    15          6           0       -4.127951   -0.454532   -0.576519
    16          6           0       -4.128532    0.451796    0.578600
 ---------------------------------------------------------------------
               Distance matrix (angstroms):
                    1        2        3        4        5
```

Supporting Information file

1	C	0.000000				
2	C	1.261937	0.000000			
3	C	1.336221	2.507282	0.000000		
4	C	2.516818	1.335205	3.587097	0.000000	
5	C	2.509089	3.516433	1.261878	4.358991	0.000000
6	C	3.593563	2.536585	4.455912	1.258200	4.974171
7	C	3.587904	4.356903	2.515463	4.893845	1.335328
8	C	4.615480	3.725173	5.232029	2.550961	5.469011
9	C	4.459452	4.975001	3.593545	5.204056	2.537889
10	C	5.521825	4.791113	5.913769	3.726193	5.900528
11	C	5.235236	5.469304	4.614670	5.369668	3.726268
12	C	6.374715	5.834295	6.518519	4.915386	6.244216
13	C	5.917586	5.901529	5.521184	5.514682	4.792558
14	C	6.520848	6.243813	6.372501	5.572708	5.834565
15	C	7.824811	7.307031	7.897915	6.372510	7.515582
16	C	7.900527	7.515363	7.823070	6.702847	7.307935

		6	7	8	9	10
6	C	0.000000				
7	C	5.200540	0.000000			
8	C	1.336555	5.366569	0.000000		
9	C	5.206733	1.258127	5.052277	0.000000	
10	C	2.568260	5.510808	1.251889	4.914999	0.000000
11	C	5.052017	2.550312	4.559203	1.336695	4.116741
12	C	3.849019	5.570345	2.587354	4.706029	1.367383
13	C	4.915894	3.725440	4.117863	2.568592	3.375893
14	C	4.706089	4.913339	3.623458	3.848696	2.581461
15	C	5.270454	6.700566	3.970999	5.689586	2.729753
16	C	5.689971	6.371391	4.454581	5.271035	3.252934

		11	12	13	14	15
11	C	0.000000				
12	C	3.622994	0.000000			
13	C	1.251912	2.581518	0.000000		
14	C	2.586826	1.448773	1.367184	0.000000	
15	C	4.453809	1.509739	3.252151	1.980149	0.000000
16	C	3.971548	1.980527	2.730463	1.510757	1.468241

		16
16	C	0.000000

Stoichiometry C16
Framework group C1[X(C16)]
Deg. of freedom 42
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.671775	-0.667468	0.012214
2	6	0	3.035208	-1.756588	0.045172
3	6	0	3.669250	0.668543	-0.011351
4	6	0	1.892277	-2.446817	0.053192
5	6	0	3.034586	1.758714	-0.043991
6	6	0	0.643693	-2.602073	0.053693
7	6	0	1.889669	2.445864	-0.053513
8	6	0	-0.653046	-2.279414	0.026533
9	6	0	0.641461	2.603532	-0.054652
10	6	0	-1.754827	-1.687667	-0.029514
11	6	0	-0.655081	2.279462	-0.028006
12	6	0	-2.700618	-0.708137	-0.154955
13	6	0	-1.756907	1.687737	0.027896
14	6	0	-2.700958	0.707047	0.155202
15	6	0	-4.127951	-0.454532	-0.576519
16	6	0	-4.128532	0.451796	0.578600

Rotational constants (GHZ): 0.8286404 0.3836542 0.2646593
Leave Link 202 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 707.7593326469 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0073441590 Hartrees.
Nuclear repulsion after empirical dispersion term = 707.7519884879 Hartrees.
Leave Link 301 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt

Supporting Information file

1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14162 LenP2D= 33380.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.11D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 564 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 2.4 elap: 0.4
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.889454862564
JPrj=0 DoOrth=F DoCkMO=F.
Leave Link 401 at Fri Aug 21 17:46:51 2026, MaxMem= 805306368 cpu: 13.5 elap: 2.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0

Supporting Information file

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.785467573105
DIIS: error= 5.21D-02 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.785467573105 IErMin= 1 ErrMin= 5.21D-02
ErrMax= 5.21D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D+00 BMatP= 1.38D+00
IDIUse=3 WtCom= 4.79D-01 WtEn= 5.21D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.245 Goal= None Shift= 0.000
GapD= 0.245 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.
Damping current iteration by 5.00D-01
RMSDP=8.53D-03 MaxDP=4.45D-01 OVMax= 1.06D-01

Cycle 2 Pass 0 IDiag 1:
RMSU= 2.66D-03 CP: 7.62D-01
E= -608.869789276275 Delta-E= -0.084321703170 Rises=F Damp=T
DIIS: error= 2.44D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.869789276275 IErMin= 2 ErrMin= 2.44D-02
ErrMax= 2.44D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.97D-01 BMatP= 1.38D+00
IDIUse=3 WtCom= 7.56D-01 WtEn= 2.44D-01
Coeff-Com: -0.793D+00 0.179D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.600D+00 0.160D+01
Gap= 0.275 Goal= None Shift= 0.000
RMSDP=4.94D-03 MaxDP=1.93D-01 DE=-8.43D-02 OVMax= 1.27D-01

Cycle 3 Pass 0 IDiag 1:
RMSU= 2.33D-03 CP: 5.45D-01 2.18D+00
E= -608.900230311374 Delta-E= -0.030441035099 Rises=F Damp=F
DIIS: error= 1.59D-02 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.900230311374 IErMin= 3 ErrMin= 1.59D-02
ErrMax= 1.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.18D-02 BMatP= 2.97D-01
IDIUse=3 WtCom= 8.41D-01 WtEn= 1.59D-01
Coeff-Com: -0.468D+00 0.101D+01 0.453D+00
Coeff-En: 0.000D+00 0.213D+00 0.787D+00
Coeff: -0.394D+00 0.888D+00 0.506D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.21D-02 MaxDP=9.49D-01 DE=-3.04D-02 OVMax= 1.09D-01

Cycle 4 Pass 0 IDiag 1:
RMSU= 1.89D-02 CP: 8.68D-01 3.00D+00 3.00D+00
E= -608.956879908755 Delta-E= -0.056649597382 Rises=F Damp=F
DIIS: error= 7.80D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.956879908755 IErMin= 4 ErrMin= 7.80D-03
ErrMax= 7.80D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-02 BMatP= 5.18D-02
IDIUse=3 WtCom= 9.22D-01 WtEn= 7.80D-02

Coeff-Com: -0.305D+00 0.660D+00 0.366D+00 0.279D+00
Coeff-En: 0.000D+00 0.000D+00 0.702D-01 0.930D+00
Coeff: -0.281D+00 0.609D+00 0.343D+00 0.329D+00
Gap= 0.224 Goal= None Shift= 0.000
RMSDP=3.20D+02 MaxDP=1.30D+04 DE=-5.66D-02 OVMax= 9.69D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 5 Pass 1 IDiag 1:
E= -608.956027483243 Delta-E= 0.000852425513 Rises=F Damp=F
DIIS: error= 6.26D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.956027483243 IErMin= 1 ErrMin= 6.26D-03
ErrMax= 6.26D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.49D-03 BMatP= 6.49D-03
IDIUse=3 WtCom= 9.37D-01 WtEn= 6.26D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.233 Goal= None Shift= 0.000
GapD= 0.233 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=2.39D-02 MaxDP=1.03D+00 DE= 8.52D-04 OVMax= 6.51D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 7.10D-03 CP: 1.80D-01
E= -608.939729452319 Delta-E= 0.016298030924 Rises=F Damp=F
DIIS: error= 1.08D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -608.956027483243 IErMin= 1 ErrMin= 6.26D-03
ErrMax= 1.08D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-02 BMatP= 6.49D-03
IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00
Coeff-En: 0.726D+00 0.274D+00
Coeff: 0.726D+00 0.274D+00
Gap= 0.225 Goal= None Shift= 0.000
RMSDP=4.19D-04 MaxDP=1.43D-02 DE= 1.63D-02 OVMax= 3.12D-02

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.61D-04 CP: 1.68D-01 1.01D+00
E= -608.962489653777 Delta-E= -0.022760201458 Rises=F Damp=F
DIIS: error= 2.26D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.962489653777 IErMin= 3 ErrMin= 2.26D-03
ErrMax= 2.26D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.42D-04 BMatP= 6.49D-03
IDIUse=3 WtCom= 9.77D-01 WtEn= 2.26D-02
Coeff-Com: 0.437D-01-0.222D+00 0.118D+01
Coeff-En: 0.105D+00 0.000D+00 0.895D+00
Coeff: 0.451D-01-0.217D+00 0.117D+01
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=8.08D-04 MaxDP=2.42D-02 DE=-2.28D-02 OVMax= 1.13D-02

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.17D-04 CP: 1.43D-01 1.02D+00 1.94D+00

Supporting Information file

E= -608.963594944859 Delta-E= -0.001105291082 Rises=F Damp=F
DIIS: error= 4.52D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.963594944859 IErMin= 4 ErrMin= 4.52D-04
ErrMax= 4.52D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.35D-05 BMatP= 9.42D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.52D-03
Coeff-Com: -0.351D-01-0.158D+00 0.672D+00 0.521D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.350D-01-0.157D+00 0.669D+00 0.523D+00
Gap= 0.226 Goal= None Shift= 0.000
RMSDP=1.32D-04 MaxDP=3.52D-03 DE=-1.11D-03 OVMax= 2.50D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 1.96D-05 CP: 1.40D-01 1.03D+00 2.08D+00 1.21D+00
E= -608.963650020709 Delta-E= -0.000055075850 Rises=F Damp=F
DIIS: error= 2.36D-04 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.963650020709 IErMin= 5 ErrMin= 2.36D-04
ErrMax= 2.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.13D-06 BMatP= 3.35D-05
IDIUse=3 WtCom= 9.98D-01 WtEn= 2.36D-03
Coeff-Com: -0.209D-01 0.207D-02-0.680D-01 0.147D+00 0.939D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.209D-01 0.207D-02-0.678D-01 0.147D+00 0.939D+00
Gap= 0.226 Goal= None Shift= 0.000
RMSDP=5.13D-05 MaxDP=1.33D-03 DE=-5.51D-05 OVMax= 3.12D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.54D-05 CP: 1.38D-01 1.03D+00 2.14D+00 1.29D+00 1.30D+00
E= -608.963673070358 Delta-E= -0.000023049649 Rises=F Damp=F
DIIS: error= 1.75D-04 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.963673070358 IErMin= 6 ErrMin= 1.75D-04
ErrMax= 1.75D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.24D-06 BMatP= 4.13D-06
IDIUse=3 WtCom= 9.98D-01 WtEn= 1.75D-03
Coeff-Com: 0.187D-02 0.704D-01-0.338D+00-0.152D+00 0.594D+00 0.824D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.186D-02 0.703D-01-0.338D+00-0.152D+00 0.593D+00 0.824D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.53D-05 MaxDP=5.31D-04 DE=-2.30D-05 OVMax= 2.82D-03

Cycle 11 Pass 1 IDiag 1:
RMSU= 6.93D-06 CP: 1.38D-01 1.03D+00 2.16D+00 1.29D+00 1.59D+00
CP: 1.75D+00
E= -608.963683721066 Delta-E= -0.000010650708 Rises=F Damp=F
DIIS: error= 7.43D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.963683721066 IErMin= 7 ErrMin= 7.43D-05
ErrMax= 7.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.08D-07 BMatP= 2.24D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.349D-02 0.280D-01-0.126D+00-0.911D-01 0.884D-01 0.355D+00
Coeff-Com: 0.742D+00
Coeff: 0.349D-02 0.280D-01-0.126D+00-0.911D-01 0.884D-01 0.355D+00

Coeff: 0.742D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=2.28D-05 MaxDP=7.10D-04 DE=-1.07D-05 OVMax= 1.06D-03

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.24D-06 CP: 1.39D-01 1.03D+00 2.13D+00 1.26D+00 1.72D+00
CP: 1.98D+00 1.22D+00
E= -608.963685106964 Delta-E= -0.000001385898 Rises=F Damp=F
DIIS: error= 3.25D-05 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.963685106964 IErMin= 8 ErrMin= 3.25D-05
ErrMax= 3.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.23D-08 BMatP= 3.08D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.129D-02-0.291D-02 0.185D-01-0.135D-01-0.101D+00-0.417D-02
Coeff-Com: 0.373D+00 0.729D+00
Coeff: 0.129D-02-0.291D-02 0.185D-01-0.135D-01-0.101D+00-0.417D-02
Coeff: 0.373D+00 0.729D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.57D-05 MaxDP=4.89D-04 DE=-1.39D-06 OVMax= 4.51D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.29D-06 CP: 1.40D-01 1.03D+00 2.12D+00 1.24D+00 1.77D+00
CP: 2.06D+00 1.38D+00 1.57D+00
E= -608.963685528414 Delta-E= -0.000000421449 Rises=F Damp=F
DIIS: error= 1.63D-05 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.963685528414 IErMin= 9 ErrMin= 1.63D-05
ErrMax= 1.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-08 BMatP= 9.23D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.478D-03-0.104D-01 0.492D-01 0.206D-01-0.699D-01-0.107D+00
Coeff-Com: -0.958D-01 0.312D+00 0.902D+00
Coeff: -0.478D-03-0.104D-01 0.492D-01 0.206D-01-0.699D-01-0.107D+00
Coeff: -0.958D-01 0.312D+00 0.902D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=7.32D-06 MaxDP=2.44D-04 DE=-4.21D-07 OVMax= 3.27D-04

Cycle 14 Pass 1 IDiag 1:
RMSU= 7.53D-07 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.79D+00
CP: 2.08D+00 1.46D+00 1.96D+00 1.62D+00
E= -608.963685699409 Delta-E= -0.000000170995 Rises=F Damp=F
DIIS: error= 8.61D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.963685699409 IErMin=10 ErrMin= 8.61D-06
ErrMax= 8.61D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.98D-09 BMatP= 2.46D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.392D-03-0.234D-02 0.989D-02 0.822D-02 0.650D-02-0.284D-01
Coeff-Com: -0.156D+00-0.118D+00 0.367D+00 0.913D+00
Coeff: -0.392D-03-0.234D-02 0.989D-02 0.822D-02 0.650D-02-0.284D-01
Coeff: -0.156D+00-0.118D+00 0.367D+00 0.913D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.40D-06 MaxDP=3.78D-05 DE=-1.71D-07 OVMax= 2.23D-04

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Cycle 15 Pass 1 IDiag 1:
RMSU= 5.68D-07 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.09D+00 1.48D+00 2.12D+00 1.86D+00 1.58D+00
E= -608.963685749107 Delta-E= -0.000000049698 Rises=F Damp=F
DIIS: error= 3.12D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.963685749107 IErMin=11 ErrMin= 3.12D-06
ErrMax= 3.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-09 BMatP= 6.98D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.325D-04 0.145D-02-0.746D-02-0.206D-02 0.183D-01 0.147D-01
Coeff-Com: -0.346D-01-0.114D+00-0.692D-01 0.313D+00 0.880D+00
Coeff: -0.325D-04 0.145D-02-0.746D-02-0.206D-02 0.183D-01 0.147D-01
Coeff: -0.346D-01-0.114D+00-0.692D-01 0.313D+00 0.880D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.96D-06 MaxDP=6.48D-05 DE=-4.97D-08 OVMax= 8.40D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 2.76D-07 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.09D+00 1.48D+00 2.08D+00 1.94D+00 1.92D+00
CP: 1.41D+00
E= -608.963685757433 Delta-E= -0.000000008326 Rises=F Damp=F
DIIS: error= 9.21D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.963685757433 IErMin=12 ErrMin= 9.21D-07
ErrMax= 9.21D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-10 BMatP= 1.20D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.440D-04 0.665D-03-0.311D-02-0.189D-02 0.207D-02 0.761D-02
Coeff-Com: 0.221D-01 0.165D-02-0.789D-01-0.120D+00 0.138D+00 0.103D+01
Coeff: 0.440D-04 0.665D-03-0.311D-02-0.189D-02 0.207D-02 0.761D-02
Coeff: 0.221D-01 0.165D-02-0.789D-01-0.120D+00 0.138D+00 0.103D+01
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=7.72D-07 MaxDP=3.06D-05 DE=-8.33D-09 OVMax= 3.26D-05

Cycle 17 Pass 1 IDiag 1:
RMSU= 9.25D-08 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.09D+00 1.49D+00 2.05D+00 1.93D+00 2.05D+00
CP: 1.62D+00 1.52D+00
E= -608.963685758613 Delta-E= -0.000000001179 Rises=F Damp=F
DIIS: error= 4.18D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.963685758613 IErMin=13 ErrMin= 4.18D-07
ErrMax= 4.18D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.16D-11 BMatP= 1.49D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.163D-04 0.549D-05 0.662D-04-0.240D-03-0.192D-02 0.435D-03
Coeff-Com: 0.125D-01 0.173D-01-0.175D-01-0.844D-01-0.791D-01 0.367D+00
Coeff-Com: 0.786D+00
Coeff: 0.163D-04 0.549D-05 0.662D-04-0.240D-03-0.192D-02 0.435D-03
Coeff: 0.125D-01 0.173D-01-0.175D-01-0.844D-01-0.791D-01 0.367D+00
Coeff: 0.786D+00
Gap= 0.227 Goal= None Shift= 0.000

RMSDP=1.39D-07 MaxDP=5.47D-06 DE=-1.18D-09 OVMax= 9.16D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 2.60D-08 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.10D+00 1.49D+00 2.04D+00 1.93D+00 2.06D+00
CP: 1.63D+00 1.71D+00 1.38D+00
E= -608.963685758719 Delta-E= -0.000000000106 Rises=F Damp=F
DIIS: error= 1.72D-07 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.963685758719 IErMin=14 ErrMin= 1.72D-07
ErrMax= 1.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.71D-12 BMatP= 3.16D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.283D-07-0.748D-04 0.358D-03 0.204D-03-0.429D-03-0.101D-02
Coeff-Com: -0.564D-03 0.221D-02 0.681D-02 0.408D-02-0.361D-01-0.810D-01
Coeff-Com: 0.141D+00 0.965D+00
Coeff: 0.283D-07-0.748D-04 0.358D-03 0.204D-03-0.429D-03-0.101D-02
Coeff: -0.564D-03 0.221D-02 0.681D-02 0.408D-02-0.361D-01-0.810D-01
Coeff: 0.141D+00 0.965D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.58D-07 MaxDP=4.64D-06 DE=-1.06D-10 OVMax= 3.53D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.24D-08 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.80D+00
CP: 2.10D+00 1.49D+00 2.04D+00 1.94D+00 2.06D+00
CP: 1.62D+00 1.76D+00 1.56D+00 1.43D+00
E= -608.963685758752 Delta-E= -0.000000000033 Rises=F Damp=F
DIIS: error= 7.16D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -608.963685758752 IErMin=15 ErrMin= 7.16D-08
ErrMax= 7.16D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.89D-13 BMatP= 3.71D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.186D-05-0.190D-04 0.779D-04 0.902D-04 0.145D-03-0.396D-03
Coeff-Com: -0.174D-02-0.183D-02 0.387D-02 0.127D-01 0.211D-02-0.688D-01
Coeff-Com: -0.845D-01 0.246D+00 0.892D+00
Coeff: -0.186D-05-0.190D-04 0.779D-04 0.902D-04 0.145D-03-0.396D-03
Coeff: -0.174D-02-0.183D-02 0.387D-02 0.127D-01 0.211D-02-0.688D-01
Coeff: -0.845D-01 0.246D+00 0.892D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=4.25D-08 MaxDP=1.29D-06 DE=-3.32D-11 OVMax= 1.61D-06

Cycle 20 Pass 1 IDiag 1:
RMSU= 5.70D-09 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.80D+00
CP: 2.10D+00 1.49D+00 2.04D+00 1.94D+00 2.05D+00
CP: 1.61D+00 1.77D+00 1.59D+00 1.64D+00 1.29D+00
E= -608.963685758750 Delta-E= 0.000000000002 Rises=F Damp=F
DIIS: error= 3.75D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -608.963685758752 IErMin=16 ErrMin= 3.75D-08
ErrMax= 3.75D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.18D-13 BMatP= 7.89D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.114D-05 0.607D-05-0.343D-04 0.697D-05 0.143D-03 0.148D-04

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Coeff-Com: -0.746D-03-0.128D-02 0.384D-03 0.518D-02 0.955D-02-0.152D-01
Coeff-Com: -0.774D-01-0.103D+00 0.448D+00 0.734D+00
Coeff: -0.114D-05 0.607D-05-0.343D-04 0.697D-05 0.143D-03 0.148D-04
Coeff: -0.746D-03-0.128D-02 0.384D-03 0.518D-02 0.955D-02-0.152D-01
Coeff: -0.774D-01-0.103D+00 0.448D+00 0.734D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=6.28D-09 MaxDP=2.53D-07 DE= 1.82D-12 OVMax= 8.53D-07

SCF Done: E(RwB97XD) = -608.963685759 A.U. after 20 cycles
NFock= 20 Conv=0.63D-08 -V/T= 2.0063
KE= 6.051483865749D+02 PE=-2.825487511843D+03 EE= 9.036234510209D+02
Leave Link 502 at Fri Aug 21 17:54:15 2026, MaxMem= 805306368 cpu: 2663.8 elap: 444.1
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

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Population analysis using the SCF Density.

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Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state is 1-A.

Alpha occ. eigenvalues -- -10.40690 -10.40650 -10.37744 -10.37670 -10.37584
Alpha occ. eigenvalues -- -10.37576 -10.37458 -10.37430 -10.37264 -10.37251
Alpha occ. eigenvalues -- -10.37144 -10.37109 -10.36674 -10.36633 -10.36232
Alpha occ. eigenvalues -- -10.36197 -1.05999 -0.98288 -0.96768 -0.94986
Alpha occ. eigenvalues -- -0.93120 -0.90373 -0.87806 -0.83889 -0.81446
Alpha occ. eigenvalues -- -0.78413 -0.75080 -0.72252 -0.69470 -0.67314
Alpha occ. eigenvalues -- -0.63827 -0.63640 -0.53512 -0.52920 -0.52039
Alpha occ. eigenvalues -- -0.51608 -0.50673 -0.50080 -0.46376 -0.46351
Alpha occ. eigenvalues -- -0.44330 -0.42870 -0.38788 -0.38377 -0.34736
Alpha occ. eigenvalues -- -0.32480 -0.31924 -0.31769
Alpha virt. eigenvalues -- -0.09094 -0.08811 -0.06639 -0.03779 -0.00340
Alpha virt. eigenvalues -- 0.02605 0.03715 0.04468 0.07072 0.08937
Alpha virt. eigenvalues -- 0.10070 0.10970 0.11335 0.12055 0.12673
Alpha virt. eigenvalues -- 0.15689 0.17021 0.18884 0.21138 0.21609
Alpha virt. eigenvalues -- 0.21664 0.22970 0.23058 0.23674 0.24865
Alpha virt. eigenvalues -- 0.26244 0.26700 0.27094 0.27999 0.28249
Alpha virt. eigenvalues -- 0.29255 0.29978 0.30712 0.30917 0.31334
Alpha virt. eigenvalues -- 0.31880 0.32712 0.33636 0.34526 0.34775
Alpha virt. eigenvalues -- 0.35562 0.36990 0.37088 0.37740 0.37765
Alpha virt. eigenvalues -- 0.38925 0.38996 0.39287 0.40559 0.41526
Alpha virt. eigenvalues -- 0.41557 0.42309 0.42360 0.43859 0.45261
Alpha virt. eigenvalues -- 0.46054 0.46117 0.46674 0.47397 0.48721
Alpha virt. eigenvalues -- 0.48922 0.49763 0.50159 0.50358 0.52303
Alpha virt. eigenvalues -- 0.52541 0.52664 0.52964 0.53837 0.54204
Alpha virt. eigenvalues -- 0.54382 0.54511 0.55485 0.55857 0.57073
Alpha virt. eigenvalues -- 0.58165 0.58417 0.58482 0.59196 0.59423
Alpha virt. eigenvalues -- 0.60685 0.62545 0.62873 0.63279 0.63667
Alpha virt. eigenvalues -- 0.64966 0.67206 0.67571 0.67633 0.68150
Alpha virt. eigenvalues -- 0.70217 0.70541 0.71511 0.72082 0.73953
Alpha virt. eigenvalues -- 0.74744 0.76060 0.76622 0.78011 0.78954

Alpha virt. eigenvalues --	0.80927	0.82709	0.83458	0.84356	0.85052
Alpha virt. eigenvalues --	0.86608	0.88275	0.89661	0.91027	0.91241
Alpha virt. eigenvalues --	0.92390	0.94524	0.95100	0.97186	0.98545
Alpha virt. eigenvalues --	0.98956	1.01019	1.01125	1.03659	1.05979
Alpha virt. eigenvalues --	1.07190	1.08687	1.08747	1.11288	1.11587
Alpha virt. eigenvalues --	1.12023	1.13912	1.14107	1.15482	1.16947
Alpha virt. eigenvalues --	1.17791	1.20372	1.21786	1.22279	1.22977
Alpha virt. eigenvalues --	1.25713	1.26192	1.26203	1.27377	1.29578
Alpha virt. eigenvalues --	1.31965	1.33063	1.33682	1.34257	1.35299
Alpha virt. eigenvalues --	1.36631	1.37452	1.37792	1.39236	1.39619
Alpha virt. eigenvalues --	1.41936	1.42298	1.42439	1.42907	1.44085
Alpha virt. eigenvalues --	1.45158	1.45496	1.46790	1.46943	1.48193
Alpha virt. eigenvalues --	1.48537	1.49287	1.49483	1.50997	1.51694
Alpha virt. eigenvalues --	1.52713	1.52832	1.54902	1.55318	1.57879
Alpha virt. eigenvalues --	1.59154	1.59282	1.61352	1.61398	1.62952
Alpha virt. eigenvalues --	1.64029	1.65346	1.67030	1.68233	1.69343
Alpha virt. eigenvalues --	1.69748	1.69957	1.71333	1.73328	1.73951
Alpha virt. eigenvalues --	1.75280	1.75578	1.76219	1.77549	1.77627
Alpha virt. eigenvalues --	1.78157	1.80551	1.82226	1.82561	1.83393
Alpha virt. eigenvalues --	1.84430	1.85205	1.88923	1.92130	1.94462
Alpha virt. eigenvalues --	1.94904	1.96375	1.97236	2.00359	2.03126
Alpha virt. eigenvalues --	2.06640	2.08108	2.11388	2.15317	2.15590
Alpha virt. eigenvalues --	2.17916	2.19108	2.19672	2.23329	2.25035
Alpha virt. eigenvalues --	2.26368	2.29808	2.33103	2.37580	2.37798
Alpha virt. eigenvalues --	2.40023	2.40672	2.43296	2.43425	2.44461
Alpha virt. eigenvalues --	2.45671	2.45890	2.45978	2.47767	2.49563
Alpha virt. eigenvalues --	2.49612	2.49851	2.52076	2.53038	2.54048
Alpha virt. eigenvalues --	2.54298	2.56845	2.57158	2.60039	2.60116
Alpha virt. eigenvalues --	2.60394	2.61715	2.62096	2.62743	2.63814
Alpha virt. eigenvalues --	2.64732	2.65694	2.68557	2.68700	2.71686
Alpha virt. eigenvalues --	2.71766	2.73222	2.73486	2.74591	2.75966
Alpha virt. eigenvalues --	2.76207	2.76590	2.77597	2.79378	2.79493
Alpha virt. eigenvalues --	2.80529	2.82441	2.82794	2.83480	2.83989
Alpha virt. eigenvalues --	2.84800	2.85391	2.85714	2.85963	2.86711
Alpha virt. eigenvalues --	2.87619	2.87852	2.87888	2.88309	2.88628
Alpha virt. eigenvalues --	2.89525	2.90250	2.90532	2.90623	2.92189
Alpha virt. eigenvalues --	2.94205	2.95921	2.95949	2.96448	2.98521
Alpha virt. eigenvalues --	2.98816	2.99596	2.99859	3.00374	3.00873
Alpha virt. eigenvalues --	3.01977	3.02713	3.03550	3.04517	3.04853
Alpha virt. eigenvalues --	3.05890	3.08265	3.08794	3.10400	3.11433
Alpha virt. eigenvalues --	3.11699	3.12798	3.13657	3.14714	3.14829
Alpha virt. eigenvalues --	3.16620	3.17281	3.17575	3.18364	3.19966
Alpha virt. eigenvalues --	3.20524	3.23800	3.24583	3.24916	3.25283
Alpha virt. eigenvalues --	3.25441	3.27026	3.28262	3.29475	3.29551
Alpha virt. eigenvalues --	3.30339	3.30824	3.31428	3.33555	3.34132
Alpha virt. eigenvalues --	3.34382	3.35017	3.35381	3.36979	3.38246
Alpha virt. eigenvalues --	3.38800	3.40529	3.41383	3.42282	3.42552
Alpha virt. eigenvalues --	3.45853	3.46699	3.46818	3.48387	3.49029

Supporting Information file

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Alpha virt. eigenvalues --    3.51456   3.51949   3.52918   3.53396   3.54830
Alpha virt. eigenvalues --    3.55909   3.58944   3.59871   3.60189   3.61996
Alpha virt. eigenvalues --    3.62781   3.68637   3.70325   3.70769   3.71758
Alpha virt. eigenvalues --    3.74026   3.78299   3.78508   3.81650   3.82991
Alpha virt. eigenvalues --    3.83287   3.83695   3.86912   3.89434   3.93028
Alpha virt. eigenvalues --    3.95765   3.99046   3.99927   4.02474   4.02659
Alpha virt. eigenvalues --    4.03871   4.04149   4.05597   4.11559   4.12337
Alpha virt. eigenvalues --    4.13711   4.17586   4.18341   4.20836   4.24842
Alpha virt. eigenvalues --    4.26572   4.31431   4.31810   4.35208   4.42212
Alpha virt. eigenvalues --    4.43172   4.46315   4.51087   4.52254   4.53026
Alpha virt. eigenvalues --    4.58309   4.62117   4.65883   4.71192   4.72864
Alpha virt. eigenvalues --    4.72888   4.74977   4.75142   4.81502   4.83137
Alpha virt. eigenvalues --    4.91778   4.91817   4.96066   5.00123   5.02929
Alpha virt. eigenvalues --    5.03424   5.07235   5.08528   5.09052   5.10261
Alpha virt. eigenvalues --    5.14230   5.16411   5.17161   5.17904   5.19066
Alpha virt. eigenvalues --    5.20071   5.23538   5.24358   5.27545   5.27626
Alpha virt. eigenvalues --    5.35726   5.36158   5.42819   5.51883   5.54656
Alpha virt. eigenvalues --    5.57667   5.67572   5.74351   5.92913   5.97855
Alpha virt. eigenvalues --    6.03944   6.11064  22.06007  22.13458  22.48653
Alpha virt. eigenvalues --   22.84147  23.07746  23.19356  23.19409  23.33661
Alpha virt. eigenvalues --   23.45384  23.53563  23.62173  23.64950  23.86424
Alpha virt. eigenvalues --   23.91611  24.14183  24.17979
      Condensed to atoms (all electrons):
               1         2         3         4         5         6
  1  C    4.798194  0.869986  0.557626 -0.077954 -0.075579 -0.043476
  2  C    0.869986  4.801135 -0.076715  0.579704 -0.038944 -0.072960
  3  C    0.557626 -0.076715  4.801360 -0.020958  0.869855 -0.007302
  4  C   -0.077954  0.579704 -0.020958  4.788184 -0.006792  0.928531
  5  C   -0.075579 -0.038944  0.869855 -0.006792  4.797278 -0.001774
  6  C   -0.043476 -0.072960 -0.007302  0.928531 -0.001774  4.906160
  7  C   -0.020761 -0.006765 -0.078473 -0.001895  0.578494 -0.000550
  8  C   -0.010157 -0.030783 -0.001644 -0.091806 -0.000422  0.557387
  9  C   -0.007204 -0.001748 -0.043144 -0.000532 -0.071634 -0.000118
 10  C   -0.002127 -0.010642 -0.000351 -0.058597 -0.000139 -0.194905
 11  C   -0.001620 -0.000396 -0.009915 -0.000171 -0.030036  0.001821
 12  C   -0.000193 -0.001115 -0.000071 -0.007119 -0.000079 -0.037944
 13  C   -0.000351 -0.000124 -0.002062 -0.000001 -0.010366  0.000303
 14  C   -0.000074 -0.000079 -0.000185 -0.000951 -0.001083 -0.009891
 15  C   -0.000001 -0.000014  0.000001 -0.000176  0.000006 -0.002319
 16  C    0.000001  0.000007 -0.000001  0.000081 -0.000013  0.001085
               7         8         9        10        11        12
  1  C   -0.020761 -0.010157 -0.007204 -0.002127 -0.001620 -0.000193
  2  C   -0.006765 -0.030783 -0.001748 -0.010642 -0.000396 -0.001115
  3  C   -0.078473 -0.001644 -0.043144 -0.000351 -0.009915 -0.000071
  4  C   -0.001895 -0.091806 -0.000532 -0.058597 -0.000171 -0.007119
  5  C    0.578494 -0.000422 -0.071634 -0.000139 -0.030036 -0.000079
  6  C   -0.000550  0.557387 -0.000118 -0.194905  0.001821 -0.037944
  7  C    4.789911 -0.000170  0.927763  0.000004 -0.090791 -0.000924
```

8	C	-0.000170	4.987906	0.001839	0.695979	0.009464	-0.138798
9	C	0.927763	0.001839	4.901054	0.000275	0.555253	-0.009800
10	C	0.000004	0.695979	0.000275	5.323346	0.001827	0.485613
11	C	-0.090791	0.009464	0.555253	0.001827	4.984459	-0.071505
12	C	-0.000924	-0.138798	-0.009800	0.485613	-0.071505	5.221782
13	C	-0.057351	0.001848	-0.192632	0.003765	0.696320	-0.058251
14	C	-0.006915	-0.071611	-0.036821	-0.059047	-0.136077	0.344902
15	C	0.000081	-0.017111	0.001072	-0.096879	0.010431	0.076592
16	C	-0.000174	0.010454	-0.002262	0.015512	-0.016753	0.090437

		13	14	15	16
1	C	-0.000351	-0.000074	-0.000001	0.000001
2	C	-0.000124	-0.000079	-0.000014	0.000007
3	C	-0.002062	-0.000185	0.000001	-0.000001
4	C	-0.000001	-0.000951	-0.000176	0.000081
5	C	-0.010366	-0.001083	0.000006	-0.000013
6	C	0.000303	-0.009891	-0.002319	0.001085
7	C	-0.057351	-0.006915	0.000081	-0.000174
8	C	0.001848	-0.071611	-0.017111	0.010454
9	C	-0.192632	-0.036821	0.001072	-0.002262
10	C	0.003765	-0.059047	-0.096879	0.015512
11	C	0.696320	-0.136077	0.010431	-0.016753
12	C	-0.058251	0.344902	0.076592	0.090437
13	C	5.317366	0.483984	0.015153	-0.096080
14	C	0.483984	5.219283	0.090908	0.076797
15	C	0.015153	0.090908	5.848828	0.125363
16	C	-0.096080	0.076797	0.125363	5.847013

Mulliken charges:

		1
1	C	0.013688
2	C	-0.010546
3	C	0.011979
4	C	-0.029547
5	C	-0.008772
6	C	-0.024046
7	C	-0.031484
8	C	0.097625
9	C	-0.021361
10	C	-0.103635
11	C	0.097689
12	C	0.106474
13	C	-0.101521
14	C	0.106860
15	C	-0.051937
16	C	-0.051467

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.013688

```
     2  C   -0.010546
     3  C    0.011979
     4  C   -0.029547
     5  C   -0.008772
     6  C   -0.024046
     7  C   -0.031484
     8  C    0.097625
     9  C   -0.021361
    10  C   -0.103635
    11  C    0.097689
    12  C    0.106474
    13  C   -0.101521
    14  C    0.106860
    15  C   -0.051937
    16  C   -0.051467
 Electronic spatial extent (au):  <R**2>=           3633.9794
 Charge=           0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=            3.9839    Y=           -0.0140    Z=           -0.0009  Tot=            3.9840
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=         -103.2801   YY=          -85.8090   ZZ=          -91.6089
   XY=           -0.0179   XZ=            0.0087   YZ=           -1.8712
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -9.7141   YY=            7.7570   ZZ=            1.9571
   XY=           -0.0179   XZ=            0.0087   YZ=           -1.8712
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=          122.6799  YYY=           -0.1474  ZZZ=           -0.0153  XYY=            5.8268
  XXY=           -0.0116  XXZ=           -0.0257  XZZ=           16.9118  YZZ=           -0.0017
  YYZ=            0.0053  XYZ=            7.8055
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=        -4254.0953 YYYY=         -1748.8643 ZZZZ=          -136.0370 XXXY=           -
0.4368
 XXXZ=            0.1687 YYYX=           -0.1109 YYYZ=           -3.9202 ZZZX=            0.0689
 ZZZY=           -4.3561 XXYY=          -912.8794 XXZZ=          -723.8826 YYZZ=           -
318.8057
 XXYZ=          -37.4656 YYXZ=           -0.0124 ZZXY=           -0.0086
 N-N= 7.077519884879D+02 E-N=-2.825487509729D+03  KE= 6.051483865749D+02
 No NMR shielding tensors so no spin-rotation constants.
 Leave Link  601 at Fri Aug 21 17:54:15 2026, MaxMem=    805306368 cpu:                1.4 elap:
0.3
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14162 LenP2D=   33380.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
```

Supporting Information file

Leave Link 701 at Fri Aug 21 17:54:15 2026, MaxMem= 805306368 cpu: 1.6 elap: 0.3
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 17:54:15 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 17:58:24 2026, MaxMem= 805306368 cpu: 1493.2 elap: 248.9
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.56740265D+00-5.50370036D-03-3.53603128D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.026122176	-0.036561762	-0.000459688
2	6	0.020024419	0.041312129	0.000389164
3	6	-0.026032801	0.036570504	0.000513453
4	6	-0.044293150	-0.003071849	-0.001763152
5	6	0.019917331	-0.041323625	-0.000485336
6	6	0.045465917	0.008118935	0.001614338
7	6	-0.044226127	0.003192823	0.001792536
8	6	-0.038935528	0.022249724	-0.004235468
9	6	0.045393096	-0.008223820	-0.001605159
10	6	0.043299844	-0.022273147	0.005391363
11	6	-0.038907177	-0.022287175	0.004223549
12	6	-0.024409829	0.033896526	0.003264056
13	6	0.043446609	0.022421201	-0.005361667
14	6	-0.024772636	-0.034074442	-0.003147689
15	6	0.024900316	0.016211880	0.021354089
16	6	0.025251893	-0.016157902	-0.021484389

Cartesian Forces: Max 0.045465917 RMS 0.025647041
Leave Link 716 at Fri Aug 21 17:58:24 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

Supporting Information file

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.051858148 RMS 0.017618546
Search for a local minimum.
Step number 1 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .17619D-01 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Second derivative matrix not updated -- first step.
ITU= 0

Eigenvalues ---	0.01281	0.01313	0.01666	0.01726	0.02624
Eigenvalues ---	0.02870	0.03117	0.03421	0.03429	0.03926
Eigenvalues ---	0.03950	0.03968	0.04046	0.08416	0.09136
Eigenvalues ---	0.24506	0.24597	0.24996	0.24997	0.24999
Eigenvalues ---	0.25000	0.25000	0.25000	0.25000	0.25000
Eigenvalues ---	0.27993	0.28436	0.32297	0.36130	0.51317
Eigenvalues ---	0.51368	0.57396	0.57823	0.57982	0.58172
Eigenvalues ---	0.58238	0.78591	0.78681	0.79707	0.80286
Eigenvalues ---	0.82175	0.82428			

RFO step: Lambda=-2.86399074D-02 EMin= 1.28103738D-02
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.05417072 RMS(Int)= 0.00133444
Iteration 2 RMS(Cart)= 0.00085692 RMS(Int)= 0.00032466
Iteration 3 RMS(Cart)= 0.00000115 RMS(Int)= 0.00032466
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00032466
ITry= 1 IFail=0 DXMaxC= 1.61D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.38472	-0.05186	0.00000	-0.06336	-0.06334	2.32138
R2	2.52509	-0.00827	0.00000	-0.01356	-0.01354	2.51156
R3	2.52317	-0.00702	0.00000	-0.01148	-0.01147	2.51170
R4	2.38460	-0.05183	0.00000	-0.06331	-0.06329	2.32131
R5	2.37765	-0.05081	0.00000	-0.06110	-0.06110	2.31655
R6	2.52340	-0.00706	0.00000	-0.01155	-0.01154	2.51187
R7	2.52572	-0.00513	0.00000	-0.00842	-0.00843	2.51729
R8	2.37752	-0.05079	0.00000	-0.06108	-0.06107	2.31644
R9	2.36573	-0.05000	0.00000	-0.05854	-0.05855	2.30718
R10	2.52599	-0.00517	0.00000	-0.00851	-0.00851	2.51748
R11	2.58398	-0.00131	0.00000	-0.00240	-0.00242	2.58156
R12	2.36577	-0.05003	0.00000	-0.05858	-0.05859	2.30718
R13	2.73778	-0.03318	0.00000	-0.08427	-0.08437	2.65342
R14	2.85299	-0.02535	0.00000	-0.07305	-0.07299	2.78000
R15	2.58360	-0.00113	0.00000	-0.00207	-0.00209	2.58151
R16	2.85492	-0.02560	0.00000	-0.07401	-0.07395	2.78096
R17	2.77457	-0.02566	0.00000	-0.06389	-0.06393	2.71064

Supporting Information file

A1	2.61084	0.00041	0.00000	0.00024	0.00030	2.61114
A2	2.64268	0.00053	0.00000	0.00070	0.00074	2.64342
A3	2.61634	0.00042	0.00000	0.00025	0.00032	2.61666
A4	2.72198	0.00022	0.00000	-0.00042	-0.00044	2.72154
A5	2.63828	0.00048	0.00000	0.00046	0.00049	2.63877
A6	2.77345	0.00081	0.00000	0.00175	0.00166	2.77512
A7	2.72665	0.00016	0.00000	-0.00073	-0.00075	2.72590
A8	2.77045	0.00080	0.00000	0.00162	0.00153	2.77198
A9	2.82874	-0.00088	0.00000	-0.00418	-0.00439	2.82435
A10	2.31893	-0.00140	0.00000	0.00294	0.00318	2.32211
A11	2.49788	0.00160	0.00000	0.01535	0.01579	2.51368
A12	1.46608	-0.00015	0.00000	-0.01767	-0.01868	1.44740
A13	2.82700	-0.00086	0.00000	-0.00415	-0.00436	2.82264
A14	2.31935	-0.00140	0.00000	0.00293	0.00317	2.32252
A15	1.46578	-0.00013	0.00000	-0.01756	-0.01858	1.44721
A16	2.49772	0.00158	0.00000	0.01529	0.01573	2.51345
A17	1.45492	-0.00264	0.00000	-0.02428	-0.02532	1.42960
A18	1.45396	-0.00250	0.00000	-0.02376	-0.02480	1.42916
A19	2.89232	0.00024	0.00000	-0.00220	-0.00234	2.88997
A20	2.89340	0.00030	0.00000	-0.00158	-0.00172	2.89168
A21	3.12157	0.00014	0.00000	0.00670	0.00662	3.12819
A22	3.12133	0.00015	0.00000	0.00688	0.00680	3.12813
D1	0.04506	0.00043	0.00000	0.00761	0.00762	0.05267
D2	-0.04271	-0.00003	0.00000	0.00055	0.00056	-0.04216
D3	-0.03109	-0.00034	0.00000	-0.00296	-0.00298	-0.03407
D4	0.04167	0.00045	0.00000	0.00790	0.00790	0.04957
D5	0.04368	-0.00014	0.00000	0.00171	0.00166	0.04534
D6	-0.02675	-0.00035	0.00000	-0.00317	-0.00319	-0.02994
D7	0.08485	-0.00105	0.00000	-0.01948	-0.01956	0.06529
D8	0.04169	-0.00014	0.00000	0.00170	0.00165	0.04334
D9	0.08811	-0.00105	0.00000	-0.01952	-0.01961	0.06850
D10	-0.52769	0.00084	0.00000	0.00831	0.00830	-0.51939
D11	2.65078	-0.00239	0.00000	-0.02937	-0.02943	2.62135
D12	0.67815	-0.00023	0.00000	0.01031	0.01070	0.68885
D13	-2.48679	0.00178	0.00000	0.03360	0.03361	-2.45318
D14	-2.48570	0.00176	0.00000	0.03346	0.03346	-2.45224
D15	0.63256	0.00377	0.00000	0.05674	0.05636	0.68892
D16	2.45954	-0.00205	0.00000	-0.03018	-0.02982	2.42972
D17	-0.65488	-0.00439	0.00000	-0.05797	-0.05762	-0.71250
D18	-0.53312	0.00086	0.00000	0.00849	0.00848	-0.52464
D19	2.64714	-0.00240	0.00000	-0.02939	-0.02946	2.61768
D20	-0.65447	-0.00444	0.00000	-0.05813	-0.05780	-0.71227
D21	2.45864	-0.00208	0.00000	-0.03021	-0.02985	2.42878
D22	0.62471	0.00205	0.00000	0.05160	0.05076	0.67547

Item	Value	Threshold	Converged?
Maximum Force	0.051858	0.000450	NO
RMS Force	0.017619	0.000300	NO
Maximum Displacement	0.161422	0.001800	NO

Supporting Information file

RMS Displacement 0.054278 0.001200 NO
Predicted change in Energy=-1.525237D-02
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 17:58:24 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.611949	-0.663657	0.016690
2	6	0	2.992478	-1.723722	0.055889
3	6	0	3.609597	0.664999	-0.015917
4	6	0	1.855475	-2.412032	0.063476
5	6	0	2.992237	1.726263	-0.054861
6	6	0	0.639091	-2.564149	0.058743
7	6	0	1.853282	2.411490	-0.063765
8	6	0	-0.653894	-2.245910	0.021513
9	6	0	0.637205	2.565589	-0.059549
10	6	0	-1.728368	-1.668931	-0.035128
11	6	0	-0.655409	2.245393	-0.022712
12	6	0	-2.668593	-0.685235	-0.155797
13	6	0	-1.730023	1.668645	0.033644
14	6	0	-2.668828	0.683839	0.155988
15	6	0	-4.043089	-0.399623	-0.595523
16	6	0	-4.043111	0.397041	0.597311

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.228420	0.000000			
3	C	1.329058	2.468193	0.000000		
4	C	2.478750	1.329137	3.542791	0.000000	
5	C	2.469996	3.451762	1.228386	4.293218	0.000000
6	C	3.528671	2.498951	4.388265	1.225867	4.894674
7	C	3.543432	4.290928	2.477330	4.825201	1.329223
8	C	4.549831	3.683734	5.162572	2.515212	5.392427
9	C	4.391235	4.894775	3.528351	5.126015	2.500134
10	C	5.434358	4.722041	5.825930	3.661401	5.814795
11	C	5.164733	5.391393	4.548402	5.291840	3.684542
12	C	6.282947	5.759426	6.423267	4.847381	6.153902
13	C	5.828943	5.814693	5.433351	5.432183	4.723441
14	C	6.425209	6.152784	6.280806	5.482910	5.760101
15	C	7.684017	7.188656	7.748094	6.267147	7.369364
16	C	7.749977	7.368194	7.681913	6.555089	7.189457

Supporting Information file

```
                6          7          8          9         10
  6  C    0.000000
  7  C    5.123109   0.000000
  8  C    1.332094   5.290046   0.000000
  9  C    5.131101   1.225809   4.982372   0.000000
 10  C    2.532803   5.429445   1.220905   4.850535   0.000000
 11  C    4.981371   2.514518   4.491521   1.332190   4.058734
 12  C    3.810134   5.481380   2.554634   4.637393   1.366104
 13  C    4.850760   3.660790   4.059796   2.533172   3.338284
 14  C    4.636940   4.845879   3.558297   3.810156   2.540968
 15  C    5.199620   6.553801   3.908472   5.566408   2.698725
 16  C    5.566123   6.265978   4.336304   5.199944   3.166426
               11         12         13         14         15
 11  C    0.000000
 12  C    3.557978   0.000000
 13  C    1.220906   2.541172   0.000000
 14  C    2.554259   1.404128   1.366076   0.000000
 15  C    4.335966   1.471113   3.166048   1.904535   0.000000
 16  C    3.908626   1.904677   2.699087   1.471623   1.434408
               16
 16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 3.53D-03
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.611845   -0.664263    0.015013
    2          6           0        2.992208   -1.724324    0.051575
    3          6           0        3.609701    0.664471   -0.014284
    4          6           0        1.855098   -2.412474    0.057455
    5          6           0        2.992507    1.725925   -0.050580
    6          6           0        0.638690   -2.564387    0.052350
    7          6           0        1.853659    2.411351   -0.057769
    8          6           0       -0.654246   -2.245855    0.015922
    9          6           0        0.637606    2.565629   -0.053161
   10          6           0       -1.728630   -1.668567   -0.039275
   11          6           0       -0.655057    2.245545   -0.017114
   12          6           0       -2.668701   -0.684427   -0.157486
   13          6           0       -1.729761    1.668827    0.037812
   14          6           0       -2.668720    0.683867    0.157708
   15          6           0       -4.043155   -0.397505   -0.596491
```

```
    16        6        0      -4.043045    0.396186    0.598324
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8539217           0.3964308           0.2735002
 Leave Link  202 at Fri Aug 21 17:58:24 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       719.6285294985 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0075423268 Hartrees.
 Nuclear repulsion after empirical dispersion term =      719.6209871716 Hartrees.
 Leave Link  301 at Fri Aug 21 17:58:24 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14229 LenP2D=   33675.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  3.73D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=          32
 NSgBfM=   565   565   565   565   565 MxSgAt=    16 MxSgA2=    16.
 Leave Link  302 at Fri Aug 21 17:58:25 2026, MaxMem=    805306368 cpu:                  2.4 elap:
0.4
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Aug 21 17:58:25 2026, MaxMem=    805306368 cpu:                  0.4 elap:
0.1
```

Supporting Information file

(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 -0.000000 0.000000
Rot= 0.999999 -0.001243 -0.000003 0.000078 Ang= -0.14 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.859453822486
Leave Link 401 at Fri Aug 21 17:58:27 2026, MaxMem= 805306368 cpu: 14.7 elap: 2.5
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.969282774191
DIIS: error= 3.74D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.969282774191 IErMin= 1 ErrMin= 3.74D-03
ErrMax= 3.74D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-02 BMatP= 1.34D-02
IDIUse=3 WtCom= 9.63D-01 WtEn= 3.74D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01

Gap= 0.952 Goal= None Shift= 0.000
GapD= 0.952 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=4.02D-03 MaxDP=1.17D-01 OVMax= 2.45D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 3.95D-03 CP: 1.09D+00
E= -608.978425951833 Delta-E= -0.009143177642 Rises=F Damp=F
DIIS: error= 1.21D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.978425951833 IErMin= 2 ErrMin= 1.21D-03
ErrMax= 1.21D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.65D-04 BMatP= 1.34D-02
IDIUse=3 WtCom= 9.88D-01 WtEn= 1.21D-02
Coeff-Com: 0.588D-01 0.941D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.581D-01 0.942D+00
Gap= 0.237 Goal= None Shift= 0.000
RMSDP=1.30D-03 MaxDP=4.19D-02 DE=-9.14D-03 OVMax= 1.27D-02

Cycle 3 Pass 0 IDiag 1:
RMSU= 1.09D-03 CP: 1.07D+00 8.29D-01
E= -608.979317444236 Delta-E= -0.000891492404 Rises=F Damp=F
DIIS: error= 1.06D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.979317444236 IErMin= 3 ErrMin= 1.06D-03
ErrMax= 1.06D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.65D-04 BMatP= 6.65D-04
IDIUse=3 WtCom= 9.89D-01 WtEn= 1.06D-02
Coeff-Com: -0.118D-01 0.328D+00 0.684D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.117D-01 0.325D+00 0.687D+00
Gap= 0.238 Goal= None Shift= 0.000
RMSDP=4.22D+02 MaxDP=1.75D+04 DE=-8.91D-04 OVMax= 9.91D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -608.979136013339 Delta-E= 0.000181430898 Rises=F Damp=F
DIIS: error= 6.73D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.979136013339 IErMin= 1 ErrMin= 6.73D-04
ErrMax= 6.73D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.65D-04 BMatP= 2.65D-04
IDIUse=3 WtCom= 9.93D-01 WtEn= 6.73D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=2.86D-03 MaxDP=6.55D-02 DE= 1.81D-04 OVMax= 8.39D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 2.51D-03 CP: 8.57D-01
E= -608.979327433085 Delta-E= -0.000191419747 Rises=F Damp=F
DIIS: error= 9.67D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -608.979327433085 IErMin= 1 ErrMin= 6.73D-04
ErrMax= 9.67D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-04 BMatP= 2.65D-04
IDIUse=3 WtCom= 9.90D-01 WtEn= 9.67D-03
Coeff-Com: 0.442D+00 0.558D+00
Coeff-En: 0.993D-01 0.901D+00
Coeff: 0.439D+00 0.561D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=1.15D-04 MaxDP=2.82D-03 DE=-1.91D-04 OVMax= 5.22D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 7.24D-05 CP: 8.52D-01 1.03D+00
E= -608.979497931207 Delta-E= -0.000170498121 Rises=F Damp=F
DIIS: error= 4.57D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.979497931207 IErMin= 3 ErrMin= 4.57D-04
ErrMax= 4.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-05 BMatP= 1.86D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.57D-03
Coeff-Com: 0.456D-01 0.307D+00 0.647D+00
Coeff-En: 0.000D+00 0.990D-01 0.901D+00
Coeff: 0.454D-01 0.306D+00 0.649D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=8.35D-05 MaxDP=1.77D-03 DE=-1.70D-04 OVMax= 2.92D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.61D-05 CP: 8.49D-01 1.05D+00 1.50D+00
E= -608.979556649518 Delta-E= -0.000058718311 Rises=F Damp=F
DIIS: error= 2.89D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.979556649518 IErMin= 4 ErrMin= 2.89D-04
ErrMax= 2.89D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.00D-06 BMatP= 4.17D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 2.89D-03
Coeff-Com: -0.453D-01 0.588D-01 0.302D+00 0.685D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.452D-01 0.587D-01 0.301D+00 0.685D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.01D-05 MaxDP=7.42D-04 DE=-5.87D-05 OVMax= 2.61D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.03D-05 CP: 8.48D-01 1.06D+00 1.73D+00 1.30D+00
E= -608.979572010534 Delta-E= -0.000015361016 Rises=F Damp=F
DIIS: error= 1.07D-04 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.979572010534 IErMin= 5 ErrMin= 1.07D-04
ErrMax= 1.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-06 BMatP= 6.00D-06
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.07D-03
Coeff-Com: -0.200D-01-0.751D-01-0.129D+00 0.148D+00 0.108D+01
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.200D-01-0.750D-01-0.129D+00 0.147D+00 0.108D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=1.23D-05 MaxDP=3.88D-04 DE=-1.54D-05 OVMax= 2.25D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 8.63D-06 CP: 8.48D-01 1.06D+00 1.80D+00 1.43D+00 1.48D+00
E= -608.979578936793 Delta-E= -0.000006926258 Rises=F Damp=F
DIIS: error= 7.85D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.979578936793 IErMin= 6 ErrMin= 7.85D-05
ErrMax= 7.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.62D-07 BMatP= 1.02D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.317D-02-0.440D-01-0.124D+00-0.108D+00 0.439D+00 0.834D+00
Coeff: 0.317D-02-0.440D-01-0.124D+00-0.108D+00 0.439D+00 0.834D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=7.17D-06 MaxDP=2.29D-04 DE=-6.93D-06 OVMax= 1.33D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 3.45D-06 CP: 8.48D-01 1.06D+00 1.79D+00 1.45D+00 1.80D+00
CP: 1.35D+00
E= -608.979580293514 Delta-E= -0.000001356721 Rises=F Damp=F
DIIS: error= 2.00D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.979580293514 IErMin= 7 ErrMin= 2.00D-05
ErrMax= 2.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.64D-08 BMatP= 2.62D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.409D-02-0.145D-01-0.520D-01-0.771D-01 0.104D+00 0.437D+00
Coeff-Com: 0.598D+00
Coeff: 0.409D-02-0.145D-01-0.520D-01-0.771D-01 0.104D+00 0.437D+00
Coeff: 0.598D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.14D-06 MaxDP=9.40D-05 DE=-1.36D-06 OVMax= 3.27D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.22D-06 CP: 8.48D-01 1.06D+00 1.78D+00 1.43D+00 1.84D+00
CP: 1.52D+00 1.20D+00
E= -608.979580500584 Delta-E= -0.000000207069 Rises=F Damp=F
DIIS: error= 1.61D-05 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.979580500584 IErMin= 8 ErrMin= 1.61D-05
ErrMax= 1.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-08 BMatP= 6.64D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.131D-04 0.121D-01 0.290D-01 0.162D-01-0.121D+00-0.184D+00
Coeff-Com: 0.131D+00 0.112D+01
Coeff: -0.131D-04 0.121D-01 0.290D-01 0.162D-01-0.121D+00-0.184D+00
Coeff: 0.131D+00 0.112D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.30D-06 MaxDP=1.17D-04 DE=-2.07D-07 OVMax= 3.23D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 8.29D-07 CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.84D+00
CP: 1.66D+00 1.40D+00 2.24D+00
E= -608.979580601792 Delta-E= -0.000000101208 Rises=F Damp=F
DIIS: error= 8.25D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.979580601792 IErMin= 9 ErrMin= 8.25D-06

ErrMax= 8.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.17D-09 BMatP= 1.22D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.138D-02 0.117D-01 0.337D-01 0.344D-01-0.946D-01-0.252D+00
Coeff-Com: -0.136D+00 0.618D+00 0.785D+00
Coeff: -0.138D-02 0.117D-01 0.337D-01 0.344D-01-0.946D-01-0.252D+00
Coeff: -0.136D+00 0.618D+00 0.785D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=1.12D-06 MaxDP=3.43D-05 DE=-1.01D-07 OVMax= 1.72D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 4.13D-07 CP: 8.49D-01 1.06D+00 1.75D+00 1.41D+00 1.84D+00
CP: 1.68D+00 1.52D+00 2.75D+00 1.49D+00
E= -608.979580627730 Delta-E= -0.000000025938 Rises=F Damp=F
DIIS: error= 2.45D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.979580627730 IErMin=10 ErrMin= 2.45D-06
ErrMax= 2.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.07D-10 BMatP= 5.17D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.319D-03 0.846D-03 0.291D-02 0.501D-02-0.126D-02-0.283D-01
Coeff-Com: -0.504D-01-0.368D-01 0.174D+00 0.934D+00
Coeff: -0.319D-03 0.846D-03 0.291D-02 0.501D-02-0.126D-02-0.283D-01
Coeff: -0.504D-01-0.368D-01 0.174D+00 0.934D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=5.59D-07 MaxDP=1.05D-05 DE=-2.59D-08 OVMax= 4.78D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 2.15D-07 CP: 8.49D-01 1.06D+00 1.75D+00 1.41D+00 1.83D+00
CP: 1.67D+00 1.51D+00 2.86D+00 1.66D+00 1.36D+00
E= -608.979580631407 Delta-E= -0.000000003677 Rises=F Damp=F
DIIS: error= 1.51D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.979580631407 IErMin=11 ErrMin= 1.51D-06
ErrMax= 1.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-10 BMatP= 5.07D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.253D-03-0.258D-02-0.755D-02-0.715D-02 0.222D-01 0.546D-01
Coeff-Com: 0.184D-01-0.161D+00-0.146D+00 0.229D+00 0.100D+01
Coeff: 0.253D-03-0.258D-02-0.755D-02-0.715D-02 0.222D-01 0.546D-01
Coeff: 0.184D-01-0.161D+00-0.146D+00 0.229D+00 0.100D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.14D-07 MaxDP=8.55D-06 DE=-3.68D-09 OVMax= 3.02D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 5.86D-08 CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
CP: 1.67D+00 1.50D+00 2.88D+00 1.73D+00 1.60D+00
CP: 1.52D+00
E= -608.979580632563 Delta-E= -0.000000001156 Rises=F Damp=F
DIIS: error= 8.13D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.979580632563 IErMin=12 ErrMin= 8.13D-07
ErrMax= 8.13D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.18D-11 BMatP= 1.37D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Supporting Information file

Coeff-Com: 0.138D-03-0.998D-03-0.295D-02-0.324D-02 0.734D-02 0.231D-01
Coeff-Com: 0.153D-01-0.463D-01-0.797D-01-0.101D+00 0.358D+00 0.831D+00
Coeff: 0.138D-03-0.998D-03-0.295D-02-0.324D-02 0.734D-02 0.231D-01
Coeff: 0.153D-01-0.463D-01-0.797D-01-0.101D+00 0.358D+00 0.831D+00
Gap=   0.239 Goal=   None   Shift=   0.000
RMSDP=6.60D-08 MaxDP=1.69D-06 DE=-1.16D-09 OVMax= 1.36D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 3.48D-08   CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
               CP: 1.67D+00 1.51D+00 2.89D+00 1.73D+00 1.64D+00
               CP: 1.63D+00 1.47D+00
E= -608.979580632860   Delta-E=   -0.000000000297 Rises=F Damp=F
DIIS: error= 4.75D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.979580632860   IErMin=13 ErrMin= 4.75D-07
ErrMax= 4.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.95D-11 BMatP= 4.18D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.288D-04 0.488D-03 0.148D-02 0.115D-02-0.507D-02-0.919D-02
Coeff-Com: 0.565D-03 0.382D-01 0.186D-01-0.143D+00-0.203D+00 0.443D+00
Coeff-Com: 0.857D+00
Coeff: -0.288D-04 0.488D-03 0.148D-02 0.115D-02-0.507D-02-0.919D-02
Coeff: 0.565D-03 0.382D-01 0.186D-01-0.143D+00-0.203D+00 0.443D+00
Coeff: 0.857D+00
Gap=   0.239 Goal=   None   Shift=   0.000
RMSDP=8.59D-08 MaxDP=1.71D-06 DE=-2.97D-10 OVMax= 9.53D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 2.25D-08   CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
               CP: 1.67D+00 1.51D+00 2.89D+00 1.73D+00 1.62D+00
               CP: 1.65D+00 1.87D+00 1.64D+00
E= -608.979580632984   Delta-E=   -0.000000000124 Rises=F Damp=F
DIIS: error= 2.57D-07 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.979580632984   IErMin=14 ErrMin= 2.57D-07
ErrMax= 2.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.99D-12 BMatP= 1.95D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.790D-04 0.740D-03 0.224D-02 0.221D-02-0.651D-02-0.158D-01
Coeff-Com: -0.664D-02 0.447D-01 0.484D-01-0.541D-01-0.279D+00-0.827D-01
Coeff-Com: 0.533D+00 0.814D+00
Coeff: -0.790D-04 0.740D-03 0.224D-02 0.221D-02-0.651D-02-0.158D-01
Coeff: -0.664D-02 0.447D-01 0.484D-01-0.541D-01-0.279D+00-0.827D-01
Coeff: 0.533D+00 0.814D+00
Gap=   0.239 Goal=   None   Shift=   0.000
RMSDP=4.71D-08 MaxDP=1.10D-06 DE=-1.24D-10 OVMax= 6.40D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.24D-08   CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
               CP: 1.67D+00 1.51D+00 2.90D+00 1.73D+00 1.61D+00
               CP: 1.64D+00 2.07D+00 2.10D+00 1.42D+00
E= -608.979580633028   Delta-E=   -0.000000000044 Rises=F Damp=F

DIIS: error= 5.98D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -608.979580633028 IErMin=15 ErrMin= 5.98D-08
ErrMax= 5.98D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.76D-13 BMatP= 6.99D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.197D-05-0.270D-04-0.530D-04 0.144D-04 0.267D-03 0.234D-03
Coeff-Com: -0.102D-02-0.301D-02 0.330D-02 0.181D-01 0.109D-01-0.866D-01
Coeff-Com: -0.926D-01 0.737D-01 0.108D+01
Coeff: -0.197D-05-0.270D-04-0.530D-04 0.144D-04 0.267D-03 0.234D-03
Coeff: -0.102D-02-0.301D-02 0.330D-02 0.181D-01 0.109D-01-0.866D-01
Coeff: -0.926D-01 0.737D-01 0.108D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=2.52D-08 MaxDP=7.35D-07 DE=-4.39D-11 OVMax= 1.87D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 7.70D-09 CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
CP: 1.67D+00 1.51D+00 2.90D+00 1.73D+00 1.60D+00
CP: 1.63D+00 2.05D+00 2.10D+00 1.58D+00 1.76D+00
E= -608.979580633025 Delta-E= 0.000000000003 Rises=F Damp=F
DIIS: error= 1.84D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -608.979580633028 IErMin=16 ErrMin= 1.84D-08
ErrMax= 1.84D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-13 BMatP= 4.76D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.112D-04-0.125D-03-0.357D-03-0.328D-03 0.110D-02 0.247D-02
Coeff-Com: 0.548D-03-0.796D-02-0.573D-02 0.148D-01 0.453D-01-0.172D-01
Coeff-Com: -0.119D+00-0.860D-01 0.387D+00 0.785D+00
Coeff: 0.112D-04-0.125D-03-0.357D-03-0.328D-03 0.110D-02 0.247D-02
Coeff: 0.548D-03-0.796D-02-0.573D-02 0.148D-01 0.453D-01-0.172D-01
Coeff: -0.119D+00-0.860D-01 0.387D+00 0.785D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=9.94D-09 MaxDP=2.85D-07 DE= 2.73D-12 OVMax= 5.24D-07

SCF Done: E(RwB97XD) = -608.979580633 A.U. after 19 cycles
NFock= 19 Conv=0.99D-08 -V/T= 2.0044
KE= 6.063388954549D+02 PE=-2.850316487064D+03 EE= 9.153770238045D+02
Leave Link 502 at Fri Aug 21 18:05:44 2026, MaxMem= 805306368 cpu: 2618.5 elap: 436.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14229 LenP2D= 33675.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 18:05:44 2026, MaxMem= 805306368 cpu: 1.6 elap: 0.3
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.

Supporting Information file

Leave Link 702 at Fri Aug 21 18:05:44 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 18:12:01 2026, MaxMem= 805306368 cpu: 2261.8 elap: 377.0
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.54326253D+00-5.66485486D-03-2.47702163D-04
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.002462975 -0.016721085 -0.000524258
2 6 0.013014191 0.010590509 0.000786127
3 6 -0.002404723 0.016738796 0.000566928
4 6 -0.015130804 -0.007220260 -0.001264458
5 6 0.012955217 -0.010618834 -0.000856015
6 6 0.015872091 -0.001797620 0.001637859
7 6 -0.015083237 0.007287560 0.001307176
8 6 -0.014916770 0.004093483 -0.001993098
9 6 0.015820067 0.001736194 -0.001647810
10 6 0.010578336 -0.008182589 0.003265646
11 6 -0.014908145 -0.004075424 0.001962257
12 6 -0.011348485 0.013227849 -0.004350077
13 6 0.010611786 0.008194740 -0.003212285
14 6 -0.011546297 -0.013272040 0.004388538
15 6 0.004367130 -0.000441283 0.003803457
16 6 0.004582618 0.000460005 -0.003869988

Cartesian Forces: Max 0.016738796 RMS 0.008899233
Leave Link 716 at Fri Aug 21 18:12:01 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.

Supporting Information file

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.012519492 RMS 0.004300779
Search for a local minimum.
Step number 2 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .43008D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2
DE= -1.59D-02 DEPred=-1.53D-02 R= 1.04D+00
TightC=F SS= 1.41D+00 RLast= 2.59D-01 DXNew= 5.0454D-01 7.7596D-01
Trust test= 1.04D+00 RLast= 2.59D-01 DXMaxT set to 5.05D-01
ITU= 1 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.01283 0.01334 0.01662 0.01726 0.02624
Eigenvalues --- 0.02870 0.03118 0.03421 0.03430 0.03926
Eigenvalues --- 0.03968 0.04046 0.04660 0.08421 0.09211
Eigenvalues --- 0.24390 0.24598 0.24995 0.24996 0.24999
Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25001
Eigenvalues --- 0.26478 0.28117 0.31408 0.33940 0.51191
Eigenvalues --- 0.51323 0.57377 0.57674 0.58063 0.58170
Eigenvalues --- 0.58236 0.78665 0.79080 0.79694 0.80909
Eigenvalues --- 0.82168 0.84474
RFO step: Lambda=-2.28359973D-03 EMin= 1.28298139D-02
Quartic linear search produced a step of 0.06826.
Iteration 1 RMS(Cart)= 0.00835754 RMS(Int)= 0.00008185
Iteration 2 RMS(Cart)= 0.00006329 RMS(Int)= 0.00005289
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005289
ITry= 1 IFail=0 DXMaxC= 2.04D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.32138	-0.00485	-0.00432	-0.00715	-0.01147	2.30991
R2	2.51156	0.01252	-0.00092	0.02286	0.02194	2.53350
R3	2.51170	0.01234	-0.00078	0.02245	0.02167	2.53338
R4	2.32131	-0.00484	-0.00432	-0.00713	-0.01144	2.30987
R5	2.31655	-0.00465	-0.00417	-0.00676	-0.01093	2.30563
R6	2.51187	0.01234	-0.00079	0.02246	0.02168	2.53355
R7	2.51729	0.01161	-0.00058	0.02126	0.02069	2.53798
R8	2.31644	-0.00461	-0.00417	-0.00671	-0.01088	2.30556
R9	2.30718	-0.00394	-0.00400	-0.00566	-0.00966	2.29752
R10	2.51748	0.01160	-0.00058	0.02125	0.02067	2.53814
R11	2.58156	0.00981	-0.00016	0.02025	0.02009	2.60165
R12	2.30718	-0.00393	-0.00400	-0.00565	-0.00965	2.29752
R13	2.65342	-0.00486	-0.00576	-0.01301	-0.01875	2.63467
R14	2.78000	-0.00474	-0.00498	-0.01653	-0.02152	2.75848
R15	2.58151	0.00984	-0.00014	0.02032	0.02017	2.60168
R16	2.78096	-0.00489	-0.00505	-0.01714	-0.02221	2.75876
R17	2.71064	-0.00262	-0.00436	-0.00731	-0.01167	2.69897

Supporting Information file

A1	2.61114	-0.00015	0.00002	-0.00071	-0.00069	2.61045
A2	2.64342	-0.00019	0.00005	-0.00087	-0.00082	2.64260
A3	2.61666	-0.00022	0.00002	-0.00098	-0.00096	2.61570
A4	2.72154	-0.00016	-0.00003	-0.00073	-0.00077	2.72077
A5	2.63877	-0.00016	0.00003	-0.00070	-0.00067	2.63810
A6	2.77512	0.00032	0.00011	0.00134	0.00143	2.77655
A7	2.72590	-0.00024	-0.00005	-0.00104	-0.00110	2.72480
A8	2.77198	0.00036	0.00010	0.00155	0.00163	2.77362
A9	2.82435	0.00064	-0.00030	0.00285	0.00250	2.82685
A10	2.32211	-0.00062	0.00022	-0.00588	-0.00567	2.31644
A11	2.51368	-0.00002	0.00108	-0.00324	-0.00216	2.51152
A12	1.44740	0.00064	-0.00128	0.00913	0.00771	1.45511
A13	2.82264	0.00066	-0.00030	0.00296	0.00262	2.82526
A14	2.32252	-0.00063	0.00022	-0.00589	-0.00568	2.31684
A15	1.44721	0.00065	-0.00127	0.00915	0.00775	1.45496
A16	2.51345	-0.00002	0.00107	-0.00327	-0.00219	2.51126
A17	1.42960	-0.00014	-0.00173	0.00690	0.00500	1.43461
A18	1.42916	-0.00005	-0.00169	0.00728	0.00541	1.43458
A19	2.88997	0.00002	-0.00016	0.00051	0.00033	2.89031
A20	2.89168	0.00002	-0.00012	0.00045	0.00032	2.89200
A21	3.12819	0.00013	0.00045	0.00595	0.00633	3.13452
A22	3.12813	0.00013	0.00046	0.00591	0.00631	3.13443
D1	0.05267	0.00016	0.00052	0.00399	0.00450	0.05718
D2	-0.04216	-0.00017	0.00004	-0.00511	-0.00507	-0.04722
D3	-0.03407	-0.00011	-0.00020	-0.00117	-0.00139	-0.03546
D4	0.04957	0.00018	0.00054	0.00443	0.00497	0.05454
D5	0.04534	0.00022	0.00011	0.00781	0.00788	0.05322
D6	-0.02994	-0.00013	-0.00022	-0.00161	-0.00185	-0.03179
D7	0.06529	-0.00026	-0.00134	0.00386	0.00244	0.06773
D8	0.04334	0.00021	0.00011	0.00784	0.00791	0.05124
D9	0.06850	-0.00027	-0.00134	0.00347	0.00206	0.07056
D10	-0.51939	-0.00079	0.00057	-0.02513	-0.02459	-0.54398
D11	2.62135	-0.00008	-0.00201	0.00176	-0.00029	2.62106
D12	0.68885	0.00058	0.00073	0.01360	0.01433	0.70317
D13	-2.45318	0.00018	0.00229	-0.00157	0.00067	-2.45251
D14	-2.45224	0.00016	0.00228	-0.00231	-0.00008	-2.45232
D15	0.68892	-0.00024	0.00385	-0.01748	-0.01374	0.67518
D16	2.42972	0.00033	-0.00204	0.00140	-0.00066	2.42906
D17	-0.71250	0.00085	-0.00393	0.02120	0.01730	-0.69519
D18	-0.52464	-0.00076	0.00058	-0.02429	-0.02374	-0.54838
D19	2.61768	-0.00009	-0.00201	0.00133	-0.00073	2.61696
D20	-0.71227	0.00081	-0.00395	0.02105	0.01714	-0.69513
D21	2.42878	0.00032	-0.00204	0.00219	0.00013	2.42891
D22	0.67547	-0.00077	0.00346	-0.01857	-0.01522	0.66025

Item	Value	Threshold	Converged?
Maximum Force	0.012519	0.000450	NO
RMS Force	0.004301	0.000300	NO
Maximum Displacement	0.020446	0.001800	NO

Supporting Information file

RMS Displacement 0.008336 0.001200 NO
Predicted change in Energy=-1.228655D-03
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 18:12:01 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.619798	-0.669410	0.016948
2	6	0	3.002568	-1.723696	0.057595
3	6	0	3.617587	0.670849	-0.016107
4	6	0	1.854674	-2.416159	0.065177
5	6	0	3.002424	1.726322	-0.056609
6	6	0	0.643685	-2.564756	0.059669
7	6	0	1.852651	2.415819	-0.065424
8	6	0	-0.659563	-2.243063	0.017052
9	6	0	0.641906	2.566146	-0.060425
10	6	0	-1.729388	-1.667920	-0.036242
11	6	0	-0.660956	2.242474	-0.018247
12	6	0	-2.679412	-0.679225	-0.160061
13	6	0	-1.730912	1.667539	0.034748
14	6	0	-2.679645	0.677754	0.159961
15	6	0	-4.047958	-0.405478	-0.587773
16	6	0	-4.047459	0.402802	0.589738

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.222353	0.000000			
3	C	1.340668	2.473364	0.000000		
4	C	2.483772	1.340606	3.555853	0.000000	
5	C	2.475094	3.451908	1.222329	4.300269	0.000000
6	C	3.528656	2.504340	4.395336	1.220085	4.898012
7	C	3.556435	4.298026	2.482408	4.833743	1.340694
8	C	4.559530	3.698998	5.175519	2.520648	5.401073
9	C	4.398028	4.897898	3.528285	5.129323	2.505467
10	C	5.441842	4.733215	5.836128	3.662738	5.823344
11	C	5.177370	5.399784	4.558064	5.295113	3.699762
12	C	6.301705	5.781280	6.441710	4.860618	6.170950
13	C	5.838814	5.822958	5.440811	5.434515	4.734582
14	C	6.443468	6.169683	6.299696	5.490112	5.782067
15	C	7.696093	7.201675	7.761821	6.269789	7.384754
16	C	7.763025	7.382957	7.693623	6.561775	7.202105

Supporting Information file

```
                6          7          8          9         10
  6  C    0.000000
  7  C    5.126731   0.000000
  8  C    1.343040   5.293694   0.000000
  9  C    5.132308   1.220052   4.982802   0.000000
 10  C    2.538699   5.432198   1.215795   4.852930   0.000000
 11  C    4.981729   2.520019   4.485676   1.343128   4.053769
 12  C    3.827072   5.488884   2.560615   4.644730   1.376733
 13  C    4.853005   3.662223   4.054740   2.539058   3.336215
 14  C    4.644185   4.859359   3.554199   3.827178   2.538438
 15  C    5.205111   6.561231   3.901763   5.577049   2.696982
 16  C    5.576218   6.268395   4.336636   5.205085   3.170677
                11         12         13         14         15
 11  C    0.000000
 12  C    3.553955   0.000000
 13  C    1.215797   2.538682   0.000000
 14  C    2.560314   1.394205   1.376752   0.000000
 15  C    4.336795   1.459724   3.170747   1.898626   0.000000
 16  C    3.901594   1.898561   2.697029   1.459871   1.428233
                16
 16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 2.65D-04
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.619654   -0.670227    0.015356
    2          6           0        3.002197   -1.724472    0.053571
    3          6           0        3.617731    0.670105   -0.014600
    4          6           0        1.854154   -2.416703    0.059564
    5          6           0        3.002795    1.725801   -0.052652
    6          6           0        0.643133   -2.565026    0.053728
    7          6           0        1.853171    2.415564   -0.059858
    8          6           0       -0.660046   -2.242954    0.011871
    9          6           0        0.642458    2.566141   -0.054496
   10          6           0       -1.729748   -1.667458   -0.040079
   11          6           0       -0.660473    2.242653   -0.013052
   12          6           0       -2.679560   -0.678275   -0.161599
   13          6           0       -1.730552    1.667828    0.038627
   14          6           0       -2.679497    0.677960    0.161561
   15          6           0       -4.048052   -0.403244   -0.588660
```

```
    16        6        0      -4.047365    0.402310    0.590718
 -------------------------------------------------------------------
 Rotational constants (GHZ):           0.8537904           0.3947969           0.2726563
 Leave Link  202 at Fri Aug 21 18:12:01 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       719.0512270591 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0075260663 Hartrees.
 Nuclear repulsion after empirical dispersion term =      719.0437009928 Hartrees.
 Leave Link  301 at Fri Aug 21 18:12:01 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14219 LenP2D=   33635.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  3.85D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=          32
 NSgBfM=   565   565   565   565   565 MxSgAt=    16 MxSgA2=    16.
 Leave Link  302 at Fri Aug 21 18:12:02 2026, MaxMem=    805306368 cpu:                  3.4 elap:
0.6
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Aug 21 18:12:02 2026, MaxMem=    805306368 cpu:                  0.5 elap:
0.1
```

Supporting Information file

(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 0.000000 -0.000000
Rot= 1.000000 0.000089 -0.000003 0.000029 Ang= 0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.860177073713
Leave Link 401 at Fri Aug 21 18:12:06 2026, MaxMem= 805306368 cpu: 24.7 elap: 4.1
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.979722802012
DIIS: error= 3.10D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.979722802012 IErMin= 1 ErrMin= 3.10D-03
ErrMax= 3.10D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-03 BMatP= 2.22D-03
IDIUse=3 WtCom= 9.69D-01 WtEn= 3.10D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01

Gap= 0.952 Goal= None Shift= 0.000
GapD= 0.952 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=4.78D-03 MaxDP=1.64D-01 OVMax= 1.06D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 4.64D-03 CP: 1.14D+00
E= -608.981036803820 Delta-E= -0.001314001808 Rises=F Damp=F
DIIS: error= 6.32D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981036803820 IErMin= 2 ErrMin= 6.32D-04
ErrMax= 6.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-04 BMatP= 2.22D-03
IDIUse=3 WtCom= 9.94D-01 WtEn= 6.32D-03
Coeff-Com: 0.526D-01 0.947D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.522D-01 0.948D+00
Gap= 0.241 Goal= None Shift= 0.000
RMSDP=1.25D-03 MaxDP=2.97D-02 DE=-1.31D-03 OVMax= 6.77D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 1.14D-03 CP: 1.13D+00 8.90D-01
E= -608.981151855228 Delta-E= -0.000115051408 Rises=F Damp=F
DIIS: error= 2.33D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981151855228 IErMin= 2 ErrMin= 6.32D-04
ErrMax= 2.33D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-04 BMatP= 1.23D-04
IDIUse=3 WtCom= 1.72D-01 WtEn= 8.28D-01
Coeff-Com: 0.306D-01 0.730D+00 0.240D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.525D-02 0.125D+00 0.869D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=4.31D+02 MaxDP=1.70D+04 DE=-1.15D-04 OVMax= 9.94D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -608.980960456240 Delta-E= 0.000191398988 Rises=F Damp=F
DIIS: error= 5.94D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.980960456240 IErMin= 1 ErrMin= 5.94D-04
ErrMax= 5.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-04 BMatP= 1.38D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 5.94D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=4.17D-03 MaxDP=1.29D-01 DE= 1.91D-04 OVMax= 5.64D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.29D-03 CP: 7.56D-01
E= -608.981059486248 Delta-E= -0.000099030008 Rises=F Damp=F
DIIS: error= 3.53D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -608.981059486248 IErMin= 2 ErrMin= 3.53D-04
ErrMax= 3.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.81D-05 BMatP= 1.38D-04
IDIUse=3 WtCom= 9.96D-01 WtEn= 3.53D-03
Coeff-Com: 0.225D+00 0.775D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.224D+00 0.776D+00
Gap= 0.242 Goal= None Shift= 0.000
RMSDP=2.37D-04 MaxDP=6.29D-03 DE=-9.90D-05 OVMax= 3.34D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.13D-04 CP: 7.44D-01 1.05D+00
E= -608.981080497832 Delta-E= -0.000021011583 Rises=F Damp=F
DIIS: error= 3.02D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981080497832 IErMin= 3 ErrMin= 3.02D-04
ErrMax= 3.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-05 BMatP= 2.81D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.02D-03
Coeff-Com: -0.950D-02 0.429D+00 0.581D+00
Coeff-En: 0.000D+00 0.278D+00 0.722D+00
Coeff: -0.947D-02 0.428D+00 0.581D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=8.34D-05 MaxDP=2.19D-03 DE=-2.10D-05 OVMax= 1.95D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.54D-05 CP: 7.39D-01 1.07D+00 1.28D+00
E= -608.981100782059 Delta-E= -0.000020284228 Rises=F Damp=F
DIIS: error= 1.02D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981100782059 IErMin= 4 ErrMin= 1.02D-04
ErrMax= 1.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-06 BMatP= 1.65D-05
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.02D-03
Coeff-Com: -0.194D-01 0.186D+00 0.319D+00 0.515D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.193D-01 0.185D+00 0.319D+00 0.515D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=1.48D-05 MaxDP=3.83D-04 DE=-2.03D-05 OVMax= 6.26D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.64D-06 CP: 7.39D-01 1.07D+00 1.34D+00 1.15D+00
E= -608.981103732968 Delta-E= -0.000002950909 Rises=F Damp=F
DIIS: error= 7.14D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981103732968 IErMin= 5 ErrMin= 7.14D-05
ErrMax= 7.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.30D-07 BMatP= 1.75D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.563D-02-0.195D+00-0.255D+00-0.426D-02 0.145D+01
Coeff: 0.563D-02-0.195D+00-0.255D+00-0.426D-02 0.145D+01
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=1.57D-05 MaxDP=3.42D-04 DE=-2.95D-06 OVMax= 1.51D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.15D-06 CP: 7.38D-01 1.07D+00 1.42D+00 1.28D+00 1.99D+00
E= -608.981105814259 Delta-E= -0.000002081291 Rises=F Damp=F
DIIS: error= 2.45D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981105814259 IErMin= 6 ErrMin= 2.45D-05
ErrMax= 2.45D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.07D-08 BMatP= 2.30D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.596D-02-0.134D+00-0.186D+00-0.807D-01 0.779D+00 0.615D+00
Coeff: 0.596D-02-0.134D+00-0.186D+00-0.807D-01 0.779D+00 0.615D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=3.62D-06 MaxDP=9.99D-05 DE=-2.08D-06 OVMax= 3.77D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.47D-06 CP: 7.38D-01 1.07D+00 1.41D+00 1.28D+00 2.23D+00
CP: 1.23D+00
E= -608.981106025962 Delta-E= -0.000000211703 Rises=F Damp=F
DIIS: error= 8.00D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981106025962 IErMin= 7 ErrMin= 8.00D-06
ErrMax= 8.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.90D-09 BMatP= 7.07D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.123D-02-0.180D-01-0.287D-01-0.302D-01 0.474D-01 0.223D+00
Coeff-Com: 0.805D+00
Coeff: 0.123D-02-0.180D-01-0.287D-01-0.302D-01 0.474D-01 0.223D+00
Coeff: 0.805D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=5.71D-06 MaxDP=1.54D-04 DE=-2.12D-07 OVMax= 1.57D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 7.72D-07 CP: 7.39D-01 1.07D+00 1.39D+00 1.24D+00 2.25D+00
CP: 1.36D+00 1.85D+00
E= -608.981106062581 Delta-E= -0.000000036619 Rises=F Damp=F
DIIS: error= 5.03D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981106062581 IErMin= 8 ErrMin= 5.03D-06
ErrMax= 5.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-09 BMatP= 7.90D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.119D-02 0.320D-01 0.419D-01 0.801D-02-0.219D+00-0.561D-01
Coeff-Com: 0.442D+00 0.753D+00
Coeff: -0.119D-02 0.320D-01 0.419D-01 0.801D-02-0.219D+00-0.561D-01
Coeff: 0.442D+00 0.753D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=3.40D-06 MaxDP=9.30D-05 DE=-3.66D-08 OVMax= 9.35D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.16D-07 CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.24D+00
CP: 1.42D+00 2.38D+00 1.59D+00
E= -608.981106076013 Delta-E= -0.000000013432 Rises=F Damp=F
DIIS: error= 2.30D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981106076013 IErMin= 9 ErrMin= 2.30D-06
ErrMax= 2.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.67D-10 BMatP= 3.14D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.842D-03 0.176D-01 0.247D-01 0.136D-01-0.893D-01-0.867D-01
Coeff-Com: -0.107D+00 0.236D+00 0.993D+00
Coeff: -0.842D-03 0.176D-01 0.247D-01 0.136D-01-0.893D-01-0.867D-01
Coeff: -0.107D+00 0.236D+00 0.993D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=7.21D-07 MaxDP=2.24D-05 DE=-1.34D-08 OVMax= 4.73D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.86D-07 CP: 7.39D-01 1.07D+00 1.37D+00 1.21D+00 2.24D+00
CP: 1.43D+00 2.55D+00 1.80D+00 1.62D+00
E= -608.981106080172 Delta-E= -0.000000004160 Rises=F Damp=F
DIIS: error= 1.10D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981106080172 IErMin=10 ErrMin= 1.10D-06
ErrMax= 1.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-10 BMatP= 5.67D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.533D-04-0.283D-02-0.343D-02 0.135D-02 0.283D-01-0.113D-01
Coeff-Com: -0.137D+00-0.121D+00 0.290D+00 0.955D+00
Coeff: 0.533D-04-0.283D-02-0.343D-02 0.135D-02 0.283D-01-0.113D-01
Coeff: -0.137D+00-0.121D+00 0.290D+00 0.955D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=7.41D-07 MaxDP=1.88D-05 DE=-4.16D-09 OVMax= 2.37D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 8.08D-08 CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.24D+00
CP: 1.43D+00 2.51D+00 1.76D+00 1.96D+00 1.54D+00
E= -608.981106080997 Delta-E= -0.000000000825 Rises=F Damp=F
DIIS: error= 5.77D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981106080997 IErMin=11 ErrMin= 5.77D-07
ErrMax= 5.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-11 BMatP= 1.09D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.153D-03-0.373D-02-0.518D-02-0.194D-02 0.231D-01 0.889D-02
Coeff-Com: -0.256D-01-0.683D-01-0.682D-01 0.312D+00 0.829D+00
Coeff: 0.153D-03-0.373D-02-0.518D-02-0.194D-02 0.231D-01 0.889D-02
Coeff: -0.256D-01-0.683D-01-0.682D-01 0.312D+00 0.829D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=3.66D-07 MaxDP=1.03D-05 DE=-8.25D-10 OVMax= 9.58D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 3.06D-08 CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.25D+00
CP: 1.43D+00 2.46D+00 1.69D+00 1.99D+00 1.73D+00
CP: 1.29D+00
E= -608.981106081146 Delta-E= -0.000000000148 Rises=F Damp=F
DIIS: error= 3.42D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981106081146 IErMin=12 ErrMin= 3.42D-07
ErrMax= 3.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.61D-12 BMatP= 2.34D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.250D-04-0.248D-03-0.476D-03-0.834D-03-0.458D-03 0.380D-02

Coeff-Com: 0.250D-01 0.122D-01-0.819D-01-0.140D+00 0.147D+00 0.104D+01
Coeff: 0.250D-04-0.248D-03-0.476D-03-0.834D-03-0.458D-03 0.380D-02
Coeff: 0.250D-01 0.122D-01-0.819D-01-0.140D+00 0.147D+00 0.104D+01
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=8.58D-08 MaxDP=2.73D-06 DE=-1.48D-10 OVMax= 6.56D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.51D-08 CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.26D+00
CP: 1.42D+00 2.45D+00 1.66D+00 1.98D+00 1.77D+00
CP: 1.47D+00 1.66D+00
E= -608.981106081205 Delta-E= -0.000000000059 Rises=F Damp=F
DIIS: error= 2.07D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981106081205 IErMin=13 ErrMin= 2.07D-07
ErrMax= 2.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.45D-12 BMatP= 6.61D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.531D-04 0.155D-02 0.206D-02 0.374D-03-0.107D-01-0.201D-02
Coeff-Com: 0.281D-01 0.399D-01-0.241D-01-0.244D+00-0.274D+00 0.727D+00
Coeff-Com: 0.756D+00
Coeff: -0.531D-04 0.155D-02 0.206D-02 0.374D-03-0.107D-01-0.201D-02
Coeff: 0.281D-01 0.399D-01-0.241D-01-0.244D+00-0.274D+00 0.727D+00
Coeff: 0.756D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=2.97D-08 MaxDP=7.17D-07 DE=-5.91D-11 OVMax= 4.68D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 8.44D-09 CP: 7.39D-01 1.07D+00 1.37D+00 1.23D+00 2.26D+00
CP: 1.42D+00 2.44D+00 1.66D+00 1.97D+00 1.77D+00
CP: 1.52D+00 2.10D+00 1.58D+00
E= -608.981106081225 Delta-E= -0.000000000020 Rises=F Damp=F
DIIS: error= 5.99D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.981106081225 IErMin=14 ErrMin= 5.99D-08
ErrMax= 5.99D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.06D-13 BMatP= 4.45D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.231D-04 0.569D-03 0.784D-03 0.330D-03-0.340D-02-0.148D-02
Coeff-Com: 0.427D-02 0.104D-01 0.856D-02-0.488D-01-0.127D+00 0.157D-01
Coeff-Com: 0.270D+00 0.870D+00
Coeff: -0.231D-04 0.569D-03 0.784D-03 0.330D-03-0.340D-02-0.148D-02
Coeff: 0.427D-02 0.104D-01 0.856D-02-0.488D-01-0.127D+00 0.157D-01
Coeff: 0.270D+00 0.870D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=4.48D-08 MaxDP=1.17D-06 DE=-2.00D-11 OVMax= 1.67D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 5.63D-09 CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.25D+00
CP: 1.42D+00 2.45D+00 1.66D+00 1.97D+00 1.76D+00
CP: 1.50D+00 2.12D+00 1.87D+00 1.42D+00
E= -608.981106081237 Delta-E= -0.000000000012 Rises=F Damp=F
DIIS: error= 2.43D-08 at cycle 15 NSaved= 15.

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NSaved=15 IEnMin=15 EnMin= -608.981106081237 IErMin=15 ErrMin= 2.43D-08
ErrMax= 2.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.27D-14 BMatP= 5.06D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.535D-05-0.187D-03-0.244D-03 0.389D-05 0.141D-02-0.148D-04
Coeff-Com: -0.513D-02-0.599D-02 0.781D-02 0.425D-01 0.240D-01-0.159D+00
Coeff-Com: -0.106D+00 0.294D+00 0.907D+00
Coeff: 0.535D-05-0.187D-03-0.244D-03 0.389D-05 0.141D-02-0.148D-04
Coeff: -0.513D-02-0.599D-02 0.781D-02 0.425D-01 0.240D-01-0.159D+00
Coeff: -0.106D+00 0.294D+00 0.907D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=2.16D-08 MaxDP=6.13D-07 DE=-1.18D-11 OVMax= 5.87D-07

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.51D-09 CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.25D+00
CP: 1.42D+00 2.46D+00 1.67D+00 1.97D+00 1.76D+00
CP: 1.47D+00 2.08D+00 1.92D+00 1.74D+00 1.54D+00
E= -608.981106081232 Delta-E= 0.000000000004 Rises=F Damp=F
DIIS: error= 7.18D-09 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -608.981106081237 IErMin=16 ErrMin= 7.18D-09
ErrMax= 7.18D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-15 BMatP= 8.27D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.253D-05-0.679D-04-0.924D-04-0.301D-04 0.416D-03 0.135D-03
Coeff-Com: -0.887D-03-0.152D-02 0.292D-03 0.832D-02 0.131D-01-0.187D-01
Coeff-Com: -0.316D-01-0.414D-01 0.977D-01 0.974D+00
Coeff: 0.253D-05-0.679D-04-0.924D-04-0.301D-04 0.416D-03 0.135D-03
Coeff: -0.887D-03-0.152D-02 0.292D-03 0.832D-02 0.131D-01-0.187D-01
Coeff: -0.316D-01-0.414D-01 0.977D-01 0.974D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=2.64D-09 MaxDP=6.32D-08 DE= 4.09D-12 OVMax= 9.82D-08

SCF Done: E(RwB97XD) = -608.981106081 A.U. after 19 cycles
NFock= 19 Conv=0.26D-08 -V/T= 2.0043
KE= 6.063506560153D+02 PE=-2.849183397747D+03 EE= 9.148079346575D+02
Leave Link 502 at Fri Aug 21 18:24:15 2026, MaxMem= 805306368 cpu: 4371.6 elap: 728.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14219 LenP2D= 33635.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 18:24:15 2026, MaxMem= 805306368 cpu: 2.3 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 18:24:16 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0

Supporting Information file

(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 18:32:51 2026, MaxMem= 805306368 cpu: 3094.5 elap: 515.8
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.53457090D+00-5.28608494D-03-3.87975051D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000154283	-0.005241617	-0.000500907
2	6	0.004345088	0.002474836	0.000754583
3	6	0.000239313	0.005272667	0.000535298
4	6	-0.004070830	-0.002930740	-0.001067360
5	6	0.004277109	-0.002535123	-0.000818853
6	6	0.004075288	-0.000736859	0.000996782
7	6	-0.004045571	0.003013648	0.001114809
8	6	-0.003974278	0.000050000	-0.000965724
9	6	0.004067988	0.000662888	-0.001012631
10	6	0.002538325	-0.002251863	0.002136582
11	6	-0.003979765	-0.000017155	0.000942031
12	6	-0.003189845	0.001811514	-0.001847456
13	6	0.002557635	0.002231574	-0.002084464
14	6	-0.003252023	-0.001798597	0.001837039
15	6	0.000087545	-0.001712116	-0.004206451
16	6	0.000169740	0.001706944	0.004186724

Cartesian Forces: Max 0.005272667 RMS 0.002647994
Leave Link 716 at Fri Aug 21 18:32:51 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.005565741 RMS 0.001771487

Supporting Information file

Search for a local minimum.
Step number 3 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .17715D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2 3
DE= -1.53D-03 DEPred=-1.23D-03 R= 1.24D+00
TightC=F SS= 1.41D+00 RLast= 9.04D-02 DXNew= 8.4853D-01 2.7111D-01
Trust test= 1.24D+00 RLast= 9.04D-02 DXMaxT set to 5.05D-01
ITU= 1 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.01281	0.01325	0.01632	0.01725	0.02624
Eigenvalues ---	0.02859	0.03105	0.03410	0.03422	0.03926
Eigenvalues ---	0.03966	0.04047	0.04725	0.08413	0.09213
Eigenvalues ---	0.23684	0.24564	0.24884	0.24996	0.24997
Eigenvalues ---	0.24999	0.25000	0.25000	0.25000	0.25000
Eigenvalues ---	0.25266	0.28151	0.32543	0.35661	0.42307
Eigenvalues ---	0.51320	0.53483	0.57377	0.57873	0.58159
Eigenvalues ---	0.58183	0.78664	0.79200	0.79694	0.81167
Eigenvalues ---	0.82167	0.88990			

RFO step: Lambda=-4.24577900D-04 EMin= 1.28124421D-02
Quartic linear search produced a step of 0.31972.
Iteration 1 RMS(Cart)= 0.01191570 RMS(Int)= 0.00015219
Iteration 2 RMS(Cart)= 0.00015562 RMS(Int)= 0.00003672
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00003672
ITry= 1 IFail=0 DXMaxC= 3.14D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.30991	0.00038	-0.00367	0.00064	-0.00302	2.30689
R2	2.53350	0.00557	0.00701	0.00772	0.01474	2.54824
R3	2.53338	0.00532	0.00693	0.00721	0.01414	2.54752
R4	2.30987	0.00038	-0.00366	0.00063	-0.00302	2.30685
R5	2.30563	0.00043	-0.00349	0.00063	-0.00286	2.30276
R6	2.53355	0.00531	0.00693	0.00720	0.01414	2.54768
R7	2.53798	0.00461	0.00661	0.00594	0.01256	2.55053
R8	2.30556	0.00042	-0.00348	0.00062	-0.00286	2.30270
R9	2.29752	0.00084	-0.00309	0.00107	-0.00202	2.29549
R10	2.53814	0.00460	0.00661	0.00593	0.01254	2.55068
R11	2.60165	0.00447	0.00642	0.00713	0.01355	2.61520
R12	2.29752	0.00084	-0.00309	0.00106	-0.00203	2.29550
R13	2.63467	0.00136	-0.00600	0.00443	-0.00159	2.63307
R14	2.75848	0.00032	-0.00688	0.00208	-0.00479	2.75369
R15	2.60168	0.00447	0.00645	0.00712	0.01356	2.61525
R16	2.75876	0.00027	-0.00710	0.00196	-0.00513	2.75363
R17	2.69897	0.00352	-0.00373	0.01478	0.01104	2.71001
A1	2.61045	0.00004	-0.00022	0.00174	0.00153	2.61199
A2	2.64260	-0.00001	-0.00026	0.00131	0.00105	2.64365

Supporting Information file

A3	2.61570	-0.00003	-0.00031	0.00143	0.00113	2.61683
A4	2.72077	-0.00014	-0.00025	0.00020	-0.00006	2.72071
A5	2.63810	0.00004	-0.00021	0.00156	0.00136	2.63945
A6	2.77655	0.00020	0.00046	0.00118	0.00161	2.77816
A7	2.72480	-0.00021	-0.00035	-0.00007	-0.00043	2.72437
A8	2.77362	0.00025	0.00052	0.00143	0.00193	2.77554
A9	2.82685	0.00037	0.00080	0.00103	0.00177	2.82862
A10	2.31644	-0.00019	-0.00181	0.00245	0.00062	2.31705
A11	2.51152	0.00002	-0.00069	0.00405	0.00341	2.51493
A12	1.45511	0.00018	0.00247	-0.00657	-0.00421	1.45091
A13	2.82526	0.00040	0.00084	0.00117	0.00195	2.82720
A14	2.31684	-0.00019	-0.00182	0.00247	0.00064	2.31748
A15	1.45496	0.00017	0.00248	-0.00661	-0.00424	1.45071
A16	2.51126	0.00002	-0.00070	0.00409	0.00344	2.51470
A17	1.43461	-0.00053	0.00160	-0.00976	-0.00827	1.42634
A18	1.43458	-0.00049	0.00173	-0.00963	-0.00801	1.42656
A19	2.89031	-0.00037	0.00011	-0.01224	-0.01218	2.87813
A20	2.89200	-0.00038	0.00010	-0.01241	-0.01236	2.87964
A21	3.13452	-0.00029	0.00202	-0.00613	-0.00409	3.13043
A22	3.13443	-0.00029	0.00202	-0.00606	-0.00403	3.13041
D1	0.05718	0.00004	0.00144	0.00128	0.00271	0.05989
D2	-0.04722	-0.00016	-0.00162	-0.00456	-0.00619	-0.05342
D3	-0.03546	-0.00015	-0.00045	-0.00371	-0.00416	-0.03962
D4	0.05454	0.00005	0.00159	0.00164	0.00323	0.05777
D5	0.05322	0.00016	0.00252	0.00614	0.00866	0.06188
D6	-0.03179	-0.00017	-0.00059	-0.00412	-0.00471	-0.03651
D7	0.06773	-0.00017	0.00078	-0.00285	-0.00206	0.06567
D8	0.05124	0.00016	0.00253	0.00618	0.00871	0.05995
D9	0.07056	-0.00018	0.00066	-0.00309	-0.00242	0.06814
D10	-0.54398	-0.00021	-0.00786	-0.01211	-0.01998	-0.56396
D11	2.62106	-0.00048	-0.00009	-0.00623	-0.00630	2.61476
D12	0.70317	0.00064	0.00458	0.02872	0.03329	0.73646
D13	-2.45251	0.00081	0.00022	0.02563	0.02584	-2.42666
D14	-2.45232	0.00080	-0.00003	0.02529	0.02527	-2.42705
D15	0.67518	0.00097	-0.00439	0.02220	0.01782	0.69301
D16	2.42906	0.00012	-0.00021	-0.02396	-0.02414	2.40492
D17	-0.69519	-0.00008	0.00553	-0.01963	-0.01403	-0.70922
D18	-0.54838	-0.00019	-0.00759	-0.01162	-0.01921	-0.56759
D19	2.61696	-0.00049	-0.00023	-0.00629	-0.00651	2.61045
D20	-0.69513	-0.00009	0.00548	-0.01965	-0.01410	-0.70923
D21	2.42891	0.00012	0.00004	-0.02356	-0.02349	2.40542
D22	0.66025	0.00047	-0.00486	0.01946	0.01456	0.67481

Item	Value	Threshold	Converged?
Maximum Force	0.005566	0.000450	NO
RMS Force	0.001771	0.000300	NO
Maximum Displacement	0.031438	0.001800	NO
RMS Displacement	0.011962	0.001200	NO

Predicted change in Energy=-3.144828D-04

Supporting Information file

Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 18:32:51 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.620486	-0.673288	0.016168
2	6	0	3.005594	-1.727069	0.057295
3	6	0	3.618433	0.674810	-0.015388
4	6	0	1.853025	-2.426249	0.065899
5	6	0	3.005453	1.729680	-0.056432
6	6	0	0.643887	-2.577540	0.063433
7	6	0	1.851107	2.426075	-0.066090
8	6	0	-0.667164	-2.259670	0.021566
9	6	0	0.642184	2.578836	-0.064030
10	6	0	-1.731249	-1.676635	-0.036300
11	6	0	-0.668510	2.259110	-0.022595
12	6	0	-2.679668	-0.677271	-0.166519
13	6	0	-1.732684	1.676199	0.034905
14	6	0	-2.679898	0.675792	0.166167
15	6	0	-4.040901	-0.391237	-0.600840
16	6	0	-4.040093	0.388456	0.602762

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220753	0.000000			
3	C	1.348468	2.479894	0.000000		
4	C	2.489832	1.348088	3.569291	0.000000	
5	C	2.481490	3.458619	1.220730	4.314488	0.000000
6	C	3.533915	2.510179	4.408165	1.218569	4.913605
7	C	3.569807	4.312386	2.488563	4.854120	1.348175
8	C	4.571715	3.711346	5.194120	2.526078	5.423017
9	C	4.410559	4.913374	3.533517	5.151106	2.511208
10	C	5.445229	4.738035	5.843700	3.663247	5.834358
11	C	5.195763	5.421720	4.570333	5.321519	3.712068
12	C	6.302803	5.785704	6.443372	4.863974	6.174636
13	C	5.846099	5.833868	5.444242	5.448702	4.739319
14	C	6.444948	6.173363	6.300947	5.493642	5.786488
15	C	7.691366	7.202130	7.755296	6.270900	7.378738
16	C	7.756021	7.376631	7.688767	6.552834	7.202301

		6	7	8	9	10
6	C	0.000000				

```
 7  C    5.148818   0.000000
 8  C    1.349685   5.320299   0.000000
 9  C    5.157952   1.218538   5.013268   0.000000
10  C    2.542212   5.446686   1.214723   4.872677   0.000000
11  C    5.012282   2.525517   4.518996   1.349763   4.076726
12  C    3.835351   5.492610   2.567008   4.652681   1.383902
13  C    4.872700   3.662795   4.077570   2.542546   3.353591
14  C    4.652125   4.862863   3.562154   3.835465   2.544571
15  C    5.212334   6.552783   3.906473   5.571425   2.702860
16  C    5.570250   6.269409   4.327471   5.212110   3.162873
            11         12         13         14         15
11  C    0.000000
12  C    3.561995   0.000000
13  C    1.214725   2.544833   0.000000
14  C    2.566750   1.393363   1.383929   0.000000
15  C    4.328016   1.457191   3.163278   1.891872   0.000000
16  C    3.906148   1.891646   2.702754   1.457158   1.434078
            16
16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 1.21D-03
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.620318   -0.674242    0.013975
    2          6           0        3.005162   -1.727994    0.051770
    3          6           0        3.618602    0.673949   -0.013307
    4          6           0        1.852419   -2.426910    0.058176
    5          6           0        3.005885    1.729098   -0.050996
    6          6           0        0.643243   -2.577890    0.055250
    7          6           0        1.851713    2.425810   -0.058428
    8          6           0       -0.667730   -2.259560    0.014412
    9          6           0        0.642828    2.578865   -0.055864
   10          6           0       -1.731669   -1.676078   -0.041588
   11          6           0       -0.667945    2.259338   -0.015422
   12          6           0       -2.679840   -0.676069   -0.168622
   13          6           0       -1.732264    1.676514    0.040248
   14          6           0       -2.679726    0.675932    0.168352
   15          6           0       -4.041008   -0.388318   -0.602012
   16          6           0       -4.039987    0.387554    0.604056
---------------------------------------------------------------------
```

Rotational constants (GHZ): 0.8455681 0.3948289 0.2719550
Leave Link 202 at Fri Aug 21 18:32:51 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 717.8042181906 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074879094 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.7967302812 Hartrees.
Leave Link 301 at Fri Aug 21 18:32:52 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14217 LenP2D= 33589.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 3.90D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 18:32:53 2026, MaxMem= 805306368 cpu: 6.4 elap: 1.1
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 18:32:53 2026, MaxMem= 805306368 cpu: 0.9 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"

Supporting Information file

B after Tr= 0.000000 -0.000000 -0.000000
Rot= 1.000000 -0.000429 -0.000002 0.000017 Ang= -0.05 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.863687939798
Leave Link 401 at Fri Aug 21 18:33:01 2026, MaxMem= 805306368 cpu: 46.7 elap: 7.8
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.980360925497
DIIS: error= 1.85D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.980360925497 IErMin= 1 ErrMin= 1.85D-03
ErrMax= 1.85D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-03 BMatP= 1.83D-03
IDIUse=3 WtCom= 9.82D-01 WtEn= 1.85D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
GapD= 0.960 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=3.94D-03 MaxDP=1.27D-01 OVMax= 7.46D-03

Cycle 2 Pass 0 IDiag 1:
RMSU= 3.84D-03 CP: 1.10D+00
E= -608.981429218990 Delta-E= -0.001068293492 Rises=F Damp=F
DIIS: error= 5.42D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981429218990 IErMin= 2 ErrMin= 5.42D-04
ErrMax= 5.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.34D-05 BMatP= 1.83D-03
IDIUse=3 WtCom= 9.95D-01 WtEn= 5.42D-03
Coeff-Com: 0.481D-02 0.995D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.478D-02 0.995D+00
Gap= 0.245 Goal= None Shift= 0.000
RMSDP=1.07D-03 MaxDP=2.92D-02 DE=-1.07D-03 OVMax= 4.01D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 1.05D-03 CP: 1.12D+00 1.06D+00
E= -608.981484156543 Delta-E= -0.000054937554 Rises=F Damp=F
DIIS: error= 2.15D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981484156543 IErMin= 2 ErrMin= 5.42D-04
ErrMax= 2.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-04 BMatP= 6.34D-05
IDIUse=3 WtCom= 1.78D-01 WtEn= 8.22D-01
Coeff-Com: 0.190D-02 0.882D+00 0.116D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.337D-03 0.157D+00 0.843D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=4.20D+02 MaxDP=1.66D+04 DE=-5.49D-05 OVMax= 9.92D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -608.981286893094 Delta-E= 0.000197263449 Rises=F Damp=F
DIIS: error= 5.88D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981286893094 IErMin= 1 ErrMin= 5.88D-04
ErrMax= 5.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-04 BMatP= 1.24D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 5.88D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=4.04D-03 MaxDP=1.25D-01 DE= 1.97D-04 OVMax= 2.69D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.24D-03 CP: 7.67D-01
E= -608.981365391536 Delta-E= -0.000078498442 Rises=F Damp=F
DIIS: error= 3.39D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981365391536 IErMin= 2 ErrMin= 3.39D-04
ErrMax= 3.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-05 BMatP= 1.24D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.39D-03
Coeff-Com: 0.138D+00 0.862D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.138D+00 0.862D+00
Gap= 0.245 Goal= None Shift= 0.000
RMSDP=2.50D-04 MaxDP=6.22D-03 DE=-7.85D-05 OVMax= 1.94D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.19D-04 CP: 7.53D-01 1.05D+00
E= -608.981362120546 Delta-E= 0.000003270990 Rises=F Damp=F
DIIS: error= 3.38D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -608.981365391536 IErMin= 3 ErrMin= 3.38D-04
ErrMax= 3.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-05 BMatP= 1.54D-05
IDIUse=3 WtCom= 3.52D-01 WtEn= 6.48D-01
Coeff-Com: -0.172D-01 0.553D+00 0.464D+00
Coeff-En: 0.000D+00 0.536D+00 0.464D+00
Coeff: -0.605D-02 0.542D+00 0.464D+00
Gap= 0.245 Goal= None Shift= 0.000
RMSDP=5.61D-05 MaxDP=1.51D-03 DE= 3.27D-06 OVMax= 1.13D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.51D-05 CP: 7.50D-01 1.06D+00 1.21D+00
E= -608.981386295772 Delta-E= -0.000024175226 Rises=F Damp=F
DIIS: error= 5.20D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981386295772 IErMin= 4 ErrMin= 5.20D-05
ErrMax= 5.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.62D-07 BMatP= 1.54D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.136D-01 0.210D+00 0.215D+00 0.589D+00
Coeff: -0.136D-01 0.210D+00 0.215D+00 0.589D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.75D-05 MaxDP=4.88D-04 DE=-2.42D-05 OVMax= 3.88D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.32D-06 CP: 7.49D-01 1.07D+00 1.29D+00 1.19D+00
E= -608.981387332955 Delta-E= -0.000001037183 Rises=F Damp=F
DIIS: error= 3.29D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981387332955 IErMin= 5 ErrMin= 3.29D-05
ErrMax= 3.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.20D-08 BMatP= 5.62D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.671D-02-0.211D+00-0.178D+00 0.256D-02 0.138D+01
Coeff: 0.671D-02-0.211D+00-0.178D+00 0.256D-02 0.138D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.78D-05 MaxDP=4.73D-04 DE=-1.04D-06 OVMax= 7.76D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.28D-06 CP: 7.49D-01 1.07D+00 1.38D+00 1.37D+00 2.12D+00
E= -608.981387981709 Delta-E= -0.000000648754 Rises=F Damp=F
DIIS: error= 1.56D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -608.981387981709 IErMin= 6 ErrMin= 1.56D-05
ErrMax= 1.56D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-08 BMatP= 8.20D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.541D-02-0.146D+00-0.127D+00-0.653D-01 0.802D+00 0.532D+00
Coeff: 0.541D-02-0.146D+00-0.127D+00-0.653D-01 0.802D+00 0.532D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.56D-06 MaxDP=4.70D-05 DE=-6.49D-07 OVMax= 1.75D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 7.71D-07 CP: 7.49D-01 1.07D+00 1.37D+00 1.37D+00 2.23D+00
CP: 1.08D+00
E= -608.981388049537 Delta-E= -0.000000067829 Rises=F Damp=F
DIIS: error= 4.74D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981388049537 IErMin= 7 ErrMin= 4.74D-06
ErrMax= 4.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-09 BMatP= 3.25D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.403D-04 0.958D-02 0.631D-02-0.261D-01-0.120D+00 0.184D+00
Coeff-Com: 0.947D+00
Coeff: -0.403D-04 0.958D-02 0.631D-02-0.261D-01-0.120D+00 0.184D+00
Coeff: 0.947D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.19D-06 MaxDP=1.35D-04 DE=-6.78D-08 OVMax= 1.14D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 6.11D-07 CP: 7.49D-01 1.07D+00 1.35D+00 1.34D+00 2.15D+00
CP: 1.08D+00 2.27D+00
E= -608.981388067291 Delta-E= -0.000000017753 Rises=F Damp=F
DIIS: error= 3.79D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981388067291 IErMin= 8 ErrMin= 3.79D-06
ErrMax= 3.79D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.04D-10 BMatP= 3.39D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.948D-03 0.293D-01 0.245D-01 0.473D-03-0.187D+00-0.725D-02
Coeff-Com: 0.399D+00 0.742D+00
Coeff: -0.948D-03 0.293D-01 0.245D-01 0.473D-03-0.187D+00-0.725D-02
Coeff: 0.399D+00 0.742D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.64D-06 MaxDP=4.66D-05 DE=-1.78D-08 OVMax= 4.85D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.53D-07 CP: 7.49D-01 1.07D+00 1.34D+00 1.32D+00 2.09D+00
CP: 1.08D+00 2.73D+00 1.34D+00
E= -608.981388070704 Delta-E= -0.000000003413 Rises=F Damp=F
DIIS: error= 1.04D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981388070704 IErMin= 9 ErrMin= 1.04D-06
ErrMax= 1.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-10 BMatP= 8.04D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.229D-03 0.442D-02 0.430D-02 0.823D-02-0.870D-02-0.545D-01
Coeff-Com: -0.196D+00 0.160D+00 0.108D+01

Coeff: -0.229D-03 0.442D-02 0.430D-02 0.823D-02-0.870D-02-0.545D-01
Coeff: -0.196D+00 0.160D+00 0.108D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.37D-07 MaxDP=1.17D-05 DE=-3.41D-09 OVMax= 2.87D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.47D-07 CP: 7.49D-01 1.07D+00 1.34D+00 1.32D+00 2.06D+00
CP: 1.06D+00 2.90D+00 1.50D+00 1.64D+00
E= -608.981388071955 Delta-E= -0.000000001251 Rises=F Damp=F
DIIS: error= 7.93D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981388071955 IErMin=10 ErrMin= 7.93D-07
ErrMax= 7.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.55D-11 BMatP= 1.58D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.111D-03-0.450D-02-0.351D-02 0.297D-02 0.368D-01-0.201D-01
Coeff-Com: -0.168D+00-0.974D-01 0.455D+00 0.799D+00
Coeff: 0.111D-03-0.450D-02-0.351D-02 0.297D-02 0.368D-01-0.201D-01
Coeff: -0.168D+00-0.974D-01 0.455D+00 0.799D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.61D-07 MaxDP=6.16D-06 DE=-1.25D-09 OVMax= 1.30D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 3.04D-08 CP: 7.49D-01 1.07D+00 1.34D+00 1.32D+00 2.07D+00
CP: 1.05D+00 2.89D+00 1.50D+00 1.94D+00 1.40D+00
E= -608.981388072164 Delta-E= -0.000000000209 Rises=F Damp=F
DIIS: error= 3.05D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981388072164 IErMin=11 ErrMin= 3.05D-07
ErrMax= 3.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-11 BMatP= 4.55D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.999D-04-0.315D-02-0.264D-02-0.109D-03 0.205D-01-0.918D-05
Coeff-Com: -0.521D-01-0.799D-01 0.398D-01 0.417D+00 0.660D+00
Coeff: 0.999D-04-0.315D-02-0.264D-02-0.109D-03 0.205D-01-0.918D-05
Coeff: -0.521D-01-0.799D-01 0.398D-01 0.417D+00 0.660D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.41D-07 MaxDP=3.74D-06 DE=-2.09D-10 OVMax= 4.46D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.43D-08 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.07D+00
CP: 1.05D+00 2.87D+00 1.49D+00 1.96D+00 1.55D+00
CP: 1.37D+00
E= -608.981388072213 Delta-E= -0.000000000049 Rises=F Damp=F
DIIS: error= 1.99D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981388072213 IErMin=12 ErrMin= 1.99D-07
ErrMax= 1.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.05D-12 BMatP= 1.35D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.436D-05 0.143D-03 0.265D-04-0.897D-03-0.293D-02 0.550D-02
Coeff-Com: 0.281D-01 0.936D-03-0.116D+00-0.655D-01 0.266D+00 0.885D+00
Coeff: 0.436D-05 0.143D-03 0.265D-04-0.897D-03-0.293D-02 0.550D-02
Coeff: 0.281D-01 0.936D-03-0.116D+00-0.655D-01 0.266D+00 0.885D+00

Gap= 0.246 Goal= None Shift= 0.000
RMSDP=6.22D-08 MaxDP=1.86D-06 DE=-4.87D-11 OVMax= 3.12D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 9.75D-09 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.08D+00
CP: 1.05D+00 2.86D+00 1.47D+00 1.94D+00 1.60D+00
CP: 1.69D+00 1.51D+00
E= -608.981388072231 Delta-E= -0.000000000018 Rises=F Damp=F
DIIS: error= 1.19D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981388072231 IErMin=13 ErrMin= 1.19D-07
ErrMax= 1.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.81D-13 BMatP= 3.05D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.326D-04 0.115D-02 0.920D-03-0.361D-03-0.810D-02 0.216D-02
Coeff-Com: 0.302D-01 0.286D-01-0.679D-01-0.171D+00-0.120D+00 0.340D+00
Coeff-Com: 0.964D+00
Coeff: -0.326D-04 0.115D-02 0.920D-03-0.361D-03-0.810D-02 0.216D-02
Coeff: 0.302D-01 0.286D-01-0.679D-01-0.171D+00-0.120D+00 0.340D+00
Coeff: 0.964D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.19D-08 MaxDP=2.40D-07 DE=-1.82D-11 OVMax= 2.47D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 5.13D-09 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.08D+00
CP: 1.06D+00 2.85D+00 1.47D+00 1.93D+00 1.61D+00
CP: 1.84D+00 1.85D+00 1.52D+00
E= -608.981388072233 Delta-E= -0.000000000002 Rises=F Damp=F
DIIS: error= 5.17D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.981388072233 IErMin=14 ErrMin= 5.17D-08
ErrMax= 5.17D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-13 BMatP= 8.81D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.397D-05 0.510D-04 0.626D-04 0.237D-03 0.273D-03-0.160D-02
Coeff-Com: -0.566D-02 0.326D-02 0.258D-01 0.864D-02-0.847D-01-0.251D+00
Coeff-Com: 0.121D+00 0.118D+01
Coeff: -0.397D-05 0.510D-04 0.626D-04 0.237D-03 0.273D-03-0.160D-02
Coeff: -0.566D-02 0.326D-02 0.258D-01 0.864D-02-0.847D-01-0.251D+00
Coeff: 0.121D+00 0.118D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.59D-08 MaxDP=6.51D-07 DE=-1.82D-12 OVMax= 1.42D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 3.27D-09 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.08D+00
CP: 1.05D+00 2.86D+00 1.47D+00 1.93D+00 1.60D+00
CP: 1.84D+00 1.90D+00 1.82D+00 1.75D+00
E= -608.981388072236 Delta-E= -0.000000000003 Rises=F Damp=F
DIIS: error= 1.25D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -608.981388072236 IErMin=15 ErrMin= 1.25D-08
ErrMax= 1.25D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-14 BMatP= 1.63D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Supporting Information file

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 Coeff-Com:  0.523D-05-0.193D-03-0.153D-03 0.724D-04 0.141D-02-0.660D-03
 Coeff-Com: -0.580D-02-0.428D-02 0.145D-01 0.307D-01 0.117D-01-0.964D-01
 Coeff-Com: -0.130D+00 0.130D+00 0.105D+01
 Coeff:      0.523D-05-0.193D-03-0.153D-03 0.724D-04 0.141D-02-0.660D-03
 Coeff:     -0.580D-02-0.428D-02 0.145D-01 0.307D-01 0.117D-01-0.964D-01
 Coeff:     -0.130D+00 0.130D+00 0.105D+01
 Gap=     0.246 Goal=   None    Shift=    0.000
 RMSDP=5.00D-09 MaxDP=1.51D-07 DE=-3.41D-12 OVMax= 4.06D-07

 SCF Done:  E(RwB97XD) =  -608.981388072     A.U. after   18 cycles
            NFock= 18  Conv=0.50D-08     -V/T= 2.0045
 KE= 6.062575326491D+02 PE=-2.846607848744D+03 EE= 9.135721977414D+02
 Leave Link  502 at Fri Aug 21 18:44:12 2026, MaxMem=    805306368 cpu:             4025.5 elap:
671.2
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14217 LenP2D=   33589.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 Leave Link  701 at Fri Aug 21 18:44:12 2026, MaxMem=    805306368 cpu:                2.2 elap:
0.4
 (Enter /home/user/gauss16/g16/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link  702 at Fri Aug 21 18:44:12 2026, MaxMem=    805306368 cpu:                0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l703.exe)
 Integral derivatives from FoFJK, PRISM(SPDF).
 Compute integral first derivatives, UseDBF=F ICtDFT=          0.
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=         800
        NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
        wScrn=  0.000000 ICntrl=      2527 IOpCl=  0 I1Cent=          0 NGrid=          0
        NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 Leave Link  703 at Fri Aug 21 18:51:28 2026, MaxMem=    805306368 cpu:             2611.4 elap:
435.3
 (Enter /home/user/gauss16/g16/l716.exe)
 Dipole        = 1.51345453D+00-4.72278216D-03-4.77546478D-04
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
```

```
     1        6         0.000134277   0.000292559  -0.000412978
     2        6        -0.000256779  -0.000172245   0.000613995
     3        6         0.000238411  -0.000264418   0.000440196
     4        6         0.000501151  -0.000232070  -0.000863098
     5        6        -0.000332742   0.000104360  -0.000670177
     6        6        -0.000479261   0.000025035   0.000862827
     7        6         0.000532306   0.000320156   0.000909665
     8        6         0.000526655  -0.000253227  -0.001090145
     9        6        -0.000484767  -0.000095891  -0.000880248
    10        6        -0.000286670   0.000839198   0.001169892
    11        6         0.000518843   0.000284454   0.001069359
    12        6        -0.000215107  -0.001473423  -0.002548339
    13        6        -0.000271391  -0.000865391  -0.001126214
    14        6        -0.000214759   0.001499044   0.002523731
    15        6         0.000043768  -0.003273910  -0.002172394
    16        6         0.000046065   0.003265772   0.002173929
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.003273910 RMS     0.001130740
 Leave Link  716 at Fri Aug 21 18:51:28 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.003236618 RMS     0.000624034
 Search for a local minimum.
 Step number   4 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .62403D-03 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
 DE= -2.82D-04 DEPred=-3.14D-04 R= 8.97D-01
 TightC=F SS=  1.41D+00  RLast= 8.74D-02 DXNew= 8.4853D-01 2.6229D-01
 Trust test= 8.97D-01 RLast= 8.74D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.01293   0.01365   0.01670   0.01734   0.02624
    Eigenvalues ---    0.02815   0.03059   0.03365   0.03423   0.03926
    Eigenvalues ---    0.03965   0.04047   0.06031   0.08438   0.09287
    Eigenvalues ---    0.19449   0.24521   0.24683   0.24993   0.24994
    Eigenvalues ---    0.24999   0.25000   0.25000   0.25000   0.25001
    Eigenvalues ---    0.25072   0.28102   0.32093   0.38069   0.43397
    Eigenvalues ---    0.51325   0.53457   0.57383   0.57862   0.58159
    Eigenvalues ---    0.58183   0.78671   0.79015   0.79698   0.80820
    Eigenvalues ---    0.82173   0.83868
 RFO step:  Lambda=-1.49434008D-04 EMin= 1.29347083D-02
```

Supporting Information file

Quartic linear search produced a step of -0.08283.
Iteration 1 RMS(Cart)= 0.00633165 RMS(Int)= 0.00005952
Iteration 2 RMS(Cart)= 0.00004072 RMS(Int)= 0.00002866
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002866
ITry= 1 IFail=0 DXMaxC= 2.16D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.30689	0.00034	0.00025	-0.00128	-0.00103	2.30586
R2	2.54824	-0.00001	-0.00122	0.00380	0.00258	2.55081
R3	2.54752	-0.00002	-0.00117	0.00365	0.00248	2.55000
R4	2.30685	0.00034	0.00025	-0.00128	-0.00103	2.30581
R5	2.30276	0.00039	0.00024	-0.00114	-0.00091	2.30185
R6	2.54768	-0.00003	-0.00117	0.00364	0.00247	2.55015
R7	2.55053	-0.00004	-0.00104	0.00325	0.00221	2.55274
R8	2.30270	0.00038	0.00024	-0.00115	-0.00091	2.30179
R9	2.29549	0.00053	0.00017	-0.00072	-0.00055	2.29494
R10	2.55068	-0.00005	-0.00104	0.00323	0.00219	2.55288
R11	2.61520	-0.00020	-0.00112	0.00335	0.00222	2.61742
R12	2.29550	0.00053	0.00017	-0.00073	-0.00056	2.29494
R13	2.63307	0.00175	0.00013	0.00360	0.00375	2.63682
R14	2.75369	-0.00000	0.00040	-0.00328	-0.00292	2.75077
R15	2.61525	-0.00021	-0.00112	0.00333	0.00221	2.61746
R16	2.75363	0.00000	0.00042	-0.00338	-0.00299	2.75064
R17	2.71001	0.00324	-0.00091	0.01120	0.01033	2.72034
A1	2.61199	0.00006	-0.00013	-0.00006	-0.00018	2.61180
A2	2.64365	0.00004	-0.00009	-0.00019	-0.00028	2.64337
A3	2.61683	-0.00001	-0.00009	-0.00043	-0.00052	2.61631
A4	2.72071	-0.00030	0.00000	-0.00163	-0.00163	2.71908
A5	2.63945	0.00009	-0.00011	0.00010	-0.00002	2.63943
A6	2.77816	0.00002	-0.00013	0.00022	0.00008	2.77823
A7	2.72437	-0.00037	0.00004	-0.00196	-0.00193	2.72244
A8	2.77554	0.00007	-0.00016	0.00049	0.00032	2.77586
A9	2.82862	0.00030	-0.00015	0.00155	0.00138	2.83000
A10	2.31705	-0.00062	-0.00005	-0.00502	-0.00506	2.31199
A11	2.51493	-0.00001	-0.00028	-0.00191	-0.00218	2.51275
A12	1.45091	0.00063	0.00035	0.00674	0.00703	1.45794
A13	2.82720	0.00032	-0.00016	0.00169	0.00151	2.82872
A14	2.31748	-0.00062	-0.00005	-0.00501	-0.00505	2.31243
A15	1.45071	0.00062	0.00035	0.00670	0.00700	1.45772
A16	2.51470	-0.00001	-0.00028	-0.00187	-0.00214	2.51256
A17	1.42634	0.00014	0.00068	0.00408	0.00469	1.43103
A18	1.42656	0.00014	0.00066	0.00418	0.00477	1.43133
A19	2.87813	0.00037	0.00101	0.00317	0.00417	2.88230
A20	2.87964	0.00036	0.00102	0.00303	0.00404	2.88369
A21	3.13043	0.00022	0.00034	0.00720	0.00753	3.13795
A22	3.13041	0.00021	0.00033	0.00711	0.00743	3.13784
D1	0.05989	0.00016	-0.00022	0.00371	0.00349	0.06338

D2	-0.05342	0.00007	0.00051	-0.00140	-0.00088	-0.05430
D3	-0.03962	-0.00005	0.00034	-0.00278	-0.00244	-0.04205
D4	0.05777	0.00018	-0.00027	0.00417	0.00390	0.06167
D5	0.06188	0.00017	-0.00072	0.00749	0.00677	0.06865
D6	-0.03651	-0.00006	0.00039	-0.00324	-0.00285	-0.03936
D7	0.06567	-0.00011	0.00017	0.00307	0.00323	0.06891
D8	0.05995	0.00017	-0.00072	0.00760	0.00687	0.06683
D9	0.06814	-0.00012	0.00020	0.00272	0.00291	0.07105
D10	-0.56396	-0.00058	0.00165	-0.01787	-0.01623	-0.58019
D11	2.61476	0.00002	0.00052	-0.00572	-0.00519	2.60956
D12	0.73646	0.00035	-0.00276	0.00360	0.00080	0.73727
D13	-2.42666	-0.00000	-0.00214	-0.00315	-0.00535	-2.43201
D14	-2.42705	-0.00000	-0.00209	-0.00362	-0.00577	-2.43283
D15	0.69301	-0.00035	-0.00148	-0.01036	-0.01192	0.68108
D16	2.40492	0.00089	0.00200	0.00603	0.00797	2.41289
D17	-0.70922	0.00134	0.00116	0.01513	0.01627	-0.69295
D18	-0.56759	-0.00057	0.00159	-0.01721	-0.01563	-0.58322
D19	2.61045	0.00002	0.00054	-0.00586	-0.00532	2.60513
D20	-0.70923	0.00134	0.00117	0.01510	0.01626	-0.69298
D21	2.40542	0.00089	0.00195	0.00661	0.00850	2.41392
D22	0.67481	-0.00067	-0.00121	-0.01186	-0.01312	0.66169

Item	Value	Threshold	Converged?
Maximum Force	0.003237	0.000450	NO
RMS Force	0.000624	0.000300	NO
Maximum Displacement	0.021642	0.001800	NO
RMS Displacement	0.006324	0.001200	NO

Predicted change in Energy=-7.735845D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.623692	-0.673916	0.017066
2	6	0	3.008781	-1.726993	0.059683
3	6	0	3.621775	0.675505	-0.016183
4	6	0	1.854749	-2.426303	0.067283
5	6	0	3.008632	1.729586	-0.058843
6	6	0	0.645777	-2.575001	0.063189
7	6	0	1.852919	2.426261	-0.067458
8	6	0	-0.665657	-2.254519	0.015860
9	6	0	0.644135	2.576223	-0.063808
10	6	0	-1.730943	-1.673869	-0.037545

11	6	0	-0.666956	2.253978	-0.016972
12	6	0	-2.684409	-0.677794	-0.168605
13	6	0	-1.732292	1.673393	0.036135
14	6	0	-2.684622	0.676321	0.168094
15	6	0	-4.048276	-0.402689	-0.596499
16	6	0	-4.047307	0.399817	0.598604

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220206	0.000000			
3	C	1.349832	2.480628	0.000000		
4	C	2.490490	1.349400	3.570792	0.000000	
5	C	2.482112	3.458610	1.220184	4.314946	0.000000
6	C	3.533303	2.510561	4.407794	1.218089	4.911969
7	C	3.571257	4.312968	2.489302	4.854434	1.349482
8	C	4.571304	3.712371	5.193086	2.526776	5.420247
9	C	4.409956	4.911667	3.532894	5.148595	2.511507
10	C	5.447477	4.741018	5.845648	3.665287	5.835026
11	C	5.194554	5.418953	4.569988	5.317060	3.713043
12	C	6.310835	5.793561	6.451558	4.869998	6.182091
13	C	5.847802	5.834462	5.446517	5.447507	4.742208
14	C	6.452966	6.180817	6.309088	5.499302	5.794308
15	C	7.701242	7.210160	7.767171	6.275454	7.391592
16	C	7.767581	7.389325	7.698622	6.565327	7.210187

		6	7	8	9	10
6	C	0.000000				
7	C	5.146540	0.000000			
8	C	1.350854	5.316001	0.000000		
9	C	5.152790	1.218057	5.005794	0.000000	
10	C	2.543813	5.445735	1.214430	4.868775	0.000000
11	C	5.004871	2.526263	4.508617	1.350924	4.069457
12	C	3.839696	5.498430	2.568161	4.656051	1.385078
13	C	4.868757	3.664871	4.070211	2.544110	3.348074
14	C	4.655497	4.868989	3.562193	3.839795	2.544639
15	C	5.214237	6.565588	3.904660	5.583583	2.701548
16	C	5.582226	6.273977	4.338277	5.213939	3.173390

		11	12	13	14	15
11	C	0.000000				
12	C	3.562077	0.000000			
13	C	1.214430	2.544902	0.000000		
14	C	2.567922	1.395347	1.385098	0.000000	
15	C	4.339016	1.455647	3.173976	1.899584	0.000000
16	C	3.904308	1.899300	2.701418	1.455577	1.439544

		16
16	C	0.000000

Stoichiometry C16

Framework group C1[X(C16)]

Supporting Information file

Deg. of freedom 42
Full point group C1 NOp 1
RotChk: IX=0 Diff= 8.27D-04
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.623506	-0.674963	0.015259
2	6	0	3.008302	-1.727976	0.055163
3	6	0	3.621962	0.674540	-0.014500
4	6	0	1.854077	-2.426983	0.060974
5	6	0	3.009111	1.728897	-0.054423
6	6	0	0.645064	-2.575335	0.056517
7	6	0	1.853592	2.425913	-0.061215
8	6	0	-0.666282	-2.254368	0.010040
9	6	0	0.644849	2.576201	-0.057156
10	6	0	-1.731408	-1.673286	-0.041844
11	6	0	-0.666331	2.254199	-0.011131
12	6	0	-2.684600	-0.676610	-0.170310
13	6	0	-1.731827	1.673775	0.040494
14	6	0	-2.684431	0.676629	0.169890
15	6	0	-4.048398	-0.400022	-0.597467
16	6	0	-4.047185	0.399390	0.599707

Rotational constants (GHZ): 0.8468943 0.3938762 0.2716111
Leave Link 202 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 717.4701327343 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.

Supporting Information file

Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074897369 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.4626429974 Hartrees.
Leave Link 301 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33574.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.01D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 563 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000292 -0.000001 0.000014 Ang= 0.03 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.864964196537
Leave Link 401 at Fri Aug 21 18:51:34 2026, MaxMem= 805306368 cpu: 31.1 elap: 5.2
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:

Supporting Information file

Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981207400464
DIIS: error= 6.29D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981207400464 IErMin= 1 ErrMin= 6.29D-04
ErrMax= 6.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.37D-04 BMatP= 5.37D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 6.29D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.959 Goal= None Shift= 0.000
RMSDP=3.35D-03 MaxDP=9.85D-02 OVMax= 3.59D-03

Cycle 2 Pass 0 IDiag 1:
RMSU= 3.28D-03 CP: 1.08D+00
E= -608.981587035798 Delta-E= -0.000379635334 Rises=F Damp=F
DIIS: error= 4.51D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981587035798 IErMin= 2 ErrMin= 4.51D-04
ErrMax= 4.51D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-05 BMatP= 5.37D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.51D-03
Coeff-Com: 0.332D-01 0.967D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.330D-01 0.967D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=9.95D-04 MaxDP=3.17D-02 DE=-3.80D-04 OVMax= 2.13D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 9.85D-04 CP: 1.09D+00 1.04D+00
E= -608.981565874565 Delta-E= 0.000021161233 Rises=F Damp=F
DIIS: error= 1.39D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -608.981587035798 IErMin= 2 ErrMin= 4.51D-04
ErrMax= 1.39D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-04 BMatP= 3.13D-05
IDIUse=3 WtCom= 2.12D-01 WtEn= 7.88D-01

Rare condition: small coef for last iteration: 0.000D+00
Coeff-Com: 0.270D-01 0.877D+00 0.964D-01
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.270D-01 0.877D+00 0.964D-01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.88D-03 MaxDP=1.13D-01 DE= 2.12D-05 OVMax= 7.47D-04

Cycle 4 Pass 0 IDiag 1:
RMSU= 1.71D-03 CP: 1.17D+00 1.71D+00 6.19D-01
E= -608.981594686058 Delta-E= -0.000028811493 Rises=F Damp=F
DIIS: error= 1.82D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981594686058 IErMin= 2 ErrMin= 4.51D-04
ErrMax= 1.82D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.79D-04 BMatP= 3.13D-05
IDIUse=3 WtCom= 1.90D-01 WtEn= 8.10D-01
Coeff-Com: -0.290D-01 0.827D+00 0.738D+00-0.536D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.551D-02 0.157D+00 0.140D+00 0.708D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.75D+02 MaxDP=1.46D+04 DE=-2.88D-05 OVMax= 9.84D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 5 Pass 1 IDiag 1:
E= -608.981372450888 Delta-E= 0.000222235170 Rises=F Damp=F
DIIS: error= 6.32D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981372450888 IErMin= 1 ErrMin= 6.32D-04
ErrMax= 6.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-04 BMatP= 1.27D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 6.32D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.72D-03 MaxDP=2.03D-01 DE= 2.22D-04 OVMax= 1.73D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 4.11D-03 CP: 6.55D-01
E= -608.981454486177 Delta-E= -0.000082035289 Rises=F Damp=F
DIIS: error= 1.02D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981454486177 IErMin= 2 ErrMin= 1.02D-04
ErrMax= 1.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-06 BMatP= 1.27D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.02D-03
Coeff-Com: -0.633D-02 0.101D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.632D-02 0.101D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.88D-04 MaxDP=9.95D-03 DE=-8.20D-05 OVMax= 1.17D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.70D-04 CP: 6.33D-01 1.06D+00
E= -608.981451868728 Delta-E= 0.000002617449 Rises=F Damp=F
DIIS: error= 1.72D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -608.981454486177 IErMin= 2 ErrMin= 1.02D-04
ErrMax= 1.72D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.94D-06 BMatP= 2.37D-06
IDIUse=3 WtCom= 4.33D-01 WtEn= 5.67D-01
Coeff-Com: -0.219D-01 0.634D+00 0.388D+00
Coeff-En: 0.000D+00 0.646D+00 0.354D+00
Coeff: -0.947D-02 0.641D+00 0.368D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.99D-05 MaxDP=5.11D-04 DE= 2.62D-06 OVMax= 4.31D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 5.26D-06 CP: 6.32D-01 1.06D+00 1.06D+00
E= -608.981457847689 Delta-E= -0.000005978960 Rises=F Damp=F
DIIS: error= 1.21D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981457847689 IErMin= 4 ErrMin= 1.21D-05
ErrMax= 1.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.25D-08 BMatP= 2.37D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.289D-02 0.339D-01 0.162D-01 0.953D+00
Coeff: -0.289D-02 0.339D-01 0.162D-01 0.953D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.05D-05 MaxDP=7.79D-04 DE=-5.98D-06 OVMax= 2.38D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.63D-06 CP: 6.30D-01 1.06D+00 1.16D+00 1.50D+00
E= -608.981458013438 Delta-E= -0.000000165750 Rises=F Damp=F
DIIS: error= 1.26D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981458013438 IErMin= 4 ErrMin= 1.21D-05
ErrMax= 1.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-08 BMatP= 4.25D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.484D-02-0.165D+00-0.102D+00 0.468D+00 0.794D+00
Coeff: 0.484D-02-0.165D+00-0.102D+00 0.468D+00 0.794D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.14D-05 MaxDP=3.00D-04 DE=-1.66D-07 OVMax= 2.58D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.08D-06 CP: 6.30D-01 1.07D+00 1.20D+00 1.65D+00 1.55D+00
E= -608.981458095696 Delta-E= -0.000000082257 Rises=F Damp=F
DIIS: error= 4.10D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981458095696 IErMin= 6 ErrMin= 4.10D-06
ErrMax= 4.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.14D-09 BMatP= 2.42D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.248D-02-0.728D-01-0.441D-01 0.902D-02 0.335D+00 0.770D+00
Coeff: 0.248D-02-0.728D-01-0.441D-01 0.902D-02 0.335D+00 0.770D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.51D-06 MaxDP=4.48D-05 DE=-8.23D-08 OVMax= 1.17D-04

Supporting Information file

Cycle 11 Pass 1 IDiag 1:
RMSU= 5.99D-07 CP: 6.30D-01 1.07D+00 1.19D+00 1.64D+00 1.57D+00
CP: 1.18D+00
E= -608.981458113165 Delta-E= -0.000000017470 Rises=F Damp=F
DIIS: error= 2.35D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981458113165 IErMin= 7 ErrMin= 2.35D-06
ErrMax= 2.35D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.77D-09 BMatP= 5.14D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.372D-03 0.202D-01 0.132D-01-0.187D+00-0.994D-01 0.452D+00
Coeff-Com: 0.801D+00
Coeff: -0.372D-03 0.202D-01 0.132D-01-0.187D+00-0.994D-01 0.452D+00
Coeff: 0.801D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.23D-06 MaxDP=9.63D-05 DE=-1.75D-08 OVMax= 8.11D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.28D-07 CP: 6.30D-01 1.06D+00 1.18D+00 1.60D+00 1.48D+00
CP: 1.24D+00 2.01D+00
E= -608.981458119197 Delta-E= -0.000000006032 Rises=F Damp=F
DIIS: error= 8.57D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981458119197 IErMin= 8 ErrMin= 8.57D-07
ErrMax= 8.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-10 BMatP= 1.77D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.423D-03 0.158D-01 0.100D-01-0.693D-01-0.676D-01 0.801D-01
Coeff-Com: 0.299D+00 0.732D+00
Coeff: -0.423D-03 0.158D-01 0.100D-01-0.693D-01-0.676D-01 0.801D-01
Coeff: 0.299D+00 0.732D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.09D-06 MaxDP=3.23D-05 DE=-6.03D-09 OVMax= 2.07D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 8.12D-08 CP: 6.30D-01 1.06D+00 1.18D+00 1.58D+00 1.43D+00
CP: 1.25D+00 2.28D+00 1.27D+00
E= -608.981458119731 Delta-E= -0.000000000534 Rises=F Damp=F
DIIS: error= 4.59D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981458119731 IErMin= 9 ErrMin= 4.59D-07
ErrMax= 4.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.27D-11 BMatP= 1.58D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.828D-05-0.108D-02-0.538D-03 0.258D-01 0.686D-02-0.907D-01
Coeff-Com: -0.113D+00 0.174D+00 0.998D+00
Coeff: -0.828D-05-0.108D-02-0.538D-03 0.258D-01 0.686D-02-0.907D-01
Coeff: -0.113D+00 0.174D+00 0.998D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.85D-07 MaxDP=1.23D-05 DE=-5.34D-10 OVMax= 1.18D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 4.57D-08 CP: 6.30D-01 1.06D+00 1.18D+00 1.57D+00 1.40D+00
CP: 1.22D+00 2.45D+00 1.46D+00 1.63D+00

E= -608.981458119909 Delta-E= -0.000000000178 Rises=F Damp=F
DIIS: error= 1.88D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981458119909 IErMin=10 ErrMin= 1.88D-07
ErrMax= 1.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.83D-12 BMatP= 3.27D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.106D-03-0.451D-02-0.277D-02 0.283D-01 0.201D-01-0.576D-01
Coeff-Com: -0.120D+00-0.107D+00 0.413D+00 0.830D+00
Coeff: 0.106D-03-0.451D-02-0.277D-02 0.283D-01 0.201D-01-0.576D-01
Coeff: -0.120D+00-0.107D+00 0.413D+00 0.830D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.02D-08 MaxDP=1.28D-06 DE=-1.78D-10 OVMax= 5.45D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.66D-08 CP: 6.30D-01 1.06D+00 1.18D+00 1.57D+00 1.40D+00
CP: 1.23D+00 2.48D+00 1.49D+00 1.84D+00 1.40D+00
E= -608.981458119942 Delta-E= -0.000000000033 Rises=F Damp=F
DIIS: error= 1.01D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981458119942 IErMin=11 ErrMin= 1.01D-07
ErrMax= 1.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.59D-13 BMatP= 7.83D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.315D-04-0.116D-02-0.735D-03 0.497D-02 0.431D-02-0.561D-02
Coeff-Com: -0.204D-01-0.533D-01-0.268D-02 0.217D+00 0.857D+00
Coeff: 0.315D-04-0.116D-02-0.735D-03 0.497D-02 0.431D-02-0.561D-02
Coeff: -0.204D-01-0.533D-01-0.268D-02 0.217D+00 0.857D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=8.49D-08 MaxDP=2.49D-06 DE=-3.27D-11 OVMax= 1.42D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 8.13D-09 CP: 6.30D-01 1.06D+00 1.18D+00 1.58D+00 1.40D+00
CP: 1.23D+00 2.46D+00 1.47D+00 1.80D+00 1.50D+00
CP: 1.44D+00
E= -608.981458119947 Delta-E= -0.000000000006 Rises=F Damp=F
DIIS: error= 5.66D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981458119947 IErMin=12 ErrMin= 5.66D-08
ErrMax= 5.66D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.10D-13 BMatP= 8.59D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.907D-05 0.476D-03 0.280D-03-0.398D-02-0.272D-02 0.108D-01
Coeff-Com: 0.183D-01-0.186D-02-0.958D-01-0.939D-01 0.475D+00 0.693D+00
Coeff: -0.907D-05 0.476D-03 0.280D-03-0.398D-02-0.272D-02 0.108D-01
Coeff: 0.183D-01-0.186D-02-0.958D-01-0.939D-01 0.475D+00 0.693D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=4.24D-08 MaxDP=1.32D-06 DE=-5.68D-12 OVMax= 6.35D-07

Cycle 17 Pass 1 IDiag 1:
RMSU= 2.91D-09 CP: 6.30D-01 1.06D+00 1.18D+00 1.58D+00 1.40D+00
CP: 1.23D+00 2.45D+00 1.46D+00 1.76D+00 1.50D+00
CP: 1.67D+00 1.52D+00
E= -608.981458119951 Delta-E= -0.000000000003 Rises=F Damp=F

Supporting Information file

DIIS: error= 3.07D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981458119951 IErMin=13 ErrMin= 3.07D-08
ErrMax= 3.07D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.26D-14 BMatP= 4.10D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.843D-05 0.375D-03 0.228D-03-0.246D-02-0.187D-02 0.581D-02
Coeff-Com: 0.112D-01 0.571D-02-0.412D-01-0.790D-01 0.901D-01 0.346D+00
Coeff-Com: 0.665D+00
Coeff: -0.843D-05 0.375D-03 0.228D-03-0.246D-02-0.187D-02 0.581D-02
Coeff: 0.112D-01 0.571D-02-0.412D-01-0.790D-01 0.901D-01 0.346D+00
Coeff: 0.665D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=6.24D-09 MaxDP=2.41D-07 DE=-3.41D-12 OVMax= 1.83D-07

SCF Done: E(RwB97XD) = -608.981458120 A.U. after 17 cycles
NFock= 17 Conv=0.62D-08 -V/T= 2.0045
KE= 6.062394251116D+02 PE=-2.845931996889D+03 EE= 9.132484706602D+02
Leave Link 502 at Fri Aug 21 19:01:46 2026, MaxMem= 805306368 cpu: 3669.8 elap: 611.9
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33574.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 19:01:46 2026, MaxMem= 805306368 cpu: 2.1 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 19:01:46 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 19:07:50 2026, MaxMem= 805306368 cpu: 2184.6 elap: 364.2
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.52170194D+00-4.32614017D-03-6.02178276D-04
***** Axes restored to original set *****

Supporting Information file

```
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number           X              Y              Z
---------------------------------------------------------------------
    1        6         0.000366109    0.001501681   -0.000429897
    2        6        -0.001136658   -0.000996602    0.000615564
    3        6         0.000466820   -0.001476295    0.000451283
    4        6         0.001568849    0.000319341   -0.000848618
    5        6        -0.001208745    0.000932572   -0.000661704
    6        6        -0.001623330    0.000289293    0.000495399
    7        6         0.001603371   -0.000239380    0.000889992
    8        6         0.001262388   -0.000730216   -0.000437065
    9        6        -0.001630788   -0.000351065   -0.000515084
   10        6        -0.000769507    0.001119645    0.000907088
   11        6         0.001256279    0.000760538    0.000424827
   12        6        -0.000549147   -0.001561225   -0.000523419
   13        6        -0.000763250   -0.001143648   -0.000878908
   14        6        -0.000539752    0.001580204    0.000514140
   15        6         0.000850168   -0.000620293   -0.001862224
   16        6         0.000847192    0.000615450    0.001858625
---------------------------------------------------------------------
Cartesian Forces:  Max     0.001862224 RMS     0.001005218
 Leave Link  716 at Fri Aug 21 19:07:50 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.001473907 RMS     0.000466734
 Search for a local minimum.
 Step number   5 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .46673D-03 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
 DE= -7.00D-05 DEPred=-7.74D-05 R= 9.05D-01
 TightC=F SS=  1.41D+00  RLast= 4.80D-02 DXNew= 8.4853D-01 1.4389D-01
 Trust test= 9.05D-01 RLast= 4.80D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  0
    Eigenvalues ---    0.01289   0.01312   0.01576   0.01731   0.02623
    Eigenvalues ---    0.02656   0.02994   0.03291   0.03423   0.03926
    Eigenvalues ---    0.03940   0.04047   0.08431   0.08693   0.09336
    Eigenvalues ---    0.16413   0.24486   0.24573   0.24987   0.24990
    Eigenvalues ---    0.24997   0.24999   0.25000   0.25000   0.25002
    Eigenvalues ---    0.25076   0.28167   0.32373   0.35757   0.49754
```

```
    Eigenvalues ---    0.51323   0.56192   0.57382   0.57878   0.58161
    Eigenvalues ---    0.58184   0.78669   0.79213   0.79697   0.81247
    Eigenvalues ---    0.82170   0.87164
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:     5    4
 RFO step:  Lambda=-4.49650053D-05.
 NNeg= 0 NGDIIS= 2 SimSw=  2.50D-01 Rises=F DC= -7.00D-05 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.3553990294D-02 NUsed= 2 OKEnD=T EnDIS=F
 InvSVX:  RCond= 5.73D-04 Info=           0 Equed=N FErr=  1.89D-15 BErr=  4.78D-17
 DidBck=F Rises=F RFO-DIIS coefs:    1.16138   -0.16138
 Iteration  1 RMS(Cart)=  0.00317740 RMS(Int)=  0.00001082
 Iteration  2 RMS(Cart)=  0.00000975 RMS(Int)=  0.00000574
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000574
  ITry=  1  IFail=0  DXMaxC=  8.45D-03  DCOld=  1.00D+10  DXMaxT=  5.05D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
   R1        2.30586   0.00077  -0.00017   0.00096   0.00079   2.30665
   R2        2.55081  -0.00085   0.00042  -0.00064  -0.00023   2.55059
   R3        2.55000  -0.00082   0.00040  -0.00061  -0.00021   2.54979
   R4        2.30581   0.00077  -0.00017   0.00096   0.00080   2.30661
   R5        2.30185   0.00082  -0.00015   0.00099   0.00084   2.30270
   R6        2.55015  -0.00082   0.00040  -0.00062  -0.00022   2.54993
   R7        2.55274  -0.00084   0.00036  -0.00070  -0.00035   2.55240
   R8        2.30179   0.00082  -0.00015   0.00099   0.00085   2.30264
   R9        2.29494   0.00061  -0.00009   0.00077   0.00068   2.29562
  R10        2.55288  -0.00084   0.00035  -0.00071  -0.00036   2.55252
  R11        2.61742  -0.00063   0.00036  -0.00063  -0.00027   2.61715
  R12        2.29494   0.00061  -0.00009   0.00077   0.00068   2.29562
  R13        2.63682   0.00082   0.00061   0.00204   0.00265   2.63947
  R14        2.75077  -0.00056  -0.00047  -0.00230  -0.00277   2.74800
  R15        2.61746  -0.00064   0.00036  -0.00064  -0.00029   2.61717
  R16        2.75064  -0.00055  -0.00048  -0.00230  -0.00278   2.74786
  R17        2.72034   0.00147   0.00167   0.00530   0.00697   2.72731
   A1        2.61180   0.00004  -0.00003   0.00042   0.00039   2.61219
   A2        2.64337   0.00005  -0.00005   0.00039   0.00034   2.64370
   A3        2.61631  -0.00003  -0.00008   0.00015   0.00007   2.61638
   A4        2.71908  -0.00015  -0.00026  -0.00056  -0.00083   2.71825
   A5        2.63943   0.00010  -0.00000   0.00061   0.00060   2.64004
   A6        2.77823   0.00009   0.00001   0.00029   0.00030   2.77853
   A7        2.72244  -0.00021  -0.00031  -0.00078  -0.00109   2.72135
   A8        2.77586   0.00013   0.00005   0.00046   0.00051   2.77637
   A9        2.83000   0.00016   0.00022   0.00043   0.00064   2.83065
  A10        2.31199  -0.00017  -0.00082  -0.00021  -0.00103   2.31096
  A11        2.51275   0.00021  -0.00035   0.00166   0.00131   2.51406
  A12        1.45794  -0.00003   0.00114  -0.00141  -0.00029   1.45765
  A13        2.82872   0.00018   0.00024   0.00053   0.00076   2.82948
  A14        2.31243  -0.00017  -0.00082  -0.00021  -0.00103   2.31140
```

A15	1.45772	-0.00004	0.00113	-0.00143	-0.00031	1.45741
A16	2.51256	0.00021	-0.00035	0.00168	0.00134	2.51390
A17	1.43103	-0.00025	0.00076	-0.00244	-0.00170	1.42933
A18	1.43133	-0.00025	0.00077	-0.00243	-0.00167	1.42966
A19	2.88230	-0.00005	0.00067	-0.00148	-0.00081	2.88148
A20	2.88369	-0.00006	0.00065	-0.00159	-0.00095	2.88274
A21	3.13795	-0.00028	0.00121	-0.00468	-0.00348	3.13448
A22	3.13784	-0.00028	0.00120	-0.00466	-0.00347	3.13437
D1	0.06338	-0.00001	0.00056	0.00011	0.00068	0.06405
D2	-0.05430	-0.00012	-0.00014	-0.00403	-0.00417	-0.05847
D3	-0.04205	-0.00013	-0.00039	-0.00425	-0.00465	-0.04670
D4	0.06167	0.00000	0.00063	0.00037	0.00100	0.06267
D5	0.06865	0.00017	0.00109	0.00436	0.00544	0.07409
D6	-0.03936	-0.00014	-0.00046	-0.00452	-0.00498	-0.04435
D7	0.06891	0.00002	0.00052	0.00664	0.00715	0.07605
D8	0.06683	0.00017	0.00111	0.00446	0.00556	0.07238
D9	0.07105	0.00001	0.00047	0.00654	0.00700	0.07805
D10	-0.58019	-0.00001	-0.00262	-0.00685	-0.00947	-0.58966
D11	2.60956	-0.00038	-0.00084	-0.00857	-0.00942	2.60015
D12	0.73727	0.00022	0.00013	0.00381	0.00394	0.74120
D13	-2.43201	0.00045	-0.00086	0.00492	0.00405	-2.42796
D14	-2.43283	0.00045	-0.00093	0.00489	0.00395	-2.42887
D15	0.68108	0.00068	-0.00192	0.00600	0.00407	0.68515
D16	2.41289	0.00017	0.00129	-0.00272	-0.00144	2.41146
D17	-0.69295	-0.00010	0.00263	-0.00399	-0.00136	-0.69431
D18	-0.58322	-0.00001	-0.00252	-0.00665	-0.00918	-0.59240
D19	2.60513	-0.00038	-0.00086	-0.00843	-0.00929	2.59584
D20	-0.69298	-0.00010	0.00262	-0.00399	-0.00136	-0.69434
D21	2.41392	0.00017	0.00137	-0.00268	-0.00131	2.41261
D22	0.66169	0.00052	-0.00212	0.00514	0.00301	0.66470

Item	Value	Threshold	Converged?
Maximum Force	0.001474	0.000450	NO
RMS Force	0.000467	0.000300	NO
Maximum Displacement	0.008451	0.001800	NO
RMS Displacement	0.003181	0.001200	NO

Predicted change in Energy=-2.250658D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 19:07:50 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.623129	-0.673877	0.015098

2	6	0	3.008357	-1.727593	0.055919
3	6	0	3.621328	0.675516	-0.014229
4	6	0	1.854860	-2.427570	0.063431
5	6	0	3.008171	1.730145	-0.055146
6	6	0	0.645400	-2.576017	0.063048
7	6	0	1.853081	2.427633	-0.063601
8	6	0	-0.666017	-2.255591	0.020331
9	6	0	0.643787	2.577171	-0.063619
10	6	0	-1.731218	-1.674031	-0.033082
11	6	0	-0.667302	2.255070	-0.021380
12	6	0	-2.684730	-0.678697	-0.167900
13	6	0	-1.732514	1.673504	0.031742
14	6	0	-2.684933	0.677220	0.167354
15	6	0	-4.046190	-0.403359	-0.598308
16	6	0	-4.045210	0.400475	0.600342

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220627	0.000000			
3	C	1.349712	2.481045	0.000000		
4	C	2.490894	1.349289	3.571496	0.000000	
5	C	2.482424	3.459522	1.220606	4.316339	0.000000
6	C	3.533738	2.510665	4.408467	1.218535	4.913215
7	C	3.571921	4.314493	2.489789	4.856864	1.349367
8	C	4.571502	3.712287	5.193641	2.527104	5.421388
9	C	4.410441	4.912889	3.533339	5.150755	2.511541
10	C	5.447170	4.740713	5.845551	3.665663	5.835298
11	C	5.194984	5.420152	4.570272	5.319362	3.712922
12	C	6.310515	5.793230	6.451656	4.870312	6.182584
13	C	5.847511	5.834715	5.446257	5.448767	4.741819
14	C	6.452929	6.181350	6.308874	5.500930	5.793927
15	C	7.698565	7.207513	7.765047	6.273572	7.389917
16	C	7.765318	7.387684	7.696048	6.564825	7.207487

		6	7	8	9	10
6	C	0.000000				
7	C	5.148887	0.000000			
8	C	1.350672	5.318410	0.000000		
9	C	5.154745	1.218505	5.007817	0.000000	
10	C	2.543842	5.447180	1.214791	4.869733	0.000000
11	C	5.006967	2.526637	4.510854	1.350736	4.070613
12	C	3.839651	5.500172	2.568506	4.657315	1.384936
13	C	4.869690	3.665282	4.071282	2.544113	3.348163
14	C	4.656774	4.869379	3.563568	3.839731	2.545216
15	C	5.212375	6.565198	3.903722	5.582592	2.700589
16	C	5.581220	6.272163	4.337054	5.212058	3.171649

		11	12	13	14	15
11	C	0.000000				

```
  12  C    3.563492   0.000000
  13  C    1.214791   2.545471   0.000000
  14  C    2.568281   1.396749   1.384946   0.000000
  15  C    4.337854   1.454179   3.172290   1.899187   0.000000
  16  C    3.903374   1.898872   2.700458   1.454105   1.443230
            16
  16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 4.76D-05
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.622934   -0.674962    0.013312
     2          6           0        3.007857   -1.728602    0.051451
     3          6           0        3.621523    0.674501   -0.012568
     4          6           0        1.854157   -2.428261    0.057195
     5          6           0        3.008671    1.729409   -0.050779
     6          6           0        0.644655   -2.576356    0.056455
     7          6           0        1.853783    2.427250   -0.057431
     8          6           0       -0.666670   -2.255443    0.014580
     9          6           0        0.644532    2.577139   -0.057045
    10          6           0       -1.731703   -1.673439   -0.037328
    11          6           0       -0.666649    2.255311   -0.015606
    12          6           0       -2.684929   -0.677488   -0.169586
    13          6           0       -1.732028    1.673919    0.036049
    14          6           0       -2.684733    0.677568    0.169131
    15          6           0       -4.046317   -0.400657   -0.599265
    16          6           0       -4.045084    0.400111    0.601435
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8461707           0.3940196           0.2716098
 Leave Link  202 at Fri Aug 21 19:07:50 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.4044189663 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
```

ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074872213 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.3969317449 Hartrees.
Leave Link 301 at Fri Aug 21 19:07:50 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33574.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.03D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 19:07:51 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 19:07:51 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000016 -0.000000 0.000006 Ang= 0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 19:07:51 2026, MaxMem= 805306368 cpu: 1.5 elap: 0.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Supporting Information file

Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981418093463
DIIS: error= 5.62D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981418093463 IErMin= 1 ErrMin= 5.62D-04
ErrMax= 5.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-04 BMatP= 1.59D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 5.62D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=3.18D-05 MaxDP=8.52D-04 OVMax= 1.56D-03

Cycle 2 Pass 1 IDiag 1:
RMSU= 3.17D-05 CP: 1.00D+00
E= -608.981488559122 Delta-E= -0.000070465659 Rises=F Damp=F
DIIS: error= 5.27D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981488559122 IErMin= 2 ErrMin= 5.27D-05
ErrMax= 5.27D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-06 BMatP= 1.59D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.276D-01 0.103D+01
Coeff: -0.276D-01 0.103D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.10D-05 MaxDP=4.06D-04 DE=-7.05D-05 OVMax= 8.97D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 1.02D-05 CP: 1.00D+00 1.11D+00
E= -608.981491935081 Delta-E= -0.000003375959 Rises=F Damp=F
DIIS: error= 3.02D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981491935081 IErMin= 3 ErrMin= 3.02D-05
ErrMax= 3.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-07 BMatP= 1.49D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.120D-01 0.228D+00 0.784D+00
Coeff: -0.120D-01 0.228D+00 0.784D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=4.70D-06 MaxDP=1.51D-04 DE=-3.38D-06 OVMax= 3.72D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 4.56D-06 CP: 1.00D+00 1.13D+00 1.07D+00
E= -608.981492491209 Delta-E= -0.000000556128 Rises=F Damp=F
DIIS: error= 2.54D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981492491209 IErMin= 4 ErrMin= 2.54D-05
ErrMax= 2.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-07 BMatP= 3.50D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.674D-04-0.993D-01 0.418D+00 0.682D+00
Coeff: -0.674D-04-0.993D-01 0.418D+00 0.682D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.71D-06 MaxDP=1.07D-04 DE=-5.56D-07 OVMax= 3.29D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 1.39D-06 CP: 1.00D+00 1.15D+00 1.29D+00 1.01D+00
E= -608.981492831449 Delta-E= -0.000000340240 Rises=F Damp=F
DIIS: error= 1.31D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981492831449 IErMin= 5 ErrMin= 1.31D-05
ErrMax= 1.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-08 BMatP= 2.02D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.243D-02-0.975D-01 0.671D-01 0.327D+00 0.701D+00
Coeff: 0.243D-02-0.975D-01 0.671D-01 0.327D+00 0.701D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.43D-06 MaxDP=3.96D-05 DE=-3.40D-07 OVMax= 1.84D-04

Cycle 6 Pass 1 IDiag 1:
RMSU= 6.41D-07 CP: 1.00D+00 1.16D+00 1.40D+00 1.09D+00 1.21D+00
E= -608.981492909410 Delta-E= -0.000000077961 Rises=F Damp=F
DIIS: error= 5.93D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981492909410 IErMin= 6 ErrMin= 5.93D-06
ErrMax= 5.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.94D-09 BMatP= 3.13D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.138D-02-0.324D-01-0.522D-01 0.291D-01 0.359D+00 0.695D+00
Coeff: 0.138D-02-0.324D-01-0.522D-01 0.291D-01 0.359D+00 0.695D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=7.47D-07 MaxDP=3.05D-05 DE=-7.80D-08 OVMax= 7.98D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.91D-07 CP: 1.00D+00 1.16D+00 1.43D+00 1.20D+00 1.33D+00
CP: 1.26D+00
E= -608.981492935472 Delta-E= -0.000000026062 Rises=F Damp=F
DIIS: error= 3.13D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981492935472 IErMin= 7 ErrMin= 3.13D-06
ErrMax= 3.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-09 BMatP= 7.94D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.497D-03 0.270D-01-0.365D-01-0.108D+00-0.186D+00 0.165D+00
Coeff-Com: 0.114D+01
Coeff: -0.497D-03 0.270D-01-0.365D-01-0.108D+00-0.186D+00 0.165D+00
Coeff: 0.114D+01

Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.96D-07 MaxDP=2.20D-05 DE=-2.61D-08 OVMax= 1.10D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.98D-07 CP: 1.00D+00 1.16D+00 1.45D+00 1.23D+00 1.53D+00
CP: 1.78D+00 1.62D+00
E= -608.981492944810 Delta-E= -0.000000009338 Rises=F Damp=F
DIIS: error= 8.22D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981492944810 IErMin= 8 ErrMin= 8.22D-07
ErrMax= 8.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-10 BMatP= 1.26D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.294D-03 0.114D-01-0.541D-02-0.332D-01-0.933D-01-0.278D-01
Coeff-Com: 0.346D+00 0.803D+00
Coeff: -0.294D-03 0.114D-01-0.541D-02-0.332D-01-0.933D-01-0.278D-01
Coeff: 0.346D+00 0.803D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.79D-07 MaxDP=5.03D-06 DE=-9.34D-09 OVMax= 2.49D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.65D-08 CP: 1.00D+00 1.16D+00 1.45D+00 1.22D+00 1.57D+00
CP: 1.92D+00 1.85D+00 1.40D+00
E= -608.981492945459 Delta-E= -0.000000000649 Rises=F Damp=F
DIIS: error= 7.10D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981492945459 IErMin= 9 ErrMin= 7.10D-07
ErrMax= 7.10D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.20D-11 BMatP= 1.53D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.134D-04-0.915D-03 0.394D-02 0.953D-02 0.210D-02-0.493D-01
Coeff-Com: -0.822D-01 0.291D+00 0.825D+00
Coeff: -0.134D-04-0.915D-03 0.394D-02 0.953D-02 0.210D-02-0.493D-01
Coeff: -0.822D-01 0.291D+00 0.825D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.14D-07 MaxDP=3.10D-06 DE=-6.49D-10 OVMax= 1.19D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.64D-08 CP: 1.00D+00 1.16D+00 1.44D+00 1.22D+00 1.57D+00
CP: 1.98D+00 2.00D+00 1.67D+00 1.31D+00
E= -608.981492945609 Delta-E= -0.000000000151 Rises=F Damp=F
DIIS: error= 5.30D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981492945609 IErMin=10 ErrMin= 5.30D-07
ErrMax= 5.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-11 BMatP= 4.20D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.668D-04-0.334D-02 0.318D-02 0.141D-01 0.250D-01-0.224D-01
Coeff-Com: -0.128D+00-0.532D-01 0.474D+00 0.691D+00
Coeff: 0.668D-04-0.334D-02 0.318D-02 0.141D-01 0.250D-01-0.224D-01
Coeff: -0.128D+00-0.532D-01 0.474D+00 0.691D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.76D-08 MaxDP=1.55D-06 DE=-1.51D-10 OVMax= 4.81D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.28D-08 CP: 1.00D+00 1.16D+00 1.44D+00 1.22D+00 1.57D+00
CP: 2.00D+00 2.07D+00 1.82D+00 1.55D+00 1.07D+00
E= -608.981492945658 Delta-E= -0.000000000048 Rises=F Damp=F
DIIS: error= 2.06D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981492945658 IErMin=11 ErrMin= 2.06D-07
ErrMax= 2.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.30D-12 BMatP= 1.63D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.279D-04-0.108D-02 0.214D-03 0.368D-02 0.916D-02 0.592D-03
Coeff-Com: -0.308D-01-0.768D-01 0.180D-02 0.274D+00 0.819D+00
Coeff: 0.279D-04-0.108D-02 0.214D-03 0.368D-02 0.916D-02 0.592D-03
Coeff: -0.308D-01-0.768D-01 0.180D-02 0.274D+00 0.819D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.26D-08 MaxDP=6.34D-07 DE=-4.84D-11 OVMax= 2.60D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 5.91D-09 CP: 1.00D+00 1.16D+00 1.44D+00 1.22D+00 1.57D+00
CP: 2.01D+00 2.09D+00 1.87D+00 1.66D+00 1.31D+00
CP: 1.33D+00
E= -608.981492945667 Delta-E= -0.000000000009 Rises=F Damp=F
DIIS: error= 4.95D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981492945667 IErMin=12 ErrMin= 4.95D-08
ErrMax= 4.95D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.19D-13 BMatP= 2.30D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.100D-04 0.590D-03-0.848D-03-0.257D-02-0.392D-02 0.564D-02
Coeff-Com: 0.257D-01-0.924D-02-0.125D+00-0.853D-01 0.197D+00 0.997D+00
Coeff: -0.100D-04 0.590D-03-0.848D-03-0.257D-02-0.392D-02 0.564D-02
Coeff: 0.257D-01-0.924D-02-0.125D+00-0.853D-01 0.197D+00 0.997D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=9.06D-09 MaxDP=3.03D-07 DE=-8.87D-12 OVMax= 1.22D-06

SCF Done: E(RwB97XD) = -608.981492946 A.U. after 12 cycles
NFock= 12 Conv=0.91D-08 -V/T= 2.0045
KE= 6.062281313365D+02 PE=-2.845787776720D+03 EE= 9.131812206933D+02
Leave Link 502 at Fri Aug 21 19:16:15 2026, MaxMem= 805306368 cpu: 3020.1 elap: 503.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33574.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 19:16:15 2026, MaxMem= 805306368 cpu: 2.4 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.

Supporting Information file

Leave Link 702 at Fri Aug 21 19:16:15 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 2804.1 elap: 467.4
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.52052001D+00-3.98676189D-03-6.17266069D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000021466	0.000902890	-0.000355004
2	6	-0.000774787	-0.000403534	0.000545450
3	6	0.000115466	-0.000878709	0.000372289
4	6	0.000807076	0.000262011	-0.000733817
5	6	-0.000843303	0.000344761	-0.000584743
6	6	-0.000792127	0.000337263	0.000595476
7	6	0.000838677	-0.000190302	0.000772042
8	6	0.000626878	-0.000329529	-0.000673302
9	6	-0.000798538	-0.000391532	-0.000615185
10	6	-0.000145826	0.000649434	0.000831218
11	6	0.000622351	0.000354605	0.000662792
12	6	-0.000515214	-0.001110012	-0.000528565
13	6	-0.000138688	-0.000666860	-0.000808893
14	6	-0.000511674	0.001120127	0.000523333
15	6	0.000748131	-0.000316335	-0.000845076
16	6	0.000740113	0.000315722	0.000841985

Cartesian Forces: Max 0.001120127 RMS 0.000635984
Leave Link 716 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.

Supporting Information file

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000864453 RMS 0.000315437
Search for a local minimum.
Step number 6 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .31544D-03 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 1 2 3 4 5
6
DE= -3.48D-05 DEPred=-2.25D-05 R= 1.55D+00
TightC=F SS= 1.41D+00 RLast= 2.78D-02 DXNew= 8.4853D-01 8.3335D-02
Trust test= 1.55D+00 RLast= 2.78D-02 DXMaxT set to 5.05D-01
ITU= 1 1 1 1 1 0
Eigenvalues --- 0.00976 0.01290 0.01453 0.01732 0.02205
Eigenvalues --- 0.02625 0.02941 0.03354 0.03422 0.03926
Eigenvalues --- 0.04047 0.04309 0.08292 0.08430 0.09348
Eigenvalues --- 0.14864 0.24488 0.24582 0.24990 0.24995
Eigenvalues --- 0.24997 0.24999 0.25000 0.25000 0.25041
Eigenvalues --- 0.25097 0.28163 0.32013 0.34279 0.42598
Eigenvalues --- 0.51322 0.53498 0.57382 0.57897 0.58160
Eigenvalues --- 0.58184 0.78669 0.79249 0.79697 0.81363
Eigenvalues --- 0.82171 0.99189
En-DIIS/RFO-DIIS/Sim-DIIS IScMMF= -3 using points: 6 5 4
RFO step: Lambda=-6.98031378D-05.
NNeg= 0 NGDIIS= 3 SimSw= 2.50D-01 Rises=F DC= -3.48D-05 SmlDif= 1.00D-05
NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj= 3.0
RMS Error= 0.8686524034D-02 NUsed= 3 OKEnD=T EnDIS=F
InvSVX: RCond= 6.75D-05 Info= 0 Equed=N FErr= 3.60D-14 BErr= 3.80D-17
DidBck=F Rises=F RFO-DIIS coefs: 2.92281 -1.56131 -0.36151
Iteration 1 RMS(Cart)= 0.00353550 RMS(Int)= 0.00003533
Iteration 2 RMS(Cart)= 0.00003195 RMS(Int)= 0.00002444
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002444
ITry= 1 IFail=0 DXMaxC= 1.07D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.30665	0.00007	0.00115	-0.00046	0.00070	2.30735
R2	2.55059	-0.00086	0.00050	-0.00150	-0.00100	2.54958
R3	2.54979	-0.00081	0.00049	-0.00138	-0.00088	2.54890
R4	2.30661	0.00007	0.00116	-0.00046	0.00071	2.30732
R5	2.30270	0.00007	0.00129	-0.00053	0.00076	2.30346
R6	2.54993	-0.00082	0.00048	-0.00139	-0.00091	2.54903
R7	2.55240	-0.00074	0.00014	-0.00112	-0.00098	2.55142
R8	2.30264	0.00007	0.00130	-0.00053	0.00077	2.30341
R9	2.29562	-0.00005	0.00111	-0.00063	0.00048	2.29610
R10	2.55252	-0.00075	0.00011	-0.00112	-0.00101	2.55151
R11	2.61715	-0.00053	0.00029	-0.00076	-0.00047	2.61668

R12	2.29562	-0.00005	0.00111	-0.00063	0.00048	2.29610
R13	2.63947	0.00051	0.00645	0.00014	0.00658	2.64605
R14	2.74800	-0.00057	-0.00639	-0.00178	-0.00817	2.73983
R15	2.61717	-0.00053	0.00024	-0.00076	-0.00052	2.61665
R16	2.74786	-0.00056	-0.00643	-0.00177	-0.00819	2.73967
R17	2.72731	0.00068	0.01713	-0.00149	0.01563	2.74294
A1	2.61219	0.00002	0.00068	-0.00005	0.00062	2.61281
A2	2.64370	0.00005	0.00054	0.00016	0.00069	2.64440
A3	2.61638	-0.00005	-0.00006	-0.00026	-0.00033	2.61605
A4	2.71825	-0.00010	-0.00218	-0.00001	-0.00221	2.71605
A5	2.64004	0.00010	0.00115	0.00034	0.00148	2.64151
A6	2.77853	0.00010	0.00061	0.00051	0.00109	2.77962
A7	2.72135	-0.00015	-0.00280	-0.00017	-0.00299	2.71836
A8	2.77637	0.00014	0.00110	0.00061	0.00168	2.77805
A9	2.83065	0.00007	0.00174	-0.00016	0.00152	2.83216
A10	2.31096	-0.00016	-0.00381	0.00045	-0.00338	2.30759
A11	2.51406	0.00021	0.00174	0.00171	0.00347	2.51753
A12	1.45765	-0.00004	0.00199	-0.00210	-0.00011	1.45754
A13	2.82948	0.00008	0.00201	-0.00009	0.00185	2.83133
A14	2.31140	-0.00016	-0.00380	0.00042	-0.00340	2.30800
A15	1.45741	-0.00004	0.00193	-0.00207	-0.00015	1.45725
A16	2.51390	0.00021	0.00181	0.00171	0.00353	2.51744
A17	1.42933	-0.00010	-0.00158	-0.00151	-0.00312	1.42621
A18	1.42966	-0.00010	-0.00149	-0.00155	-0.00307	1.42659
A19	2.88148	-0.00000	-0.00006	-0.00145	-0.00155	2.87994
A20	2.88274	-0.00001	-0.00036	-0.00150	-0.00190	2.88084
A21	3.13448	0.00005	-0.00397	0.01199	0.00797	3.14244
A22	3.13437	0.00005	-0.00399	0.01204	0.00799	3.14236
D1	0.06405	0.00010	0.00256	0.00470	0.00729	0.07134
D2	-0.05847	0.00003	-0.00834	0.00522	-0.00309	-0.06156
D3	-0.04670	-0.00009	-0.00981	-0.00047	-0.01028	-0.05697
D4	0.06267	0.00010	0.00333	0.00480	0.00816	0.07082
D5	0.07409	0.00010	0.01291	0.00285	0.01575	0.08984
D6	-0.04435	-0.00010	-0.01062	-0.00067	-0.01129	-0.05563
D7	0.07605	-0.00010	0.01491	-0.01079	0.00408	0.08014
D8	0.07238	0.00011	0.01317	0.00297	0.01612	0.08851
D9	0.07805	-0.00010	0.01451	-0.01078	0.00368	0.08173
D10	-0.58966	-0.00010	-0.02408	-0.00186	-0.02596	-0.61563
D11	2.60015	-0.00029	-0.01998	-0.00494	-0.02494	2.57521
D12	0.74120	0.00012	0.00786	0.00091	0.00875	0.74996
D13	-2.42796	0.00024	0.00585	0.00253	0.00837	-2.41959
D14	-2.42887	0.00024	0.00551	0.00279	0.00828	-2.42059
D15	0.68515	0.00036	0.00351	0.00441	0.00790	0.69305
D16	2.41146	0.00014	0.00012	-0.00210	-0.00198	2.40948
D17	-0.69431	0.00000	0.00327	-0.00439	-0.00110	-0.69541
D18	-0.59240	-0.00010	-0.02331	-0.00194	-0.02527	-0.61768
D19	2.59584	-0.00029	-0.01978	-0.00459	-0.02439	2.57145
D20	-0.69434	0.00000	0.00326	-0.00439	-0.00111	-0.69544

D21 2.41261 0.00014 0.00055 -0.00242 -0.00187 2.41074
D22 0.66470 0.00032 0.00104 0.00466 0.00570 0.67039
Item Value Threshold Converged?
Maximum Force 0.000864 0.000450 NO
RMS Force 0.000315 0.000300 NO
Maximum Displacement 0.010717 0.001800 NO
RMS Displacement 0.003554 0.001200 NO
Predicted change in Energy=-3.505190D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.621413	-0.673513	0.016004
2	6	0	3.006863	-1.727693	0.059215
3	6	0	3.619958	0.675306	-0.015233
4	6	0	1.854626	-2.428861	0.064763
5	6	0	3.006567	1.730131	-0.058679
6	6	0	0.644621	-2.576164	0.064452
7	6	0	1.853000	2.429231	-0.064873
8	6	0	-0.666262	-2.256528	0.016222
9	6	0	0.643092	2.577125	-0.064859
10	6	0	-1.731138	-1.673437	-0.032526
11	6	0	-0.667501	2.256040	-0.017052
12	6	0	-2.685711	-0.679890	-0.170407
13	6	0	-1.732278	1.672747	0.031426
14	6	0	-2.685895	0.678374	0.169840
15	6	0	-4.041135	-0.402545	-0.603979
16	6	0	-4.040220	0.399675	0.605688

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220997	0.000000			
3	C	1.349182	2.481095	0.000000		
4	C	2.491016	1.348821	3.571925	0.000000	
5	C	2.482161	3.459834	1.220980	4.317340	0.000000
6	C	3.533231	2.510004	4.408065	1.218938	4.913057
7	C	3.572234	4.315880	2.490152	4.859822	1.348887
8	C	4.570569	3.711249	5.193103	2.527238	5.421138
9	C	4.409488	4.912664	3.532861	5.152137	2.510667
10	C	5.445366	4.739200	5.843896	3.665765	5.833593

```
  11  C    5.194051   5.420046   4.569576   5.321289   3.711750
  12  C    6.309882   5.792756   6.451518   4.871228   6.182452
  13  C    5.845271   5.832943   5.444584   5.448869   4.740049
  14  C    6.452395   6.181334   6.308568   5.502934   5.793318
  15  C    7.692363   7.202092   7.758913   6.270022   7.383479
  16  C    7.758872   7.381444   7.690243   6.560673   7.201993
                6          7          8          9         10
   6  C    0.000000
   7  C    5.150814   0.000000
   8  C    1.350151   5.320676   0.000000
   9  C    5.154912   1.218913   5.008511   0.000000
  10  C    2.543334   5.447842   1.215043   4.868809   0.000000
  11  C    5.007845   2.526897   4.512691   1.350199   4.070916
  12  C    3.839548   5.502515   2.568811   4.658349   1.384687
  13  C    4.868674   3.665482   4.071341   2.543533   3.346795
  14  C    4.657839   4.870539   3.565973   3.839596   2.546278
  15  C    5.208429   6.561282   3.900214   5.577730   2.697743
  16  C    5.576405   6.268875   4.334337   5.208103   3.168118
               11         12         13         14         15
  11  C    0.000000
  12  C    3.566002   0.000000
  13  C    1.215044   2.546501   0.000000
  14  C    2.568632   1.400232   1.384673   0.000000
  15  C    4.335200   1.449855   3.168816   1.898383   0.000000
  16  C    3.899888   1.898020   2.697607   1.449770   1.451500
               16
  16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 6.92D-05
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.621195   -0.674726    0.014197
    2          6           0        3.006304   -1.728815    0.054688
    3          6           0        3.620176    0.674170   -0.013546
    4          6           0        1.853840   -2.429622    0.058440
    5          6           0        3.007126    1.729303   -0.054250
    6          6           0        0.643787   -2.576531    0.057768
    7          6           0        1.853786    2.428791   -0.058613
    8          6           0       -0.666993   -2.256346    0.010389
    9          6           0        0.643927    2.577076   -0.058196
```

```
    10        6        0       -1.731680   -1.672786   -0.036830
    11        6        0       -0.666770    2.256293   -0.011198
    12        6        0       -2.685934   -0.678576   -0.172121
    13        6        0       -1.731735    1.673221    0.035788
    14        6        0       -2.685672    0.678803    0.171643
    15        6        0       -4.041275   -0.399670   -0.604951
    16        6        0       -4.040080    0.399414    0.606791
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8455567           0.3943858           0.2717769
 Leave Link  202 at Fri Aug 21 19:24:03 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.4564325114 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000  wLong=    0.200000  cFull=    0.222036  cShort=    0.000000  cLong=
0.777964
  DFx    wShort=    0.000000  wLong=    0.200000  cFull=    0.000000  cShort=    0.000000  cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0074870116 Hartrees.
 Nuclear repulsion after empirical dispersion term =      717.4489454998 Hartrees.
 Leave Link  301 at Fri Aug 21 19:24:03 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14214 LenP2D=   33578.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  4.18D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=         32
 NSgBfM=   564   564   564   564   564 MxSgAt=    16 MxSgA2=    16.
```

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 Leave Link  302 at Fri Aug 21 19:24:03 2026, MaxMem=    805306368 cpu:                3.4 elap:
0.6
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Aug 21 19:24:04 2026, MaxMem=    805306368 cpu:                0.5 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca.chk"
 B after Tr=    -0.000000    0.000000   -0.000000
       Rot=    1.000000   -0.000017    0.000000    0.000017 Ang=  -0.00 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Leave Link  401 at Fri Aug 21 19:24:04 2026, MaxMem=    805306368 cpu:                1.9 elap:
0.3
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804634234 LenY=   804301882
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
       NFxFlg=          0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=          0 NGrid=          0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -608.981346938310
 DIIS: error= 5.51D-04 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -608.981346938310     IErMin= 1 ErrMin= 5.51D-04
 ErrMax= 5.51D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-04 BMatP= 2.40D-04
 IDIUse=3 WtCom= 9.94D-01 WtEn= 5.51D-03
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=     0.960 Goal=   None    Shift=    0.000
 RMSDP=1.17D-04 MaxDP=2.84D-03             OVMax= 3.31D-03

 Cycle   2  Pass 1  IDiag  1:
 RMSU=  1.14D-04    CP:  9.97D-01
 E= -608.981504442509     Delta-E=       -0.000157504199 Rises=F Damp=F
 DIIS: error= 1.00D-04 at cycle   2 NSaved=   2.
```

NSaved= 2 IEnMin= 2 EnMin= -608.981504442509 IErMin= 2 ErrMin= 1.00D-04
ErrMax= 1.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.13D-06 BMatP= 2.40D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.00D-03
Coeff-Com: -0.309D-01 0.103D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.309D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.09D-05 MaxDP=9.02D-04 DE=-1.58D-04 OVMax= 2.24D-03

Cycle 3 Pass 1 IDiag 1:
RMSU= 1.78D-05 CP: 9.96D-01 1.09D+00
E= -608.981518282894 Delta-E= -0.000013840385 Rises=F Damp=F
DIIS: error= 8.16D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981518282894 IErMin= 3 ErrMin= 8.16D-05
ErrMax= 8.16D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-06 BMatP= 5.13D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.236D-01 0.345D+00 0.679D+00
Coeff: -0.236D-01 0.345D+00 0.679D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=8.83D-06 MaxDP=3.25D-04 DE=-1.38D-05 OVMax= 9.23D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 8.29D-06 CP: 9.97D-01 1.10D+00 9.09D-01
E= -608.981521772383 Delta-E= -0.000003489489 Rises=F Damp=F
DIIS: error= 5.60D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981521772383 IErMin= 4 ErrMin= 5.60D-05
ErrMax= 5.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.88D-07 BMatP= 2.16D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.289D-03-0.162D+00 0.334D+00 0.828D+00
Coeff: 0.289D-03-0.162D+00 0.334D+00 0.828D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=6.02D-06 MaxDP=2.81D-04 DE=-3.49D-06 OVMax= 8.85D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.21D-06 CP: 9.97D-01 1.10D+00 1.18D+00 1.18D+00
E= -608.981523731732 Delta-E= -0.000001959349 Rises=F Damp=F
DIIS: error= 2.76D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981523731732 IErMin= 5 ErrMin= 2.76D-05
ErrMax= 2.76D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-07 BMatP= 7.88D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.411D-02-0.141D+00 0.614D-01 0.409D+00 0.667D+00
Coeff: 0.411D-02-0.141D+00 0.614D-01 0.409D+00 0.667D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.74D-06 MaxDP=1.11D-04 DE=-1.96D-06 OVMax= 4.60D-04

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.47D-06 CP: 9.97D-01 1.10D+00 1.30D+00 1.30D+00 1.17D+00
E= -608.981524145941 Delta-E= -0.000000414209 Rises=F Damp=F

DIIS: error= 1.19D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981524145941 IErMin= 6 ErrMin= 1.19D-05
ErrMax= 1.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.88D-08 BMatP= 1.51D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.233D-02-0.285D-01-0.754D-01-0.369D-01 0.354D+00 0.784D+00
Coeff: 0.233D-02-0.285D-01-0.754D-01-0.369D-01 0.354D+00 0.784D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.04D-06 MaxDP=1.05D-04 DE=-4.14D-07 OVMax= 2.56D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 8.65D-07 CP: 9.97D-01 1.10D+00 1.33D+00 1.48D+00 1.40D+00
CP: 1.28D+00
E= -608.981524300102 Delta-E= -0.000000154161 Rises=F Damp=F
DIIS: error= 4.90D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981524300102 IErMin= 7 ErrMin= 4.90D-06
ErrMax= 4.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.88D-09 BMatP= 3.88D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.605D-03 0.314D-01-0.300D-01-0.101D+00-0.114D+00 0.114D+00
Coeff-Com: 0.110D+01
Coeff: -0.605D-03 0.314D-01-0.300D-01-0.101D+00-0.114D+00 0.114D+00
Coeff: 0.110D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.13D-06 MaxDP=4.58D-05 DE=-1.54D-07 OVMax= 1.99D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.61D-07 CP: 9.97D-01 1.10D+00 1.35D+00 1.55D+00 1.58D+00
CP: 1.58D+00 1.38D+00
E= -608.981524331009 Delta-E= -0.000000030907 Rises=F Damp=F
DIIS: error= 3.27D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981524331009 IErMin= 8 ErrMin= 3.27D-06
ErrMax= 3.27D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.42D-10 BMatP= 3.88D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.451D-03 0.149D-01-0.601D-02-0.330D-01-0.779D-01-0.300D-01
Coeff-Com: 0.433D+00 0.700D+00
Coeff: -0.451D-03 0.149D-01-0.601D-02-0.330D-01-0.779D-01-0.300D-01
Coeff: 0.433D+00 0.700D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.54D-07 MaxDP=8.84D-06 DE=-3.09D-08 OVMax= 4.69D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 1.28D-07 CP: 9.97D-01 1.10D+00 1.35D+00 1.56D+00 1.59D+00
CP: 1.67D+00 1.50D+00 1.27D+00
E= -608.981524333915 Delta-E= -0.000000002907 Rises=F Damp=F
DIIS: error= 1.92D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981524333915 IErMin= 9 ErrMin= 1.92D-06
ErrMax= 1.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-10 BMatP= 9.42D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.818D-04-0.928D-03 0.526D-02 0.144D-01-0.115D-01-0.603D-01

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Coeff-Com: -0.825D-01 0.421D+00 0.715D+00
Coeff: -0.818D-04-0.928D-03 0.526D-02 0.144D-01-0.115D-01-0.603D-01
Coeff: -0.825D-01 0.421D+00 0.715D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.73D-07 MaxDP=5.17D-06 DE=-2.91D-09 OVMax= 2.63D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 6.71D-08 CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.60D+00
CP: 1.70D+00 1.59D+00 1.54D+00 1.28D+00
E= -608.981524335260 Delta-E= -0.000000001344 Rises=F Damp=F
DIIS: error= 7.67D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981524335260 IErMin=10 ErrMin= 7.67D-07
ErrMax= 7.67D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.22D-11 BMatP= 4.17D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.111D-03-0.489D-02 0.262D-02 0.158D-01 0.210D-01-0.157D-01
Coeff-Com: -0.155D+00-0.650D-01 0.230D+00 0.972D+00
Coeff: 0.111D-03-0.489D-02 0.262D-02 0.158D-01 0.210D-01-0.157D-01
Coeff: -0.155D+00-0.650D-01 0.230D+00 0.972D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.26D-07 MaxDP=4.13D-06 DE=-1.34D-09 OVMax= 1.70D-05

Cycle 11 Pass 1 IDiag 1:
RMSU= 3.52D-08 CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.60D+00
CP: 1.72D+00 1.64D+00 1.72D+00 1.66D+00 1.57D+00
E= -608.981524335633 Delta-E= -0.000000000373 Rises=F Damp=F
DIIS: error= 3.59D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981524335633 IErMin=11 ErrMin= 3.59D-07
ErrMax= 3.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.54D-12 BMatP= 6.22D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.418D-04-0.112D-02-0.324D-03 0.215D-02 0.726D-02 0.557D-02
Coeff-Com: -0.268D-01-0.902D-01-0.487D-01 0.250D+00 0.902D+00
Coeff: 0.418D-04-0.112D-02-0.324D-03 0.215D-02 0.726D-02 0.557D-02
Coeff: -0.268D-01-0.902D-01-0.487D-01 0.250D+00 0.902D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.16D-08 MaxDP=1.13D-06 DE=-3.73D-10 OVMax= 5.96D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.44D-08 CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.61D+00
CP: 1.73D+00 1.65D+00 1.76D+00 1.80D+00 1.84D+00
CP: 1.38D+00
E= -608.981524335692 Delta-E= -0.000000000059 Rises=F Damp=F
DIIS: error= 1.84D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981524335692 IErMin=12 ErrMin= 1.84D-07
ErrMax= 1.84D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.91D-12 BMatP= 9.54D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.132D-04 0.800D-03-0.772D-03-0.300D-02-0.253D-02 0.574D-02
Coeff-Com: 0.275D-01-0.163D-01-0.710D-01-0.146D+00 0.334D+00 0.871D+00
Coeff: -0.132D-04 0.800D-03-0.772D-03-0.300D-02-0.253D-02 0.574D-02

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Coeff: 0.275D-01-0.163D-01-0.710D-01-0.146D+00 0.334D+00 0.871D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.73D-08 MaxDP=5.63D-07 DE=-5.91D-11 OVMax= 3.33D-06

Cycle 13 Pass 1 IDiag 1:
RMSU= 8.83D-09 CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.60D+00
CP: 1.73D+00 1.65D+00 1.76D+00 1.84D+00 1.97D+00
CP: 1.62D+00 1.30D+00
E= -608.981524335716 Delta-E= -0.000000000025 Rises=F Damp=F
DIIS: error= 9.44D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981524335716 IErMin=13 ErrMin= 9.44D-08
ErrMax= 9.44D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-12 BMatP= 2.91D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.172D-04 0.693D-03-0.324D-03-0.215D-02-0.298D-02 0.175D-02
Coeff-Com: 0.208D-01 0.131D-01-0.269D-01-0.131D+00-0.355D-01 0.447D+00
Coeff-Com: 0.716D+00
Coeff: -0.172D-04 0.693D-03-0.324D-03-0.215D-02-0.298D-02 0.175D-02
Coeff: 0.208D-01 0.131D-01-0.269D-01-0.131D+00-0.355D-01 0.447D+00
Coeff: 0.716D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=7.39D-09 MaxDP=2.22D-07 DE=-2.46D-11 OVMax= 1.69D-06

SCF Done: E(RwB97XD) = -608.981524336 A.U. after 13 cycles
NFock= 13 Conv=0.74D-08 -V/T= 2.0045
KE= 6.062244414788D+02 PE=-2.845882832050D+03 EE= 9.132279207355D+02
Leave Link 502 at Fri Aug 21 19:33:40 2026, MaxMem= 805306368 cpu: 3454.3 elap: 576.0
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14214 LenP2D= 33578.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 19:33:40 2026, MaxMem= 805306368 cpu: 2.2 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 19:33:40 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

```
      NFxFlg=           0 DoJE=F BraDBF=F KetDBF=F FulRan=T
      wScrn=  0.000000 ICntrl=       2527 IOpCl=  0 I1Cent=           0 NGrid=           0
      NMat0=     1 NMatS0=       1 NMatT0=     0 NMatD0=     1 NMtDS0=     0 NMtDT0=     0
 Symmetry not used in FoFCou.
 Leave Link  703 at Fri Aug 21 19:40:31 2026, MaxMem=    805306368 cpu:              2465.1 elap:
411.0
 (Enter /home/user/gauss16/g16/l716.exe)
 Dipole        = 1.51961950D+00-3.02113427D-03-5.87945115D-04
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
     1        6         -0.000265558   -0.000020332   -0.000334886
     2        6         -0.000103310    0.000235385    0.000434918
     3        6         -0.000191714    0.000038929    0.000340126
     4        6         -0.000172783    0.000123021   -0.000591187
     5        6         -0.000159097   -0.000278344   -0.000451126
     6        6          0.000250443    0.000194974    0.000236237
     7        6         -0.000146623   -0.000074358    0.000615618
     8        6         -0.000185489    0.000120610   -0.000036054
     9        6          0.000243032   -0.000229011   -0.000254287
    10        6          0.000384268    0.000033002    0.000294546
    11        6         -0.000186095   -0.000107392    0.000029924
    12        6         -0.000051501   -0.000077549   -0.000361099
    13        6          0.000392697   -0.000036483   -0.000283553
    14        6         -0.000057920    0.000070676    0.000358308
    15        6          0.000136621    0.000393613    0.000827645
    16        6          0.000113029   -0.000386741   -0.000825130
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000827645 RMS     0.000308833
 Leave Link  716 at Fri Aug 21 19:40:31 2026, MaxMem=    805306368 cpu:                 0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000690566 RMS     0.000239370
 Search for a local minimum.
 Step number   7 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .23937D-03 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                      6    7
```

Supporting Information file

DE= -3.14D-05 DEPred=-3.51D-05 R= 8.96D-01
TightC=F SS= 1.41D+00 RLast= 6.64D-02 DXNew= 8.4853D-01 1.9913D-01
Trust test= 8.96D-01 RLast= 6.64D-02 DXMaxT set to 5.05D-01
ITU= 1 1 1 1 1 1 0
Eigenvalues --- 0.00696 0.01290 0.01541 0.01732 0.02380
Eigenvalues --- 0.02626 0.02939 0.03413 0.03422 0.03926
Eigenvalues --- 0.04047 0.04753 0.08286 0.08440 0.09362
Eigenvalues --- 0.15854 0.24430 0.24571 0.24988 0.24993
Eigenvalues --- 0.24994 0.24998 0.25000 0.25000 0.25048
Eigenvalues --- 0.25292 0.28162 0.31615 0.34593 0.40147
Eigenvalues --- 0.51322 0.53330 0.57381 0.57901 0.58162
Eigenvalues --- 0.58185 0.78669 0.79194 0.79696 0.81312
Eigenvalues --- 0.82168 0.87719
En-DIIS/RFO-DIIS/Sim-DIIS IScMMF= -3 using points: 7 6 5 4
RFO step: Lambda=-1.55547474D-05.
NNeg= 0 NGDIIS= 4 SimSw= 2.50D-01 Rises=F DC= -3.14D-05 SmlDif= 1.00D-05
NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj= 3.0
RMS Error= 0.3559269524D-02 NUsed= 4 OKEnD=T EnDIS=F
InvSVX: RCond= 2.68D-05 Info= 0 Equed=N FErr= 1.19D-13 BErr= 6.21D-17
DidBck=T Rises=F RFO-DIIS coefs: 0.76669 1.02114 -0.65717 -0.13066
Iteration 1 RMS(Cart)= 0.00278217 RMS(Int)= 0.00001226
Iteration 2 RMS(Cart)= 0.00000605 RMS(Int)= 0.00001159
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001159
ITry= 1 IFail=0 DXMaxC= 7.00D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.30735	-0.00051	0.00033	-0.00086	-0.00053	2.30682
R2	2.54958	-0.00044	0.00039	-0.00111	-0.00071	2.54887
R3	2.54890	-0.00041	0.00036	-0.00102	-0.00066	2.54824
R4	2.30732	-0.00051	0.00033	-0.00086	-0.00053	2.30679
R5	2.30346	-0.00053	0.00037	-0.00090	-0.00054	2.30292
R6	2.54903	-0.00042	0.00036	-0.00103	-0.00067	2.54836
R7	2.55142	-0.00029	0.00025	-0.00074	-0.00050	2.55092
R8	2.30341	-0.00053	0.00037	-0.00090	-0.00053	2.30288
R9	2.29610	-0.00051	0.00035	-0.00088	-0.00053	2.29557
R10	2.55151	-0.00029	0.00024	-0.00075	-0.00050	2.55100
R11	2.61668	-0.00021	0.00019	-0.00056	-0.00037	2.61630
R12	2.29610	-0.00051	0.00035	-0.00088	-0.00053	2.29557
R13	2.64605	-0.00020	0.00104	-0.00109	-0.00005	2.64600
R14	2.73983	-0.00019	-0.00066	-0.00025	-0.00092	2.73891
R15	2.61665	-0.00021	0.00018	-0.00055	-0.00037	2.61628
R16	2.73967	-0.00018	-0.00067	-0.00022	-0.00090	2.73877
R17	2.74294	-0.00069	0.00319	-0.00418	-0.00099	2.74195
A1	2.61281	-0.00003	0.00014	-0.00026	-0.00012	2.61269
A2	2.64440	0.00001	0.00007	-0.00007	-0.00000	2.64439
A3	2.61605	-0.00008	0.00006	-0.00035	-0.00029	2.61576
A4	2.71605	0.00003	-0.00035	0.00031	-0.00004	2.71601

A5	2.64151	0.00005	0.00013	0.00002	0.00014	2.64166
A6	2.77962	0.00009	-0.00001	0.00031	0.00029	2.77991
A7	2.71836	-0.00000	-0.00042	0.00025	-0.00017	2.71819
A8	2.77805	0.00010	0.00005	0.00033	0.00037	2.77842
A9	2.83216	0.00001	0.00033	-0.00026	0.00005	2.83221
A10	2.30759	-0.00010	-0.00068	0.00021	-0.00049	2.30710
A11	2.51753	0.00015	-0.00006	0.00039	0.00033	2.51786
A12	1.45754	-0.00006	0.00072	-0.00056	0.00016	1.45770
A13	2.83133	0.00002	0.00036	-0.00024	0.00010	2.83143
A14	2.30800	-0.00010	-0.00068	0.00017	-0.00052	2.30749
A15	1.45725	-0.00005	0.00070	-0.00052	0.00018	1.45743
A16	2.51744	0.00015	-0.00005	0.00037	0.00033	2.51777
A17	1.42621	0.00011	-0.00000	0.00048	0.00047	1.42667
A18	1.42659	0.00009	0.00002	0.00042	0.00043	1.42702
A19	2.87994	-0.00000	0.00026	0.00008	0.00032	2.88026
A20	2.88084	-0.00000	0.00023	0.00008	0.00029	2.88113
A21	3.14244	-0.00024	-0.00362	0.00033	-0.00331	3.13913
A22	3.14236	-0.00024	-0.00363	0.00034	-0.00331	3.13905
D1	0.07134	-0.00005	-0.00071	0.00076	0.00006	0.07140
D2	-0.06156	-0.00019	-0.00268	-0.00016	-0.00282	-0.06438
D3	-0.05697	-0.00010	-0.00158	-0.00143	-0.00300	-0.05998
D4	0.07082	-0.00005	-0.00061	0.00073	0.00013	0.07096
D5	0.08984	0.00018	0.00150	0.00081	0.00230	0.09214
D6	-0.05563	-0.00010	-0.00167	-0.00146	-0.00313	-0.05876
D7	0.08014	0.00019	0.00510	0.00056	0.00564	0.08577
D8	0.08851	0.00019	0.00152	0.00089	0.00240	0.09090
D9	0.08173	0.00019	0.00503	0.00062	0.00562	0.08735
D10	-0.61563	-0.00006	-0.00353	0.00030	-0.00324	-0.61886
D11	2.57521	0.00004	-0.00228	-0.00103	-0.00331	2.57190
D12	0.74996	-0.00005	0.00116	-0.00194	-0.00079	0.74917
D13	-2.41959	-0.00011	0.00054	-0.00139	-0.00087	-2.42046
D14	-2.42059	-0.00010	0.00043	-0.00115	-0.00073	-2.42132
D15	0.69305	-0.00016	-0.00020	-0.00060	-0.00081	0.69224
D16	2.40948	-0.00005	0.00037	0.00050	0.00086	2.41035
D17	-0.69541	0.00002	0.00131	-0.00049	0.00082	-0.69459
D18	-0.61768	-0.00006	-0.00338	0.00015	-0.00325	-0.62092
D19	2.57145	0.00004	-0.00232	-0.00076	-0.00309	2.56836
D20	-0.69544	0.00003	0.00131	-0.00049	0.00083	-0.69461
D21	2.41074	-0.00005	0.00051	0.00019	0.00070	2.41143
D22	0.67039	-0.00005	-0.00067	0.00011	-0.00057	0.66982

Item	Value	Threshold	Converged?
Maximum Force	0.000691	0.000450	NO
RMS Force	0.000239	0.000300	YES
Maximum Displacement	0.007000	0.001800	NO
RMS Displacement	0.002783	0.001200	NO

Predicted change in Energy=-6.481618D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Supporting Information file

Leave Link 103 at Fri Aug 21 19:40:31 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.621144	-0.673346	0.014334
2	6	0	3.006590	-1.727268	0.055827
3	6	0	3.619745	0.675169	-0.013595
4	6	0	1.854521	-2.428045	0.061249
5	6	0	3.006261	1.729686	-0.055321
6	6	0	0.644764	-2.575020	0.063740
7	6	0	1.852910	2.428465	-0.061358
8	6	0	-0.666001	-2.255378	0.019886
9	6	0	0.643240	2.575949	-0.064131
10	6	0	-1.730854	-1.672824	-0.028821
11	6	0	-0.667233	2.254873	-0.020680
12	6	0	-2.685862	-0.680270	-0.168840
13	6	0	-1.731972	1.672088	0.027772
14	6	0	-2.686047	0.678732	0.168338
15	6	0	-4.041019	-0.404323	-0.602516
16	6	0	-4.040189	0.401510	0.604119

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220717	0.000000			
3	C	1.348805	2.480420	0.000000		
4	C	2.490406	1.348473	3.570932	0.000000	
5	C	2.481431	3.458741	1.220701	4.315880	0.000000
6	C	3.532370	2.509375	4.406838	1.218655	4.911347
7	C	3.571220	4.314490	2.489585	4.858057	1.348534
8	C	4.569734	3.710541	5.191998	2.526768	5.419584
9	C	4.408173	4.910956	3.532011	5.150037	2.510001
10	C	5.444695	4.738513	5.843134	3.665159	5.832498
11	C	5.192868	5.418513	4.568775	5.319369	3.711008
12	C	6.309669	5.792295	6.451511	4.870599	6.182316
13	C	5.844407	5.831842	5.443936	5.447489	4.739311
14	C	6.452325	6.181231	6.308418	5.502753	5.792832
15	C	7.691659	7.200860	7.758830	6.268447	7.383601
16	C	7.758814	7.381695	7.689672	6.561151	7.200789

		6	7	8	9	10
6	C	0.000000				
7	C	5.148798	0.000000			
8	C	1.349889	5.318825	0.000000		

```
   9  C    5.152556   1.218631   5.006285   0.000000
  10  C    2.542850   5.446558   1.214765   4.867201   0.000000
  11  C    5.005630   2.526443   4.510434   1.349933   4.069172
  12  C    3.838912   5.502384   2.568350   4.657987   1.384489
  13  C    4.867041   3.664892   4.069563   2.543038   3.345391
  14  C    4.657483   4.869955   3.565337   3.838963   2.545797
  15  C    5.206956   6.561703   3.899300   5.578007   2.697236
  16  C    5.576785   6.267378   4.334228   5.206655   3.168044
                11         12         13         14         15
  11  C    0.000000
  12  C    3.565372   0.000000
  13  C    1.214765   2.546006   0.000000
  14  C    2.568182   1.400205   1.384477   0.000000
  15  C    4.335007   1.449370   3.168666   1.898202   0.000000
  16  C    3.898995   1.897871   2.697112   1.449295   1.450977
                16
  16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 1.52D-04
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.620925   -0.674559    0.012603
    2          6           0        3.006028   -1.728380    0.051489
    3          6           0        3.619965    0.674022   -0.011977
    4          6           0        1.853732   -2.428793    0.055190
    5          6           0        3.006823    1.728839   -0.051075
    6          6           0        0.643927   -2.575380    0.057336
    7          6           0        1.853700    2.428007   -0.055358
    8          6           0       -0.666735   -2.255203    0.014297
    9          6           0        0.644078    2.575891   -0.057746
   10          6           0       -1.731399   -1.672184   -0.032947
   11          6           0       -0.666500    2.255135   -0.015070
   12          6           0       -2.686086   -0.678974   -0.170485
   13          6           0       -1.731427    1.672578    0.031952
   14          6           0       -2.685824    0.679186    0.170066
   15          6           0       -4.041160   -0.401510   -0.603453
   16          6           0       -4.040049    0.401324    0.605179
---------------------------------------------------------------------
Rotational constants (GHZ):           0.8462479           0.3944465           0.2718532
```

Supporting Information file

Leave Link 202 at Fri Aug 21 19:40:31 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 717.6062848131 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074903768 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.5987944362 Hartrees.
Leave Link 301 at Fri Aug 21 19:40:32 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14214 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.17D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 19:40:32 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 19:40:32 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000054 0.000000 0.000001 Ang= 0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 19:40:33 2026, MaxMem= 805306368 cpu: 1.9 elap: 0.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981484875068
DIIS: error= 4.87D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981484875068 IErMin= 1 ErrMin= 4.87D-04
ErrMax= 4.87D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-04 BMatP= 1.10D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.87D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=1.99D-05 MaxDP=4.25D-04 OVMax= 9.48D-04

Cycle 2 Pass 1 IDiag 1:
RMSU= 1.97D-05 CP: 1.00D+00
E= -608.981529019781 Delta-E= -0.000044144714 Rises=F Damp=F
DIIS: error= 3.76D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981529019781 IErMin= 2 ErrMin= 3.76D-05
ErrMax= 3.76D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.82D-07 BMatP= 1.10D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.308D-01 0.103D+01
Coeff: -0.308D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.88D-06 MaxDP=1.50D-04 DE=-4.41D-05 OVMax= 3.36D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.84D-06 CP: 1.00D+00 1.03D+00
E= -608.981530579122 Delta-E= -0.000001559340 Rises=F Damp=F
DIIS: error= 1.98D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981530579122 IErMin= 3 ErrMin= 1.98D-05
ErrMax= 1.98D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-07 BMatP= 6.82D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.997D-02 0.187D+00 0.823D+00
Coeff: -0.997D-02 0.187D+00 0.823D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.30D-06 MaxDP=6.40D-05 DE=-1.56D-06 OVMax= 1.74D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 1.99D-06 CP: 1.00D+00 1.03D+00 1.19D+00
E= -608.981530704336 Delta-E= -0.000000125214 Rises=F Damp=F
DIIS: error= 2.66D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981530704336 IErMin= 3 ErrMin= 1.98D-05
ErrMax= 2.66D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-07 BMatP= 1.44D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.645D-03-0.112D+00 0.514D+00 0.597D+00
Coeff: 0.645D-03-0.112D+00 0.514D+00 0.597D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.45D-06 MaxDP=3.53D-05 DE=-1.25D-07 OVMax= 1.27D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 9.88D-07 CP: 1.00D+00 1.02D+00 1.37D+00 1.06D+00
E= -608.981530861839 Delta-E= -0.000000157504 Rises=F Damp=F
DIIS: error= 5.53D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981530861839 IErMin= 5 ErrMin= 5.53D-06
ErrMax= 5.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.62D-09 BMatP= 1.29D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.188D-02-0.781D-01 0.902D-01 0.255D+00 0.731D+00
Coeff: 0.188D-02-0.781D-01 0.902D-01 0.255D+00 0.731D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=6.73D-07 MaxDP=1.71D-05 DE=-1.58D-07 OVMax= 4.67D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.18D-07 CP: 1.00D+00 1.02D+00 1.45D+00 1.22D+00 1.07D+00
E= -608.981530879252 Delta-E= -0.000000017413 Rises=F Damp=F
DIIS: error= 1.42D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981530879252 IErMin= 6 ErrMin= 1.42D-06
ErrMax= 1.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-09 BMatP= 9.62D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.559D-03-0.110D-01-0.395D-01 0.195D-02 0.252D+00 0.796D+00
Coeff: 0.559D-03-0.110D-01-0.395D-01 0.195D-02 0.252D+00 0.796D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.27D-07 MaxDP=1.38D-05 DE=-1.74D-08 OVMax= 2.45D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.48D-07 CP: 1.00D+00 1.02D+00 1.47D+00 1.31D+00 1.24D+00
CP: 1.34D+00
E= -608.981530882359 Delta-E= -0.000000003107 Rises=F Damp=F
DIIS: error= 9.48D-07 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981530882359 IErMin= 7 ErrMin= 9.48D-07
ErrMax= 9.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-10 BMatP= 1.25D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.293D-03 0.158D-01-0.334D-01-0.641D-01-0.107D+00 0.241D+00
Coeff-Com: 0.948D+00
Coeff: -0.293D-03 0.158D-01-0.334D-01-0.641D-01-0.107D+00 0.241D+00
Coeff: 0.948D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.04D-07 MaxDP=9.33D-06 DE=-3.11D-09 OVMax= 1.62D-05

Cycle 8 Pass 1 IDiag 1:
RMSU= 8.32D-08 CP: 1.00D+00 1.02D+00 1.47D+00 1.35D+00 1.35D+00
CP: 1.68D+00 1.44D+00
E= -608.981530883060 Delta-E= -0.000000000700 Rises=F Damp=F
DIIS: error= 9.54D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981530883060 IErMin= 7 ErrMin= 9.48D-07
ErrMax= 9.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.58D-11 BMatP= 2.37D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.236D-03 0.105D-01-0.153D-01-0.380D-01-0.887D-01 0.481D-01
Coeff-Com: 0.560D+00 0.524D+00
Coeff: -0.236D-03 0.105D-01-0.153D-01-0.380D-01-0.887D-01 0.481D-01
Coeff: 0.560D+00 0.524D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.76D-08 MaxDP=2.11D-06 DE=-7.00D-10 OVMax= 3.99D-06

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.18D-08 CP: 1.00D+00 1.02D+00 1.47D+00 1.35D+00 1.37D+00
CP: 1.77D+00 1.59D+00 1.12D+00
E= -608.981530883213 Delta-E= -0.000000000153 Rises=F Damp=F
DIIS: error= 2.07D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981530883213 IErMin= 9 ErrMin= 2.07D-07
ErrMax= 2.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.44D-12 BMatP= 9.58D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.116D-04-0.931D-04 0.239D-02 0.155D-02-0.386D-02-0.373D-01
Coeff-Com: -0.300D-01 0.177D+00 0.890D+00
Coeff: -0.116D-04-0.931D-04 0.239D-02 0.155D-02-0.386D-02-0.373D-01
Coeff: -0.300D-01 0.177D+00 0.890D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.63D-08 MaxDP=1.36D-06 DE=-1.53D-10 OVMax= 2.83D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.12D-08 CP: 1.00D+00 1.02D+00 1.47D+00 1.35D+00 1.38D+00
CP: 1.83D+00 1.73D+00 1.37D+00 1.35D+00
E= -608.981530883226 Delta-E= -0.000000000013 Rises=F Damp=F

DIIS: error= 8.71D-08 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981530883226 IErMin=10 ErrMin= 8.71D-08
ErrMax= 8.71D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-12 BMatP= 7.44D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.364D-04-0.189D-02 0.381D-02 0.735D-02 0.140D-01-0.268D-01
Coeff-Com: -0.115D+00-0.582D-02 0.382D+00 0.742D+00
Coeff: 0.364D-04-0.189D-02 0.381D-02 0.735D-02 0.140D-01-0.268D-01
Coeff: -0.115D+00-0.582D-02 0.382D+00 0.742D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.99D-08 MaxDP=5.12D-07 DE=-1.34D-11 OVMax= 1.46D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 7.04D-09 CP: 1.00D+00 1.02D+00 1.46D+00 1.35D+00 1.37D+00
CP: 1.84D+00 1.78D+00 1.51D+00 1.45D+00 1.15D+00
E= -608.981530883229 Delta-E= -0.000000000003 Rises=F Damp=F
DIIS: error= 5.43D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981530883229 IErMin=11 ErrMin= 5.43D-08
ErrMax= 5.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.62D-13 BMatP= 1.69D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.125D-04-0.505D-03 0.564D-03 0.167D-02 0.497D-02-0.407D-03
Coeff-Com: -0.250D-01-0.329D-01-0.702D-01 0.188D+00 0.934D+00
Coeff: 0.125D-04-0.505D-03 0.564D-03 0.167D-02 0.497D-02-0.407D-03
Coeff: -0.250D-01-0.329D-01-0.702D-01 0.188D+00 0.934D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=7.86D-09 MaxDP=1.86D-07 DE=-2.73D-12 OVMax= 7.87D-07

SCF Done: E(RwB97XD) = -608.981530883 A.U. after 11 cycles
NFock= 11 Conv=0.79D-08 -V/T= 2.0045
KE= 6.062400375314D+02 PE=-2.846196658125D+03 EE= 9.133762952744D+02
Leave Link 502 at Fri Aug 21 19:48:04 2026, MaxMem= 805306368 cpu: 2710.3 elap: 451.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14214 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 19:48:05 2026, MaxMem= 805306368 cpu: 2.2 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 19:48:05 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Supporting Information file

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 19:56:25 2026, MaxMem= 805306368 cpu: 2999.7 elap: 500.1
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.51995985D+00-2.88711103D-03-5.41129412D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000026476	0.000082985	-0.000305987
2	6	-0.000075764	-0.000079040	0.000413196
3	6	0.000095902	-0.000065273	0.000310616
4	6	0.000082831	0.000004516	-0.000503254
5	6	-0.000127633	0.000038372	-0.000427881
6	6	-0.000052520	0.000065103	0.000349726
7	6	0.000107095	0.000041222	0.000526290
8	6	0.000041604	-0.000087507	-0.000236160
9	6	-0.000058946	-0.000097397	-0.000367517
10	6	-0.000025773	0.000126774	0.000304796
11	6	0.000039905	0.000100447	0.000230563
12	6	0.000109040	-0.000110010	-0.000190401
13	6	-0.000017488	-0.000130458	-0.000291650
14	6	0.000101753	0.000104734	0.000184077
15	6	-0.000112800	0.000348082	0.000424988
16	6	-0.000133682	-0.000342550	-0.000421399

Cartesian Forces: Max 0.000526290 RMS 0.000228542
Leave Link 716 at Fri Aug 21 19:56:25 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000426578 RMS 0.000079605
Search for a local minimum.
Step number 8 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)

Supporting Information file

RMS Force = .79605D-04 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 1 2 3 4 5
6 7 8
DE= -6.55D-06 DEPred=-6.48D-06 R= 1.01D+00
TightC=F SS= 1.41D+00 RLast= 1.34D-02 DXNew= 8.4853D-01 4.0069D-02
Trust test= 1.01D+00 RLast= 1.34D-02 DXMaxT set to 5.05D-01
ITU= 1 1 1 1 1 1 1 0
Eigenvalues --- 0.00716 0.01290 0.01554 0.01732 0.02369
Eigenvalues --- 0.02625 0.02913 0.03422 0.03422 0.03926
Eigenvalues --- 0.04047 0.06019 0.08167 0.08437 0.09356
Eigenvalues --- 0.15990 0.23880 0.24444 0.24735 0.24989
Eigenvalues --- 0.24994 0.24996 0.24998 0.25000 0.25000
Eigenvalues --- 0.25060 0.28164 0.31343 0.32172 0.40829
Eigenvalues --- 0.51321 0.53346 0.57380 0.57872 0.58159
Eigenvalues --- 0.58183 0.78668 0.79313 0.79696 0.81411
Eigenvalues --- 0.82169 0.92688
En-DIIS/RFO-DIIS/Sim-DIIS IScMMF= -3 using points: 8 7 6 5 4
RFO step: Lambda=-3.94495644D-06.
NNeg= 0 NGDIIS= 5 SimSw= 2.50D-01 Rises=F DC= -6.55D-06 SmlDif= 1.00D-05
NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj= 3.0
RMS Error= 0.2024303191D-02 NUsed= 5 OKEnD=F EnDIS=F
InvSVX: RCond= 2.47D-06 Info= 0 Equed=N FErr= 2.23D-13 BErr= 6.05D-17
DidBck=F Rises=F RFO-DIIS coefs: 1.86245 -0.66575 -0.40010 0.19083 0.01256
Iteration 1 RMS(Cart)= 0.00148293 RMS(Int)= 0.00000229
Iteration 2 RMS(Cart)= 0.00000213 RMS(Int)= 0.00000153
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000153
ITry= 1 IFail=0 DXMaxC= 4.56D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.30682	0.00007	-0.00047	0.00056	0.00009	2.30692
R2	2.54887	-0.00004	-0.00080	0.00043	-0.00036	2.54851
R3	2.54824	-0.00004	-0.00073	0.00037	-0.00036	2.54788
R4	2.30679	0.00007	-0.00046	0.00056	0.00010	2.30689
R5	2.30292	0.00005	-0.00047	0.00054	0.00006	2.30299
R6	2.54836	-0.00005	-0.00074	0.00037	-0.00037	2.54799
R7	2.55092	-0.00001	-0.00058	0.00032	-0.00026	2.55066
R8	2.30288	0.00005	-0.00047	0.00054	0.00007	2.30295
R9	2.29557	0.00005	-0.00049	0.00053	0.00004	2.29562
R10	2.55100	-0.00001	-0.00059	0.00032	-0.00027	2.55073
R11	2.61630	-0.00003	-0.00039	0.00012	-0.00027	2.61604
R12	2.29557	0.00005	-0.00049	0.00053	0.00004	2.29562
R13	2.64600	-0.00004	0.00066	-0.00024	0.00042	2.64643
R14	2.73891	0.00009	-0.00180	0.00154	-0.00025	2.73866
R15	2.61628	-0.00003	-0.00039	0.00013	-0.00026	2.61602
R16	2.73877	0.00010	-0.00178	0.00158	-0.00020	2.73857

R17	2.74195	-0.00043	0.00068	-0.00133	-0.00065	2.74130
A1	2.61269	-0.00004	-0.00006	-0.00011	-0.00017	2.61251
A2	2.64439	-0.00001	0.00007	-0.00010	-0.00003	2.64436
A3	2.61576	-0.00009	-0.00032	-0.00020	-0.00052	2.61523
A4	2.71601	0.00003	-0.00028	0.00021	-0.00008	2.71593
A5	2.64166	0.00003	0.00029	-0.00002	0.00027	2.64193
A6	2.77991	0.00008	0.00040	0.00011	0.00051	2.78042
A7	2.71819	-0.00001	-0.00049	0.00015	-0.00034	2.71785
A8	2.77842	0.00010	0.00054	0.00014	0.00068	2.77909
A9	2.83221	-0.00001	0.00019	-0.00020	-0.00001	2.83220
A10	2.30710	-0.00003	-0.00081	0.00014	-0.00067	2.30643
A11	2.51786	0.00009	0.00073	-0.00001	0.00072	2.51858
A12	1.45770	-0.00006	0.00008	-0.00015	-0.00006	1.45763
A13	2.83143	-0.00000	0.00027	-0.00018	0.00009	2.83152
A14	2.30749	-0.00004	-0.00084	0.00012	-0.00072	2.30677
A15	1.45743	-0.00005	0.00010	-0.00012	-0.00002	1.45742
A16	2.51777	0.00009	0.00073	-0.00002	0.00072	2.51849
A17	1.42667	0.00008	0.00008	0.00026	0.00034	1.42701
A18	1.42702	0.00006	0.00005	0.00021	0.00026	1.42728
A19	2.88026	0.00000	0.00009	-0.00011	-0.00002	2.88024
A20	2.88113	-0.00000	0.00002	-0.00013	-0.00012	2.88101
A21	3.13913	0.00000	-0.00068	0.00014	-0.00054	3.13859
A22	3.13905	0.00000	-0.00067	0.00018	-0.00050	3.13855
D1	0.07140	0.00004	0.00130	0.00075	0.00206	0.07345
D2	-0.06438	-0.00006	-0.00218	-0.00059	-0.00278	-0.06716
D3	-0.05998	-0.00007	-0.00364	-0.00090	-0.00453	-0.06451
D4	0.07096	0.00004	0.00147	0.00073	0.00220	0.07316
D5	0.09214	0.00011	0.00389	0.00089	0.00478	0.09692
D6	-0.05876	-0.00007	-0.00387	-0.00091	-0.00477	-0.06353
D7	0.08577	0.00004	0.00417	-0.00029	0.00388	0.08966
D8	0.09090	0.00011	0.00402	0.00096	0.00499	0.09589
D9	0.08735	0.00004	0.00412	-0.00034	0.00378	0.09113
D10	-0.61886	-0.00007	-0.00577	-0.00028	-0.00605	-0.62492
D11	2.57190	-0.00002	-0.00578	0.00048	-0.00530	2.56659
D12	0.74917	-0.00005	0.00023	0.00035	0.00058	0.74975
D13	-2.42046	-0.00008	0.00014	-0.00016	-0.00001	-2.42047
D14	-2.42132	-0.00008	0.00027	-0.00010	0.00017	-2.42115
D15	0.69224	-0.00011	0.00018	-0.00061	-0.00042	0.69182
D16	2.41035	-0.00008	0.00055	-0.00080	-0.00025	2.41010
D17	-0.69459	-0.00004	0.00057	-0.00023	0.00033	-0.69425
D18	-0.62092	-0.00007	-0.00571	-0.00026	-0.00597	-0.62689
D19	2.56836	-0.00001	-0.00551	0.00060	-0.00490	2.56346
D20	-0.69461	-0.00004	0.00057	-0.00023	0.00034	-0.69427
D21	2.41143	-0.00008	0.00039	-0.00086	-0.00047	2.41096
D22	0.66982	-0.00002	0.00018	-0.00034	-0.00017	0.66965

Item	Value	Threshold	Converged?
Maximum Force	0.000427	0.000450	YES
RMS Force	0.000080	0.000300	YES

Supporting Information file

Maximum Displacement 0.004565 0.001800 NO
RMS Displacement 0.001483 0.001200 NO
Predicted change in Energy=-1.950728D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 19:56:25 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.621585	-0.673243	0.013425
2	6	0	3.006759	-1.727084	0.054430
3	6	0	3.620302	0.675114	-0.012769
4	6	0	1.854674	-2.427473	0.059238
5	6	0	3.006358	1.729444	-0.054000
6	6	0	0.644839	-2.574046	0.063509
7	6	0	1.853089	2.427983	-0.059335
8	6	0	-0.665908	-2.254692	0.021351
9	6	0	0.643319	2.574913	-0.063851
10	6	0	-1.730931	-1.672323	-0.026406
11	6	0	-0.667143	2.254181	-0.022033
12	6	0	-2.686312	-0.680566	-0.168123
13	6	0	-1.732018	1.671521	0.025475
14	6	0	-2.686516	0.679000	0.167706
15	6	0	-4.041381	-0.405050	-0.601905
16	6	0	-4.040716	0.402319	0.603288

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220767	0.000000			
3	C	1.348613	2.480223	0.000000		
4	C	2.490259	1.348283	3.570528	0.000000	
5	C	2.481120	3.458228	1.220753	4.314991	0.000000
6	C	3.532219	2.509201	4.406386	1.218689	4.910254
7	C	3.570781	4.313755	2.489530	4.856904	1.348338
8	C	4.569862	3.710518	5.191967	2.526782	5.418907
9	C	4.407557	4.909889	3.531893	5.148436	2.509754
10	C	5.445106	4.738696	5.843488	3.665263	5.832211
11	C	5.192712	5.417921	4.568996	5.318275	3.710927
12	C	6.310513	5.792736	6.452549	4.870722	6.182852
13	C	5.844581	5.831583	5.444412	5.446765	4.739396
14	C	6.453255	6.181864	6.309400	5.503121	5.793219
15	C	7.692308	7.201029	7.759846	6.268235	7.384232

```
  16  C    7.759873   7.382581   7.690588   6.561962   7.201009
             6          7          8          9          10
   6  C    0.000000
   7  C    5.147354   0.000000
   8  C    1.349749   5.317829   0.000000
   9  C    5.150534   1.218668   5.004639   0.000000
  10  C    2.542730   5.445990   1.214787   4.865951   0.000000
  11  C    5.004037   2.526493   4.509081   1.349788   4.068059
  12  C    3.838683   5.502824   2.568230   4.657838   1.384348
  13  C    4.865772   3.665027   4.068385   2.542896   3.344247
  14  C    4.657369   4.870164   3.565224   3.838737   2.545495
  15  C    5.206532   6.562411   3.899158   5.578180   2.697287
  16  C    5.577144   6.267322   4.334476   5.206287   3.167927
             11         12         13         14         15
  11  C    0.000000
  12  C    3.565267   0.000000
  13  C    1.214787   2.545677   0.000000
  14  C    2.568085   1.400429   1.384339   0.000000
  15  C    4.335117   1.449237   3.168424   1.898190   0.000000
  16  C    3.898899   1.897926   2.697189   1.449187   1.450633
             16
  16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 7.13D-05
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.621366   -0.674452    0.011736
    2          6           0        3.006198   -1.728189    0.050186
    3          6           0        3.620521    0.673966   -0.011178
    4          6           0        1.853886   -2.428213    0.053307
    5          6           0        3.006919    1.728592   -0.049836
    6          6           0        0.644003   -2.574402    0.057238
    7          6           0        1.853878    2.427518   -0.053455
    8          6           0       -0.666641   -2.254520    0.015876
    9          6           0        0.644156    2.574851   -0.057597
   10          6           0       -1.731476   -1.671691   -0.030449
   11          6           0       -0.666410    2.254445   -0.016541
   12          6           0       -2.686536   -0.679281   -0.169739
   13          6           0       -1.731474    1.672018    0.029565
   14          6           0       -2.686292    0.679464    0.169396
```

```
    15        6        0       -4.041520   -0.402271   -0.602831
    16        6        0       -4.040577    0.402164    0.604323
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8467271           0.3943751           0.2718574
 Leave Link  202 at Fri Aug 21 19:56:25 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.6441226232 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0074916892 Hartrees.
 Nuclear repulsion after empirical dispersion term =      717.6366309340 Hartrees.
 Leave Link  301 at Fri Aug 21 19:56:25 2026, MaxMem=    805306368 cpu:                  0.5 elap:
0.1
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33578.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  4.20D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=           5 IRanWt=          -1 IRanGd=           0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=           0 NUsed=           0 NTot=          32
 NSgBfM=   562   562   562   562   562 MxSgAt=    16 MxSgA2=    16.
 Leave Link  302 at Fri Aug 21 19:56:26 2026, MaxMem=    805306368 cpu:                  6.9 elap:
1.2
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
```

Supporting Information file

```
 Leave Link  303 at Fri Aug 21 19:56:27 2026, MaxMem=    805306368 cpu:                1.0 elap:
0.2
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca.chk"
 B after Tr=    -0.000000   -0.000000    0.000000
       Rot=    1.000000    0.000025    0.000001   -0.000000 Ang=   0.00 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Leave Link  401 at Fri Aug 21 19:56:27 2026, MaxMem=    805306368 cpu:                3.9 elap:
0.7
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804634234 LenY=   804301882
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -608.981520241532
 DIIS: error= 2.60D-04 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -608.981520241532     IErMin= 1 ErrMin= 2.60D-04
 ErrMax= 2.60D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.24D-05 BMatP= 3.24D-05
 IDIUse=3 WtCom= 9.97D-01 WtEn= 2.60D-03
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=     0.960 Goal=   None    Shift=    0.000
 RMSDP=2.35D-05 MaxDP=6.26D-04             OVMax= 5.20D-04

 Cycle   2  Pass 1  IDiag  1:
 RMSU=  2.28D-05    CP:  9.99D-01
 E= -608.981533431867     Delta-E=       -0.000013190335 Rises=F Damp=F
 DIIS: error= 1.98D-05 at cycle   2 NSaved=   2.
 NSaved= 2 IEnMin= 2 EnMin= -608.981533431867     IErMin= 2 ErrMin= 1.98D-05
 ErrMax= 1.98D-05  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-07 BMatP= 3.24D-05
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: -0.301D-01 0.103D+01
```

Coeff: -0.301D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.73D-06 MaxDP=1.11D-04 DE=-1.32D-05 OVMax= 1.96D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 3.54D-06 CP: 9.99D-01 1.13D+00
E= -608.981533894336 Delta-E= -0.000000462469 Rises=F Damp=F
DIIS: error= 1.57D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981533894336 IErMin= 3 ErrMin= 1.57D-05
ErrMax= 1.57D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.62D-08 BMatP= 2.23D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.147D-01 0.344D+00 0.670D+00
Coeff: -0.147D-01 0.344D+00 0.670D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.53D-06 MaxDP=4.92D-05 DE=-4.62D-07 OVMax= 1.02D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 1.40D-06 CP: 9.99D-01 1.15D+00 1.07D+00
E= -608.981533976241 Delta-E= -0.000000081905 Rises=F Damp=F
DIIS: error= 1.51D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981533976241 IErMin= 4 ErrMin= 1.51D-05
ErrMax= 1.51D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-08 BMatP= 8.62D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.828D-03-0.119D+00 0.394D+00 0.724D+00
Coeff: 0.828D-03-0.119D+00 0.394D+00 0.724D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.04D-06 MaxDP=2.74D-05 DE=-8.19D-08 OVMax= 9.87D-05

Cycle 5 Pass 1 IDiag 1:
RMSU= 5.54D-07 CP: 9.99D-01 1.17D+00 1.29D+00 1.10D+00
E= -608.981534031807 Delta-E= -0.000000055566 Rises=F Damp=F
DIIS: error= 4.24D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981534031807 IErMin= 5 ErrMin= 4.24D-06
ErrMax= 4.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.78D-09 BMatP= 3.96D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.214D-02-0.989D-01 0.120D+00 0.359D+00 0.619D+00
Coeff: 0.214D-02-0.989D-01 0.120D+00 0.359D+00 0.619D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.66D-07 MaxDP=1.06D-05 DE=-5.56D-08 OVMax= 3.87D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.27D-07 CP: 9.99D-01 1.17D+00 1.36D+00 1.17D+00 1.05D+00
E= -608.981534040992 Delta-E= -0.000000009185 Rises=F Damp=F
DIIS: error= 3.09D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981534040992 IErMin= 6 ErrMin= 3.09D-06
ErrMax= 3.09D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.14D-10 BMatP= 4.78D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.549D-03-0.615D-02-0.488D-01-0.510D-01 0.206D+00 0.899D+00

Coeff: 0.549D-03-0.615D-02-0.488D-01-0.510D-01 0.206D+00 0.899D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.65D-07 MaxDP=9.93D-06 DE=-9.19D-09 OVMax= 3.91D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.14D-07 CP: 9.99D-01 1.17D+00 1.39D+00 1.27D+00 1.27D+00
CP: 1.14D+00
E= -608.981534044533 Delta-E= -0.000000003541 Rises=F Damp=F
DIIS: error= 1.49D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981534044533 IErMin= 7 ErrMin= 1.49D-06
ErrMax= 1.49D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-10 BMatP= 7.14D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.412D-03 0.233D-01-0.396D-01-0.105D+00-0.112D+00 0.212D+00
Coeff-Com: 0.102D+01
Coeff: -0.412D-03 0.233D-01-0.396D-01-0.105D+00-0.112D+00 0.212D+00
Coeff: 0.102D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.41D-07 MaxDP=5.37D-06 DE=-3.54D-09 OVMax= 2.83D-05

Cycle 8 Pass 1 IDiag 1:
RMSU= 6.90D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.29D+00 1.40D+00
CP: 1.46D+00 1.41D+00
E= -608.981534045836 Delta-E= -0.000000001302 Rises=F Damp=F
DIIS: error= 7.98D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981534045836 IErMin= 8 ErrMin= 7.98D-07
ErrMax= 7.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.98D-11 BMatP= 1.71D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.350D-03 0.139D-01-0.104D-01-0.449D-01-0.103D+00-0.863D-01
Coeff-Com: 0.531D+00 0.700D+00
Coeff: -0.350D-03 0.139D-01-0.104D-01-0.449D-01-0.103D+00-0.863D-01
Coeff: 0.531D+00 0.700D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.43D-08 MaxDP=1.15D-06 DE=-1.30D-09 OVMax= 1.37D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.42D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.29D+00 1.43D+00
CP: 1.54D+00 1.67D+00 1.25D+00
E= -608.981534046165 Delta-E= -0.000000000330 Rises=F Damp=F
DIIS: error= 5.01D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981534046165 IErMin= 9 ErrMin= 5.01D-07
ErrMax= 5.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-11 BMatP= 6.98D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.408D-04-0.387D-03 0.649D-02 0.901D-02-0.147D-01-0.979D-01
Coeff-Com: -0.565D-01 0.318D+00 0.836D+00
Coeff: -0.408D-04-0.387D-03 0.649D-02 0.901D-02-0.147D-01-0.979D-01
Coeff: -0.565D-01 0.318D+00 0.836D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.77D-08 MaxDP=8.02D-07 DE=-3.30D-10 OVMax= 8.42D-06

Supporting Information file

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.44D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.29D+00 1.43D+00
CP: 1.57D+00 1.80D+00 1.60D+00 1.41D+00
E= -608.981534046282 Delta-E= -0.000000000117 Rises=F Damp=F
DIIS: error= 2.51D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981534046282 IErMin=10 ErrMin= 2.51D-07
ErrMax= 2.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.79D-12 BMatP= 1.94D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.135D-03-0.643D-02 0.816D-02 0.254D-01 0.402D-01-0.150D-01
Coeff-Com: -0.286D+00-0.130D+00 0.456D+00 0.907D+00
Coeff: 0.135D-03-0.643D-02 0.816D-02 0.254D-01 0.402D-01-0.150D-01
Coeff: -0.286D+00-0.130D+00 0.456D+00 0.907D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.65D-08 MaxDP=1.06D-06 DE=-1.17D-10 OVMax= 7.09D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.19D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.27D+00 1.42D+00
CP: 1.60D+00 1.86D+00 1.91D+00 1.81D+00 1.49D+00
E= -608.981534046327 Delta-E= -0.000000000044 Rises=F Damp=F
DIIS: error= 8.03D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981534046327 IErMin=11 ErrMin= 8.03D-08
ErrMax= 8.03D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.72D-13 BMatP= 6.79D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.115D-04-0.158D-03-0.903D-03-0.792D-03 0.504D-02 0.175D-01
Coeff-Com: -0.305D-02-0.651D-01-0.129D+00 0.662D-01 0.111D+01
Coeff: 0.115D-04-0.158D-03-0.903D-03-0.792D-03 0.504D-02 0.175D-01
Coeff: -0.305D-02-0.651D-01-0.129D+00 0.662D-01 0.111D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.26D-08 MaxDP=5.19D-07 DE=-4.43D-11 OVMax= 2.15D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.30D-09 CP: 9.99D-01 1.17D+00 1.40D+00 1.27D+00 1.41D+00
CP: 1.61D+00 1.85D+00 1.97D+00 1.95D+00 1.94D+00
CP: 1.46D+00
E= -608.981534046337 Delta-E= -0.000000000010 Rises=F Damp=F
DIIS: error= 2.51D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981534046337 IErMin=12 ErrMin= 2.51D-08
ErrMax= 2.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.82D-13 BMatP= 5.72D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.186D-04 0.106D-02-0.185D-02-0.482D-02-0.487D-02 0.111D-01
Coeff-Com: 0.478D-01-0.828D-02-0.132D+00-0.131D+00 0.487D+00 0.736D+00
Coeff: -0.186D-04 0.106D-02-0.185D-02-0.482D-02-0.487D-02 0.111D-01
Coeff: 0.478D-01-0.828D-02-0.132D+00-0.131D+00 0.487D+00 0.736D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.34D-09 MaxDP=2.11D-07 DE=-1.00D-11 OVMax= 5.85D-07

SCF Done: E(RwB97XD) = -608.981534046 A.U. after 12 cycles

```
          NFock= 12  Conv=0.53D-08     -V/T= 2.0045
 KE= 6.062426096206D+02 PE=-2.846274015989D+03 EE= 9.134132413882D+02
 Leave Link  502 at Fri Aug 21 20:05:08 2026, MaxMem=    805306368 cpu:             3122.5 elap:
520.6
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33578.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 Leave Link  701 at Fri Aug 21 20:05:08 2026, MaxMem=    805306368 cpu:                2.3 elap:
0.4
 (Enter /home/user/gauss16/g16/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link  702 at Fri Aug 21 20:05:09 2026, MaxMem=    805306368 cpu:                0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l703.exe)
 Integral derivatives from FoFJK, PRISM(SPDF).
 Compute integral first derivatives, UseDBF=F ICtDFT=          0.
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=         800
        NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
        wScrn=  0.000000 ICntrl=      2527 IOpCl=  0 I1Cent=          0 NGrid=          0
        NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 Leave Link  703 at Fri Aug 21 20:12:29 2026, MaxMem=    805306368 cpu:             2641.9 elap:
440.4
 (Enter /home/user/gauss16/g16/l716.exe)
 Dipole        = 1.51933063D+00-2.59526006D-03-4.54353626D-04
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
     1        6          0.000014453   -0.000076431   -0.000281433
     2        6          0.000057539   -0.000000858    0.000364959
     3        6          0.000076187    0.000092428    0.000284321
     4        6         -0.000034635   -0.000054553   -0.000419566
     5        6          0.000011496   -0.000035296   -0.000375863
     6        6          0.000021507    0.000022913    0.000350701
     7        6         -0.000013825    0.000094932    0.000438757
     8        6         -0.000010571   -0.000053761   -0.000258083
     9        6          0.000017045   -0.000051870   -0.000365379
    10        6         -0.000045238    0.000025222    0.000216794
```

```
    11        6       -0.000012636   0.000065345   0.000250789
    12        6        0.000170463   0.000045910  -0.000017219
    13        6       -0.000038542  -0.000028629  -0.000201681
    14        6        0.000160635  -0.000049319   0.000011899
    15        6       -0.000181603   0.000278616   0.000242923
    16        6       -0.000192274  -0.000274650  -0.000241917
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.000438757 RMS     0.000189954
 Leave Link  716 at Fri Aug 21 20:12:29 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000303081 RMS     0.000072937
 Search for a local minimum.
 Step number   9 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .72937D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                      6    7    8    9
 DE= -3.16D-06 DEPred=-1.95D-06 R= 1.62D+00
 TightC=F SS=  1.41D+00  RLast= 1.64D-02 DXNew= 8.4853D-01 4.9113D-02
 Trust test= 1.62D+00 RLast= 1.64D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  1  1  1  1  0
    Eigenvalues ---    0.00419   0.01290   0.01571   0.01731   0.02291
    Eigenvalues ---    0.02625   0.02821   0.03355   0.03422   0.03926
    Eigenvalues ---    0.04047   0.06567   0.08079   0.08436   0.09389
    Eigenvalues ---    0.13340   0.23546   0.24440   0.24712   0.24988
    Eigenvalues ---    0.24995   0.24996   0.25000   0.25000   0.25004
    Eigenvalues ---    0.25099   0.28166   0.33023   0.33856   0.44130
    Eigenvalues ---    0.51321   0.54180   0.57379   0.58091   0.58166
    Eigenvalues ---    0.58218   0.78667   0.79284   0.79696   0.81395
    Eigenvalues ---    0.82168   0.97740
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:     9    8    7    6    5    4
 RFO step:  Lambda=-5.44266118D-06.
 NNeg= 0 NGDIIS= 6 SimSw=  2.50D-01 Rises=F DC= -3.16D-06 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.3713657610D-02 NUsed= 6 OKEnD=F EnDIS=F
 InvSVX:  RCond= 7.49D-08 Info=          0 Equed=N FErr=  9.81D-12 BErr=  4.13D-17
 DIIS inversion failure, remove point   6.
 InvSVX:  RCond= 9.04D-08 Info=          0 Equed=N FErr=  7.74D-12 BErr=  2.72D-17
 DIIS inversion failure, remove point   5.
 InvSVX:  RCond= 1.19D-07 Info=          0 Equed=N FErr=  5.07D-12 BErr=  3.67D-17
```

Supporting Information file

Old DIIS coefficients: 3.33103 -2.83973 0.49672 0.01198 0.00000
Old DIIS coefficients: 0.00000
RFO-DIIS uses 4 points instead of 6
DidBck=F Rises=F RFO-DIIS coefs: 2.60255 -2.00000 0.38809 0.00936 0.00000
RFO-DIIS coefs: 0.00000
Iteration 1 RMS(Cart)= 0.00175225 RMS(Int)= 0.00000613
Iteration 2 RMS(Cart)= 0.00000487 RMS(Int)= 0.00000363
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000363
ITry= 1 IFail=0 DXMaxC= 5.97D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.30692	0.00006	0.00036	-0.00033	0.00003	2.30694
R2	2.54851	0.00012	-0.00029	0.00018	-0.00011	2.54840
R3	2.54788	0.00010	-0.00031	0.00013	-0.00017	2.54771
R4	2.30689	0.00006	0.00036	-0.00033	0.00003	2.30692
R5	2.30299	0.00005	0.00031	-0.00031	-0.00000	2.30299
R6	2.54799	0.00009	-0.00032	0.00012	-0.00020	2.54779
R7	2.55066	0.00007	-0.00022	0.00006	-0.00016	2.55050
R8	2.30295	0.00005	0.00032	-0.00031	0.00001	2.30296
R9	2.29562	0.00007	0.00027	-0.00024	0.00003	2.29565
R10	2.55073	0.00007	-0.00023	0.00005	-0.00018	2.55055
R11	2.61604	0.00003	-0.00027	0.00003	-0.00024	2.61579
R12	2.29562	0.00007	0.00027	-0.00024	0.00003	2.29565
R13	2.64643	-0.00008	0.00064	-0.00063	0.00001	2.64643
R14	2.73866	0.00017	0.00004	0.00049	0.00053	2.73919
R15	2.61602	0.00004	-0.00027	0.00004	-0.00023	2.61579
R16	2.73857	0.00017	0.00011	0.00050	0.00061	2.73917
R17	2.74130	-0.00030	-0.00080	-0.00138	-0.00217	2.73912
A1	2.61251	-0.00002	-0.00024	-0.00004	-0.00028	2.61223
A2	2.64436	-0.00002	-0.00006	-0.00008	-0.00015	2.64422
A3	2.61523	-0.00006	-0.00072	-0.00035	-0.00107	2.61416
A4	2.71593	0.00002	-0.00009	0.00006	-0.00004	2.71589
A5	2.64193	0.00002	0.00036	0.00020	0.00056	2.64248
A6	2.78042	0.00004	0.00069	0.00023	0.00091	2.78133
A7	2.71785	-0.00001	-0.00044	-0.00016	-0.00061	2.71725
A8	2.77909	0.00006	0.00092	0.00038	0.00129	2.78038
A9	2.83220	-0.00004	-0.00005	-0.00025	-0.00031	2.83189
A10	2.30643	0.00002	-0.00085	0.00006	-0.00080	2.30563
A11	2.51858	0.00002	0.00099	0.00008	0.00107	2.51965
A12	1.45763	-0.00004	-0.00016	-0.00014	-0.00030	1.45733
A13	2.83152	-0.00003	0.00008	-0.00017	-0.00009	2.83143
A14	2.30677	0.00002	-0.00092	0.00001	-0.00092	2.30585
A15	1.45742	-0.00004	-0.00010	-0.00010	-0.00020	1.45722
A16	2.51849	0.00002	0.00099	0.00008	0.00107	2.51956
A17	1.42701	0.00004	0.00038	0.00015	0.00053	1.42754
A18	1.42728	0.00003	0.00027	0.00011	0.00038	1.42766
A19	2.88024	-0.00000	-0.00015	-0.00020	-0.00035	2.87989

A20	2.88101	-0.00001	-0.00028	-0.00030	-0.00059	2.88042
A21	3.13859	0.00008	0.00038	0.00097	0.00136	3.13995
A22	3.13855	0.00008	0.00045	0.00088	0.00132	3.13988
D1	0.07345	0.00006	0.00321	0.00256	0.00577	0.07922
D2	-0.06716	-0.00002	-0.00330	-0.00233	-0.00562	-0.07278
D3	-0.06451	-0.00005	-0.00598	-0.00342	-0.00939	-0.07391
D4	0.07316	0.00006	0.00340	0.00261	0.00601	0.07916
D5	0.09692	0.00007	0.00660	0.00400	0.01060	0.10752
D6	-0.06353	-0.00006	-0.00630	-0.00360	-0.00990	-0.07343
D7	0.08966	-0.00002	0.00395	0.00065	0.00460	0.09426
D8	0.09589	0.00008	0.00689	0.00419	0.01108	0.10697
D9	0.09113	-0.00002	0.00378	0.00051	0.00430	0.09543
D10	-0.62492	-0.00005	-0.00817	-0.00317	-0.01134	-0.63626
D11	2.56659	-0.00003	-0.00695	-0.00296	-0.00990	2.55669
D12	0.74975	-0.00005	0.00116	0.00005	0.00121	0.75096
D13	-2.42047	-0.00006	0.00024	-0.00020	0.00004	-2.42043
D14	-2.42115	-0.00006	0.00048	-0.00007	0.00041	-2.42074
D15	0.69182	-0.00007	-0.00043	-0.00032	-0.00076	0.69106
D16	2.41010	-0.00008	-0.00072	-0.00038	-0.00110	2.40900
D17	-0.69425	-0.00006	0.00022	-0.00022	-0.00000	-0.69426
D18	-0.62689	-0.00005	-0.00803	-0.00303	-0.01107	-0.63795
D19	2.56346	-0.00002	-0.00640	-0.00260	-0.00900	2.55445
D20	-0.69427	-0.00006	0.00023	-0.00022	0.00001	-0.69426
D21	2.41096	-0.00008	-0.00101	-0.00054	-0.00156	2.40940
D22	0.66965	-0.00002	-0.00009	-0.00015	-0.00024	0.66941

Item	Value	Threshold	Converged?
Maximum Force	0.000303	0.000450	YES
RMS Force	0.000073	0.000300	YES
Maximum Displacement	0.005971	0.001800	NO
RMS Displacement	0.001752	0.001200	NO

Predicted change in Energy=-2.546054D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 20:12:29 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.622483	-0.673185	0.012360
2	6	0	3.007218	-1.726778	0.053555
3	6	0	3.621458	0.675154	-0.011833
4	6	0	1.854872	-2.426569	0.056876
5	6	0	3.006639	1.728988	-0.053240
6	6	0	0.644974	-2.572529	0.063471

7	6	0	1.853331	2.427268	-0.056935
8	6	0	-0.665890	-2.253908	0.022075
9	6	0	0.643452	2.573256	-0.063764
10	6	0	-1.731113	-1.671677	-0.023246
11	6	0	-0.667151	2.253408	-0.022641
12	6	0	-2.686879	-0.680793	-0.167209
13	6	0	-1.732150	1.670754	0.022532
14	6	0	-2.687122	0.679179	0.166986
15	6	0	-4.042240	-0.405414	-0.601099
16	6	0	-4.041883	0.402845	0.602112

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220781	0.000000			
3	C	1.348556	2.480090	0.000000		
4	C	2.490138	1.348191	3.570187	0.000000	
5	C	2.480726	3.457416	1.220772	4.313624	0.000000
6	C	3.532093	2.509101	4.405970	1.218688	4.908577
7	C	3.570365	4.312744	2.489621	4.855172	1.348231
8	C	4.570441	3.710873	5.192486	2.526908	5.418173
9	C	4.406790	4.908304	3.531856	5.145906	2.509492
10	C	5.446031	4.739274	5.844465	3.665457	5.831956
11	C	5.192989	5.417442	4.569811	5.316871	3.711157
12	C	6.311921	5.793579	6.454289	4.870878	6.183540
13	C	5.845190	5.831449	5.445505	5.445729	4.739752
14	C	6.454759	6.182799	6.311115	5.503409	5.793920
15	C	7.693895	7.202044	7.761903	6.268487	7.385290
16	C	7.761968	7.384174	7.692716	6.563123	7.202069

		6	7	8	9	10
6	C	0.000000				
7	C	5.145152	0.000000			
8	C	1.349666	5.316590	0.000000		
9	C	5.147358	1.218674	5.002325	0.000000	
10	C	2.542606	5.445247	1.214804	4.864119	0.000000
11	C	5.001876	2.526704	4.507538	1.349694	4.066732
12	C	3.838375	5.503245	2.568056	4.657321	1.384219
13	C	4.863933	3.665283	4.066925	2.542723	3.342744
14	C	4.656950	4.870489	3.565022	3.838423	2.544929
15	C	5.206536	6.563380	3.899361	5.578254	2.697896
16	C	5.577599	6.267868	4.334986	5.206384	3.167707

		11	12	13	14	15
11	C	0.000000				
12	C	3.565072	0.000000			
13	C	1.214804	2.545050	0.000000		
14	C	2.567963	1.400433	1.384218	0.000000	
15	C	4.335341	1.449517	3.167950	1.898063	0.000000
16	C	3.899194	1.897936	2.697846	1.449507	1.449482

Supporting Information file

```
                16
  16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 5.38D-05
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.622268   -0.674369    0.010709
     2          6           0        3.006667   -1.727862    0.049387
     3          6           0        3.621674    0.674024   -0.010255
     4          6           0        1.854098   -2.427291    0.051045
     5          6           0        3.007190    1.728150   -0.049131
     6          6           0        0.644153   -2.572880    0.057303
     7          6           0        1.854105    2.426805   -0.051141
     8          6           0       -0.666610   -2.253742    0.016684
     9          6           0        0.644273    2.573196   -0.057608
    10          6           0       -1.731647   -1.671063   -0.027231
    11          6           0       -0.666432    2.253669   -0.017237
    12          6           0       -2.687097   -0.679533   -0.168810
    13          6           0       -1.731616    1.671248    0.026552
    14          6           0       -2.686903    0.679636    0.168641
    15          6           0       -4.042375   -0.402683   -0.602025
    16          6           0       -4.041748    0.402693    0.603118
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8474306           0.3942233           0.2718438
 Leave Link  202 at Fri Aug 21 20:12:29 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons        48 beta electrons
       nuclear repulsion energy       717.6774361154 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000  wLong=    0.200000  cFull=    0.222036  cShort=    0.000000  cLong=
0.777964
```

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074931591 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.6699429562 Hartrees.
Leave Link 301 at Fri Aug 21 20:12:29 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33582.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.29D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 20:12:30 2026, MaxMem= 805306368 cpu: 3.3 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 20:12:30 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000019 0.000002 -0.000003 Ang= 0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 20:12:30 2026, MaxMem= 805306368 cpu: 1.9 elap: 0.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Supporting Information file

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981514296594
DIIS: error= 2.70D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981514296594 IErMin= 1 ErrMin= 2.70D-04
ErrMax= 2.70D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.45D-05 BMatP= 5.45D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 2.70D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=6.38D-05 MaxDP=1.65D-03 OVMax= 7.06D-04

Cycle 2 Pass 1 IDiag 1:
RMSU= 6.15D-05 CP: 9.98D-01
E= -608.981536952752 Delta-E= -0.000022656157 Rises=F Damp=F
DIIS: error= 2.75D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981536952752 IErMin= 2 ErrMin= 2.75D-05
ErrMax= 2.75D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.33D-07 BMatP= 5.45D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.297D-01 0.103D+01
Coeff: -0.297D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=7.97D-06 MaxDP=2.28D-04 DE=-2.27D-05 OVMax= 3.44D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 4.95D-06 CP: 9.98D-01 1.10D+00
E= -608.981537837741 Delta-E= -0.000000884990 Rises=F Damp=F
DIIS: error= 2.13D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981537837741 IErMin= 3 ErrMin= 2.13D-05
ErrMax= 2.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.35D-07 BMatP= 4.33D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.177D-01 0.420D+00 0.598D+00
Coeff: -0.177D-01 0.420D+00 0.598D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.40D-06 MaxDP=8.27D-05 DE=-8.85D-07 OVMax= 1.67D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 2.22D-06 CP: 9.98D-01 1.10D+00 9.29D-01
E= -608.981538105512 Delta-E= -0.000000267770 Rises=F Damp=F
DIIS: error= 1.69D-05 at cycle 4 NSaved= 4.

Supporting Information file

NSaved= 4 IEnMin= 4 EnMin= -608.981538105512 IErMin= 4 ErrMin= 1.69D-05
ErrMax= 1.69D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.75D-08 BMatP= 2.35D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.123D-02-0.135D+00 0.279D+00 0.856D+00
Coeff: 0.123D-02-0.135D+00 0.279D+00 0.856D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.53D-06 MaxDP=4.63D-05 DE=-2.68D-07 OVMax= 1.72D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 8.09D-07 CP: 9.98D-01 1.12D+00 1.12D+00 1.18D+00
E= -608.981538226637 Delta-E= -0.000000121125 Rises=F Damp=F
DIIS: error= 7.96D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981538226637 IErMin= 5 ErrMin= 7.96D-06
ErrMax= 7.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-08 BMatP= 5.75D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.279D-02-0.124D+00 0.875D-01 0.477D+00 0.557D+00
Coeff: 0.279D-02-0.124D+00 0.875D-01 0.477D+00 0.557D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.43D-07 MaxDP=1.87D-05 DE=-1.21D-07 OVMax= 8.51D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.93D-07 CP: 9.98D-01 1.12D+00 1.19D+00 1.20D+00 1.11D+00
E= -608.981538259018 Delta-E= -0.000000032381 Rises=F Damp=F
DIIS: error= 5.82D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981538259018 IErMin= 6 ErrMin= 5.82D-06
ErrMax= 5.82D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-09 BMatP= 1.45D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.121D-03 0.225D-01-0.745D-01-0.204D+00 0.102D+00 0.115D+01
Coeff: 0.121D-03 0.225D-01-0.745D-01-0.204D+00 0.102D+00 0.115D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.26D-07 MaxDP=1.95D-05 DE=-3.24D-08 OVMax= 1.08D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.19D-07 CP: 9.98D-01 1.12D+00 1.22D+00 1.32D+00 1.46D+00
CP: 1.40D+00
E= -608.981538278401 Delta-E= -0.000000019383 Rises=F Damp=F
DIIS: error= 3.14D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981538278401 IErMin= 7 ErrMin= 3.14D-06
ErrMax= 3.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.92D-10 BMatP= 2.16D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.768D-03 0.412D-01-0.447D-01-0.196D+00-0.135D+00 0.325D+00
Coeff-Com: 0.101D+01
Coeff: -0.768D-03 0.412D-01-0.447D-01-0.196D+00-0.135D+00 0.325D+00
Coeff: 0.101D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.07D-07 MaxDP=8.48D-06 DE=-1.94D-08 OVMax= 7.10D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.20D-07 CP: 9.98D-01 1.12D+00 1.24D+00 1.33D+00 1.65D+00
CP: 1.76D+00 1.57D+00
E= -608.981538284068 Delta-E= -0.000000005668 Rises=F Damp=F
DIIS: error= 1.32D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981538284068 IErMin= 8 ErrMin= 1.32D-06
ErrMax= 1.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-10 BMatP= 5.92D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.401D-03 0.144D-01-0.508D-02-0.475D-01-0.846D-01-0.974D-01
Coeff-Com: 0.453D+00 0.767D+00
Coeff: -0.401D-03 0.144D-01-0.508D-02-0.475D-01-0.846D-01-0.974D-01
Coeff: 0.453D+00 0.767D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.17D-07 MaxDP=2.62D-06 DE=-5.67D-09 OVMax= 2.99D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.87D-08 CP: 9.98D-01 1.12D+00 1.25D+00 1.33D+00 1.67D+00
CP: 1.87D+00 1.95D+00 1.26D+00
E= -608.981538285120 Delta-E= -0.000000001051 Rises=F Damp=F
DIIS: error= 7.66D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981538285120 IErMin= 9 ErrMin= 7.66D-07
ErrMax= 7.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.20D-11 BMatP= 1.80D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.246D-04-0.263D-02 0.852D-02 0.237D-01-0.126D-01-0.136D+00
Coeff-Com: -0.113D-01 0.406D+00 0.725D+00
Coeff: -0.246D-04-0.263D-02 0.852D-02 0.237D-01-0.126D-01-0.136D+00
Coeff: -0.113D-01 0.406D+00 0.725D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=6.63D-08 MaxDP=1.98D-06 DE=-1.05D-09 OVMax= 1.32D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.53D-08 CP: 9.98D-01 1.12D+00 1.25D+00 1.32D+00 1.67D+00
CP: 1.90D+00 2.12D+00 1.55D+00 1.29D+00
E= -608.981538285392 Delta-E= -0.000000000272 Rises=F Damp=F
DIIS: error= 2.80D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981538285392 IErMin=10 ErrMin= 2.80D-07
ErrMax= 2.80D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-11 BMatP= 6.20D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.131D-03-0.628D-02 0.560D-02 0.282D-01 0.275D-01-0.260D-01
Coeff-Com: -0.186D+00-0.880D-01 0.339D+00 0.906D+00
Coeff: 0.131D-03-0.628D-02 0.560D-02 0.282D-01 0.275D-01-0.260D-01
Coeff: -0.186D+00-0.880D-01 0.339D+00 0.906D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.49D-08 MaxDP=2.16D-06 DE=-2.72D-10 OVMax= 8.49D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.72D-08 CP: 9.98D-01 1.12D+00 1.25D+00 1.31D+00 1.65D+00
CP: 1.93D+00 2.22D+00 1.73D+00 1.63D+00 1.55D+00
E= -608.981538285468 Delta-E= -0.000000000076 Rises=F Damp=F

DIIS: error= 8.78D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981538285468 IErMin=11 ErrMin= 8.78D-08
ErrMax= 8.78D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-12 BMatP= 1.46D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.211D-04-0.469D-03-0.554D-03 0.973D-04 0.696D-02 0.190D-01
Coeff-Com: -0.296D-01-0.816D-01-0.583D-01 0.185D+00 0.959D+00
Coeff: 0.211D-04-0.469D-03-0.554D-03 0.973D-04 0.696D-02 0.190D-01
Coeff: -0.296D-01-0.816D-01-0.583D-01 0.185D+00 0.959D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.64D-08 MaxDP=8.92D-07 DE=-7.59D-11 OVMax= 2.01D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 7.36D-09 CP: 9.98D-01 1.12D+00 1.25D+00 1.31D+00 1.65D+00
CP: 1.93D+00 2.22D+00 1.76D+00 1.75D+00 1.91D+00
CP: 1.34D+00
E= -608.981538285479 Delta-E= -0.000000000011 Rises=F Damp=F
DIIS: error= 4.99D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981538285479 IErMin=12 ErrMin= 4.99D-08
ErrMax= 4.99D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.53D-13 BMatP= 1.54D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.191D-04 0.116D-02-0.150D-02-0.629D-02-0.263D-02 0.162D-01
Coeff-Com: 0.244D-01-0.222D-01-0.978D-01-0.104D+00 0.457D+00 0.735D+00
Coeff: -0.191D-04 0.116D-02-0.150D-02-0.629D-02-0.263D-02 0.162D-01
Coeff: 0.244D-01-0.222D-01-0.978D-01-0.104D+00 0.457D+00 0.735D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=8.04D-09 MaxDP=4.31D-07 DE=-1.14D-11 OVMax= 9.20D-07

SCF Done: E(RwB97XD) = -608.981538285 A.U. after 12 cycles
NFock= 12 Conv=0.80D-08 -V/T= 2.0045
KE= 6.062447872355D+02 PE=-2.846341858416D+03 EE= 9.134455899387D+02
Leave Link 502 at Fri Aug 21 20:22:34 2026, MaxMem= 805306368 cpu: 3620.5 elap: 603.6
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33582.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 20:22:34 2026, MaxMem= 805306368 cpu: 4.2 elap: 0.7
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 20:22:35 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Supporting Information file

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 20:30:25 2026, MaxMem= 805306368 cpu: 2822.9 elap: 470.5
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.51754080D+00-1.89892547D-03-3.05358975D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000021870	-0.000090482	-0.000240125
2	6	0.000102458	-0.000007855	0.000269207
3	6	0.000066036	0.000102335	0.000240202
4	6	-0.000029972	-0.000057410	-0.000272002
5	6	0.000069323	-0.000018003	-0.000272452
6	6	-0.000019026	-0.000047678	0.000254688
7	6	-0.000016049	0.000086206	0.000281359
8	6	0.000031974	-0.000016601	-0.000135226
9	6	-0.000020969	0.000026426	-0.000265317
10	6	-0.000140932	-0.000062026	-0.000008948
11	6	0.000030412	0.000023565	0.000132523
12	6	0.000212045	0.000202252	0.000194385
13	6	-0.000137323	0.000059898	0.000024268
14	6	0.000202828	-0.000200725	-0.000200428
15	6	-0.000188190	0.000050152	-0.000060347
16	6	-0.000184484	-0.000050053	0.000058212

Cartesian Forces: Max 0.000281359 RMS 0.000145596
Leave Link 716 at Fri Aug 21 20:30:25 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000183572 RMS 0.000074995
Search for a local minimum.
Step number 10 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)

Supporting Information file

```
 RMS Force = .74995D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                                      6    7    8    9   10
 DE= -4.24D-06 DEPred=-2.55D-06 R= 1.66D+00
 TightC=F SS=  1.41D+00  RLast= 3.19D-02 DXNew= 8.4853D-01 9.5654D-02
 Trust test= 1.66D+00 RLast= 3.19D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  1  1  1  1  1  0
    Eigenvalues ---    0.00330   0.01290   0.01570   0.01731   0.02119
    Eigenvalues ---    0.02626   0.02785   0.03335   0.03422   0.03926
    Eigenvalues ---    0.04047   0.06915   0.08126   0.08439   0.09397
    Eigenvalues ---    0.10628   0.24385   0.24426   0.24687   0.24988
    Eigenvalues ---    0.24994   0.24995   0.25000   0.25000   0.25012
    Eigenvalues ---    0.25650   0.28166   0.32710   0.36018   0.43155
    Eigenvalues ---    0.51320   0.54132   0.57377   0.58118   0.58172
    Eigenvalues ---    0.58400   0.78666   0.79237   0.79695   0.81366
    Eigenvalues ---    0.82167   0.92886
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    10    9    8    7    6    5    4
 RFO step:  Lambda=-2.27660351D-06.
 NNeg= 0 NGDIIS= 7 SimSw=  2.50D-01 Rises=F DC= -4.24D-06 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.2276392689D-02 NUsed= 7 OKEnD=F EnDIS=F
 InvSVX:  RCond= 1.08D-08 Info=          0 Equed=N FErr=  7.70D-11 BErr=  4.84D-17
 DIIS inversion failure, remove point   7.
 InvSVX:  RCond= 1.77D-08 Info=          0 Equed=N FErr=  5.46D-11 BErr=  2.97D-17
 DIIS inversion failure, remove point   6.
 InvSVX:  RCond= 2.76D-08 Info=          0 Equed=N FErr=  3.59D-11 BErr=  3.38D-17
 DIIS inversion failure, remove point   5.
 InvSVX:  RCond= 5.72D-08 Info=          0 Equed=N FErr=  1.99D-11 BErr=  5.59D-17
 DIIS inversion failure, remove point   4.
 InvSVX:  RCond= 2.50D-07 Info=          0 Equed=N FErr=  3.36D-12 BErr=  5.42D-17
 RFO-DIIS uses    3 points instead of    7
 DidBck=F Rises=F RFO-DIIS coefs:    1.94016   -1.67111    0.73095    0.00000    0.00000
              RFO-DIIS coefs:    0.00000    0.00000
 Iteration  1 RMS(Cart)=  0.00071248 RMS(Int)=  0.00000254
 Iteration  2 RMS(Cart)=  0.00000137 RMS(Int)=  0.00000144
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000144
  ITry=  1 IFail=0 DXMaxC=  2.59D-03 DCOld=  1.00D+10 DXMaxT=  5.05D-01 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)    (Quad)   (Total)
    R1       2.30694   0.00010  -0.00004   0.00015   0.00011   2.30705
    R2       2.54840   0.00018   0.00017   0.00006   0.00023   2.54863
    R3       2.54771   0.00016   0.00010   0.00006   0.00016   2.54787
    R4       2.30692   0.00010  -0.00004   0.00015   0.00011   2.30704
    R5       2.30299   0.00011  -0.00005   0.00016   0.00011   2.30310
    R6       2.54779   0.00015   0.00008   0.00005   0.00013   2.54792
```

R7	2.55050	0.00009	0.00004	0.00000	0.00005	2.55055
R8	2.30296	0.00011	-0.00004	0.00016	0.00012	2.30308
R9	2.29565	0.00012	-0.00000	0.00015	0.00015	2.29580
R10	2.55055	0.00009	0.00003	0.00000	0.00003	2.55059
R11	2.61579	0.00005	-0.00003	-0.00003	-0.00007	2.61573
R12	2.29565	0.00012	-0.00000	0.00015	0.00015	2.29579
R13	2.64643	-0.00010	-0.00030	-0.00033	-0.00063	2.64580
R14	2.73919	0.00018	0.00068	0.00052	0.00120	2.74039
R15	2.61579	0.00005	-0.00002	-0.00004	-0.00006	2.61573
R16	2.73917	0.00018	0.00072	0.00051	0.00123	2.74040
R17	2.73912	-0.00002	-0.00157	-0.00013	-0.00169	2.73743
A1	2.61223	0.00003	-0.00013	0.00017	0.00004	2.61227
A2	2.64422	-0.00001	-0.00011	-0.00004	-0.00016	2.64406
A3	2.61416	-0.00000	-0.00062	0.00009	-0.00054	2.61362
A4	2.71589	0.00000	0.00002	0.00001	0.00003	2.71592
A5	2.64248	0.00001	0.00033	0.00003	0.00036	2.64284
A6	2.78133	-0.00004	0.00048	-0.00026	0.00022	2.78155
A7	2.71725	-0.00002	-0.00033	-0.00005	-0.00037	2.71687
A8	2.78038	-0.00002	0.00072	-0.00023	0.00049	2.78088
A9	2.83189	-0.00006	-0.00028	-0.00019	-0.00048	2.83141
A10	2.30563	0.00009	-0.00026	0.00047	0.00020	2.30583
A11	2.51965	-0.00010	0.00048	-0.00047	0.00001	2.51966
A12	1.45733	0.00000	-0.00024	0.00001	-0.00022	1.45711
A13	2.83143	-0.00005	-0.00015	-0.00018	-0.00033	2.83109
A14	2.30585	0.00009	-0.00034	0.00046	0.00013	2.30597
A15	1.45722	0.00001	-0.00017	0.00001	-0.00016	1.45705
A16	2.51956	-0.00010	0.00048	-0.00046	0.00002	2.51958
A17	1.42754	-0.00002	0.00025	-0.00005	0.00020	1.42774
A18	1.42766	-0.00002	0.00017	-0.00004	0.00013	1.42779
A19	2.87989	-0.00000	-0.00032	0.00004	-0.00028	2.87961
A20	2.88042	-0.00001	-0.00047	0.00004	-0.00043	2.87999
A21	3.13995	0.00009	0.00167	-0.00028	0.00139	3.14134
A22	3.13988	0.00009	0.00161	0.00003	0.00164	3.14152
D1	0.07922	0.00006	0.00392	0.00087	0.00480	0.08402
D2	-0.07278	-0.00001	-0.00326	-0.00120	-0.00446	-0.07724
D3	-0.07391	-0.00003	-0.00552	-0.00079	-0.00630	-0.08021
D4	0.07916	0.00006	0.00404	0.00085	0.00490	0.08406
D5	0.10752	0.00003	0.00648	0.00080	0.00728	0.11480
D6	-0.07343	-0.00003	-0.00582	-0.00078	-0.00660	-0.08003
D7	0.09426	-0.00004	0.00149	-0.00068	0.00081	0.09506
D8	0.10697	0.00003	0.00677	0.00084	0.00761	0.11458
D9	0.09543	-0.00004	0.00128	-0.00078	0.00050	0.09592
D10	-0.63626	-0.00000	-0.00623	0.00112	-0.00511	-0.64137
D11	2.55669	-0.00002	-0.00543	0.00065	-0.00479	2.55190
D12	0.75096	-0.00002	0.00071	-0.00064	0.00007	0.75102
D13	-2.42043	-0.00002	0.00005	-0.00031	-0.00026	-2.42069
D14	-2.42074	-0.00002	0.00026	-0.00038	-0.00012	-2.42086
D15	0.69106	-0.00001	-0.00040	-0.00005	-0.00045	0.69061

D16 2.40900 -0.00004 -0.00085 0.00022 -0.00063 2.40836
D17 -0.69426 -0.00005 -0.00025 -0.00015 -0.00040 -0.69466
D18 -0.63795 0.00000 -0.00604 0.00130 -0.00474 -0.64269
D19 2.55445 -0.00001 -0.00488 0.00069 -0.00419 2.55027
D20 -0.69426 -0.00005 -0.00024 -0.00015 -0.00039 -0.69465
D21 2.40940 -0.00004 -0.00112 0.00032 -0.00080 2.40860
D22 0.66941 -0.00003 -0.00010 -0.00009 -0.00020 0.66921

Item	Value	Threshold	Converged?
Maximum Force	0.000184	0.000450	YES
RMS Force	0.000075	0.000300	YES
Maximum Displacement	0.002588	0.001800	NO
RMS Displacement	0.000713	0.001200	YES

Predicted change in Energy=-1.023448D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 20:30:25 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.622838	-0.673225	0.011716
2	6	0	3.007490	-1.726810	0.053562
3	6	0	3.621999	0.675252	-0.011480
4	6	0	1.854973	-2.426482	0.055949
5	6	0	3.006776	1.728897	-0.053436
6	6	0	0.645010	-2.572333	0.063750
7	6	0	1.853460	2.427305	-0.055958
8	6	0	-0.665950	-2.254040	0.022016
9	6	0	0.643485	2.572960	-0.063840
10	6	0	-1.731260	-1.671693	-0.021876
11	6	0	-0.667229	2.253563	-0.022166
12	6	0	-2.686802	-0.680760	-0.166639
13	6	0	-1.732278	1.670718	0.021456
14	6	0	-2.687114	0.679138	0.166459
15	6	0	-4.042735	-0.405345	-0.600841
16	6	0	-4.042663	0.402855	0.601329

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220838	0.000000			
3	C	1.348676	2.480273	0.000000		
4	C	2.490224	1.348274	3.570390	0.000000	
5	C	2.480719	3.457363	1.220831	4.313443	0.000000

6	C	3.532248	2.509248	4.406237	1.218746	4.908385
7	C	3.570513	4.312825	2.489860	4.855077	1.348302
8	C	4.570862	3.711216	5.193108	2.527041	5.418338
9	C	4.406809	4.908190	3.532079	5.145530	2.509521
10	C	5.446506	4.739671	5.845138	3.665628	5.832151
11	C	5.193449	5.417810	4.570411	5.316994	3.711410
12	C	6.312164	5.793762	6.454751	4.870812	6.183534
13	C	5.845633	5.831778	5.446129	5.445788	4.740002
14	C	6.455101	6.183030	6.311624	5.503421	5.794026
15	C	7.694673	7.202791	7.762937	6.268917	7.385814
16	C	7.763085	7.385133	7.693945	6.563893	7.202895

		6	7	8	9	10
6	C	0.000000				
7	C	5.145003	0.000000			
8	C	1.349692	5.316812	0.000000		
9	C	5.146875	1.218736	5.002191	0.000000	
10	C	2.542665	5.445472	1.214883	4.863975	0.000000
11	C	5.001861	2.526896	4.507819	1.349713	4.066914
12	C	3.838241	5.503299	2.568003	4.657046	1.384184
13	C	4.863822	3.665506	4.067035	2.542748	3.342692
14	C	4.656787	4.870562	3.565039	3.838293	2.544707
15	C	5.206964	6.563987	3.899782	5.578471	2.698473
16	C	5.578083	6.268548	4.335537	5.206899	3.167762

		11	12	13	14	15
11	C	0.000000				
12	C	3.565080	0.000000			
13	C	1.214882	2.544788	0.000000		
14	C	2.567942	1.400099	1.384185	0.000000	
15	C	4.335746	1.450152	3.167886	1.898041	0.000000
16	C	3.899669	1.897987	2.698446	1.450157	1.448586

		16
16	C	0.000000

Stoichiometry C16
Framework group C1[X(C16)]
Deg. of freedom 42
Full point group C1 NOp 1
RotChk: IX=0 Diff= 1.19D-05
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.622628	-0.674380	0.010077
2	6	0	3.006952	-1.727871	0.049402
3	6	0	3.622209	0.674148	-0.009889
4	6	0	1.854217	-2.427187	0.050122

```
     5        6        0        3.007314    1.728083   -0.049316
     6        6        0        0.644209   -2.572679    0.057583
     7        6        0        1.854216    2.426854   -0.050156
     8        6        0       -0.666652   -2.253878    0.016621
     9        6        0        0.644287    2.572905   -0.057680
    10        6        0       -1.731781   -1.671096   -0.025869
    11        6        0       -0.666527    2.253817   -0.016762
    12        6        0       -2.687015   -0.679522   -0.168250
    13        6        0       -1.731757    1.671202    0.025471
    14        6        0       -2.686902    0.679575    0.168105
    15        6        0       -4.042865   -0.402644   -0.601781
    16        6        0       -4.042533    0.402673    0.602322
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8474928           0.3941534           0.2718102
 Leave Link  202 at Fri Aug 21 20:30:25 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.6511336511 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0074926751 Hartrees.
 Nuclear repulsion after empirical dispersion term =      717.6436409760 Hartrees.
 Leave Link  301 at Fri Aug 21 20:30:25 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33580.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  4.36D-06  NBF=   496
```

Supporting Information file

NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 564 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 20:30:26 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 20:30:26 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000000 0.000002 -0.000004 Ang= -0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 20:30:26 2026, MaxMem= 805306368 cpu: 2.0 elap: 0.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981532932494
DIIS: error= 1.42D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981532932494 IErMin= 1 ErrMin= 1.42D-04
ErrMax= 1.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-05 BMatP= 1.42D-05
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.42D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=4.81D-05 MaxDP=1.23D-03 OVMax= 4.38D-04

Cycle 2 Pass 1 IDiag 1:
RMSU= 4.61D-05 CP: 9.98D-01
E= -608.981539607835 Delta-E= -0.000006675341 Rises=F Damp=F
DIIS: error= 1.71D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981539607835 IErMin= 2 ErrMin= 1.71D-05
ErrMax= 1.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-07 BMatP= 1.42D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.327D-01 0.103D+01
Coeff: -0.327D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.47D-06 MaxDP=1.35D-04 DE=-6.68D-06 OVMax= 3.09D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 2.67D-06 CP: 9.98D-01 1.08D+00
E= -608.981540007872 Delta-E= -0.000000400037 Rises=F Damp=F
DIIS: error= 1.14D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981540007872 IErMin= 3 ErrMin= 1.14D-05
ErrMax= 1.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.49D-08 BMatP= 1.45D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.171D-01 0.324D+00 0.693D+00
Coeff: -0.171D-01 0.324D+00 0.693D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.48D-06 MaxDP=5.38D-05 DE=-4.00D-07 OVMax= 1.24D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 1.40D-06 CP: 9.98D-01 1.08D+00 9.08D-01
E= -608.981540105893 Delta-E= -0.000000098021 Rises=F Damp=F
DIIS: error= 8.95D-06 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981540105893 IErMin= 4 ErrMin= 8.95D-06
ErrMax= 8.95D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-08 BMatP= 5.49D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.349D-02-0.203D+00 0.317D+00 0.882D+00
Coeff: 0.349D-02-0.203D+00 0.317D+00 0.882D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=9.79D-07 MaxDP=4.81D-05 DE=-9.80D-08 OVMax= 1.35D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 5.81D-07 CP: 9.98D-01 1.08D+00 1.19D+00 1.01D+00
E= -608.981540169085 Delta-E= -0.000000063191 Rises=F Damp=F
DIIS: error= 5.47D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981540169085 IErMin= 5 ErrMin= 5.47D-06
ErrMax= 5.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-09 BMatP= 1.94D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.288D-02-0.936D-01 0.219D-01 0.238D+00 0.831D+00
Coeff: 0.288D-02-0.936D-01 0.219D-01 0.238D+00 0.831D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.84D-07 MaxDP=1.12D-05 DE=-6.32D-08 OVMax= 7.69D-05

Supporting Information file

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.22D-07 CP: 9.98D-01 1.08D+00 1.27D+00 1.09D+00 1.31D+00
E= -608.981540183043 Delta-E= -0.000000013958 Rises=F Damp=F
DIIS: error= 4.51D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981540183043 IErMin= 6 ErrMin= 4.51D-06
ErrMax= 4.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-09 BMatP= 2.45D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.354D-03 0.285D-01-0.127D+00-0.246D+00 0.536D+00 0.807D+00
Coeff: 0.354D-03 0.285D-01-0.127D+00-0.246D+00 0.536D+00 0.807D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.43D-07 MaxDP=1.13D-05 DE=-1.40D-08 OVMax= 6.94D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.56D-07 CP: 9.98D-01 1.09D+00 1.32D+00 1.20D+00 1.62D+00
CP: 1.47D+00
E= -608.981540191591 Delta-E= -0.000000008548 Rises=F Damp=F
DIIS: error= 1.92D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981540191591 IErMin= 7 ErrMin= 1.92D-06
ErrMax= 1.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.59D-10 BMatP= 1.54D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.955D-03 0.443D-01-0.493D-01-0.166D+00-0.124D+00 0.271D+00
Coeff-Com: 0.102D+01
Coeff: -0.955D-03 0.443D-01-0.493D-01-0.166D+00-0.124D+00 0.271D+00
Coeff: 0.102D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.35D-07 MaxDP=6.86D-06 DE=-8.55D-09 OVMax= 5.00D-05

Cycle 8 Pass 1 IDiag 1:
RMSU= 8.78D-08 CP: 9.98D-01 1.09D+00 1.36D+00 1.21D+00 1.79D+00
CP: 1.96D+00 1.53D+00
E= -608.981540193959 Delta-E= -0.000000002368 Rises=F Damp=F
DIIS: error= 6.79D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981540193959 IErMin= 8 ErrMin= 6.79D-07
ErrMax= 6.79D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.20D-11 BMatP= 2.59D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.434D-03 0.137D-01-0.324D-02-0.338D-01-0.115D+00 0.358D-02
Coeff-Com: 0.375D+00 0.760D+00
Coeff: -0.434D-03 0.137D-01-0.324D-02-0.338D-01-0.115D+00 0.358D-02
Coeff: 0.375D+00 0.760D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=7.44D-08 MaxDP=2.39D-06 DE=-2.37D-09 OVMax= 1.36D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.57D-08 CP: 9.98D-01 1.09D+00 1.36D+00 1.21D+00 1.80D+00
CP: 2.12D+00 1.72D+00 1.28D+00
E= -608.981540194243 Delta-E= -0.000000000284 Rises=F Damp=F
DIIS: error= 3.63D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -608.981540194243 IErMin= 9 ErrMin= 3.63D-07
ErrMax= 3.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-11 BMatP= 5.20D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.884D-04-0.793D-02 0.145D-01 0.383D-01-0.139D-01-0.929D-01
Coeff-Com: -0.172D+00 0.411D+00 0.823D+00
Coeff: 0.884D-04-0.793D-02 0.145D-01 0.383D-01-0.139D-01-0.929D-01
Coeff: -0.172D+00 0.411D+00 0.823D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.22D-08 MaxDP=1.85D-06 DE=-2.84D-10 OVMax= 8.82D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.24D-08 CP: 9.98D-01 1.09D+00 1.37D+00 1.20D+00 1.79D+00
CP: 2.20D+00 1.86D+00 1.55D+00 1.30D+00
E= -608.981540194354 Delta-E= -0.000000000111 Rises=F Damp=F
DIIS: error= 1.45D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981540194354 IErMin=10 ErrMin= 1.45D-07
ErrMax= 1.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.06D-12 BMatP= 2.23D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.141D-03-0.674D-02 0.687D-02 0.248D-01 0.271D-01-0.440D-01
Coeff-Com: -0.181D+00-0.756D-02 0.384D+00 0.796D+00
Coeff: 0.141D-03-0.674D-02 0.687D-02 0.248D-01 0.271D-01-0.440D-01
Coeff: -0.181D+00-0.756D-02 0.384D+00 0.796D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.34D-08 MaxDP=1.03D-06 DE=-1.11D-10 OVMax= 3.70D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 8.33D-09 CP: 9.98D-01 1.09D+00 1.37D+00 1.19D+00 1.79D+00
CP: 2.22D+00 1.89D+00 1.65D+00 1.58D+00 1.46D+00
E= -608.981540194374 Delta-E= -0.000000000020 Rises=F Damp=F
DIIS: error= 5.34D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981540194374 IErMin=11 ErrMin= 5.34D-08
ErrMax= 5.34D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.97D-13 BMatP= 5.06D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.204D-04-0.139D-03-0.142D-02-0.180D-02 0.148D-01 0.877D-02
Coeff-Com: -0.231D-01-0.110D+00-0.596D-01 0.308D+00 0.865D+00
Coeff: 0.204D-04-0.139D-03-0.142D-02-0.180D-02 0.148D-01 0.877D-02
Coeff: -0.231D-01-0.110D+00-0.596D-01 0.308D+00 0.865D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.26D-08 MaxDP=6.10D-07 DE=-2.05D-11 OVMax= 1.53D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.69D-09 CP: 9.98D-01 1.09D+00 1.37D+00 1.19D+00 1.79D+00
CP: 2.21D+00 1.88D+00 1.67D+00 1.77D+00 1.75D+00
CP: 1.40D+00
E= -608.981540194379 Delta-E= -0.000000000005 Rises=F Damp=F
DIIS: error= 3.00D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981540194379 IErMin=12 ErrMin= 3.00D-08
ErrMax= 3.00D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.90D-13 BMatP= 9.97D-13

Supporting Information file

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.220D-04 0.143D-02-0.219D-02-0.669D-02 0.221D-02 0.145D-01
Coeff-Com: 0.258D-01-0.534D-01-0.109D+00-0.150D-01 0.432D+00 0.710D+00
Coeff: -0.220D-04 0.143D-02-0.219D-02-0.669D-02 0.221D-02 0.145D-01
Coeff: 0.258D-01-0.534D-01-0.109D+00-0.150D-01 0.432D+00 0.710D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=6.40D-09 MaxDP=2.78D-07 DE=-5.00D-12 OVMax= 6.68D-07

SCF Done: E(RwB97XD) = -608.981540194 A.U. after 12 cycles
NFock= 12 Conv=0.64D-08 -V/T= 2.0045
KE= 6.062420690731D+02 PE=-2.846286594698D+03 EE= 9.134193444550D+02
Leave Link 502 at Fri Aug 21 20:38:11 2026, MaxMem= 805306368 cpu: 2786.4 elap: 464.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 20:38:11 2026, MaxMem= 805306368 cpu: 2.1 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 20:38:11 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 2462.4 elap: 410.4
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.51648605D+00-1.36620676D-03-1.34471627D-04
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.000026695 -0.000040585 -0.000199513

```
     2        6        0.000064794   0.000017116   0.000201414
     3        6        0.000005232   0.000048433   0.000198632
     4        6       -0.000029035  -0.000005914  -0.000184797
     5        6        0.000041019  -0.000035041  -0.000201661
     6        6        0.000000939  -0.000053202   0.000163728
     7        6       -0.000017699   0.000026579   0.000189342
     8        6        0.000014154   0.000044764  -0.000031415
     9        6       -0.000002106   0.000037122  -0.000162680
    10        6       -0.000075257  -0.000105408  -0.000118629
    11        6        0.000014127  -0.000038161   0.000013713
    12        6        0.000110816   0.000188858   0.000193858
    13        6       -0.000074866   0.000102600   0.000136547
    14        6        0.000105351  -0.000185022  -0.000193038
    15        6       -0.000070758  -0.000082644  -0.000131243
    16        6       -0.000060019   0.000080508   0.000125743
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.000201661 RMS     0.000111407
 Leave Link  716 at Fri Aug 21 20:45:02 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000108465 RMS     0.000041757
 Search for a local minimum.
 Step number  11 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .41757D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                                      6    7    8    9   10
                                                     11
 DE= -1.91D-06 DEPred=-1.02D-06 R= 1.87D+00
 TightC=F SS=  1.41D+00  RLast= 1.91D-02 DXNew= 8.4853D-01 5.7341D-02
 Trust test= 1.87D+00 RLast= 1.91D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  1  1  1  1  1  1  0
    Eigenvalues ---    0.00288   0.01290   0.01565   0.01615   0.01735
    Eigenvalues ---    0.02626   0.02770   0.03294   0.03422   0.03926
    Eigenvalues ---    0.04057   0.07224   0.08044   0.08443   0.09471
    Eigenvalues ---    0.10199   0.24404   0.24561   0.24696   0.24988
    Eigenvalues ---    0.24993   0.24995   0.25000   0.25000   0.25020
    Eigenvalues ---    0.26628   0.28165   0.31862   0.35533   0.40320
    Eigenvalues ---    0.51320   0.53500   0.57376   0.57991   0.58167
    Eigenvalues ---    0.58204   0.78666   0.79299   0.79695   0.81379
    Eigenvalues ---    0.82166   0.87958
```

Supporting Information file

```
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=      -3 using points:    11   10    9    8    7    6    5    4
 RFO step:  Lambda=-1.17424508D-06.
 NNeg= 0 NGDIIS= 8 SimSw=  2.50D-01 Rises=F DC= -1.91D-06 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.1583635339D-02 NUsed= 8 OKEnD=F EnDIS=F
 InvSVX:  RCond= 7.43D-09 Info=          0 Equed=N FErr=  6.55D-11 BErr=  1.42D-17
 DIIS inversion failure, remove point   8.
 InvSVX:  RCond= 9.29D-09 Info=          0 Equed=N FErr=  5.13D-11 BErr=  5.12D-17
 DIIS inversion failure, remove point   7.
 InvSVX:  RCond= 1.39D-08 Info=          0 Equed=N FErr=  3.39D-11 BErr=  8.73D-17
 DIIS inversion failure, remove point   6.
 InvSVX:  RCond= 1.66D-08 Info=          0 Equed=N FErr=  3.13D-11 BErr=  8.65D-17
 DIIS inversion failure, remove point   5.
 InvSVX:  RCond= 5.70D-08 Info=          0 Equed=N FErr=  9.36D-12 BErr=  5.34D-17
 DIIS inversion failure, remove point   4.
 InvSVX:  RCond= 6.27D-07 Info=          0 Equed=N FErr=  4.75D-13 BErr=  3.70D-17
 RFO-DIIS uses    3 points instead of    8
 DidBck=F Rises=F RFO-DIIS coefs:    2.48602   -1.99894    0.51292    0.00000    0.00000
              RFO-DIIS coefs:    0.00000    0.00000    0.00000
 Iteration  1 RMS(Cart)=  0.00060599 RMS(Int)=  0.00000187
 Iteration  2 RMS(Cart)=  0.00000083 RMS(Int)=  0.00000158
  ITry=  1  IFail=0  DXMaxC=  1.75D-03  DCOld=  1.00D+10  DXMaxT=  5.05D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)    (Quad)   (Total)
    R1       2.30705   0.00001   0.00015  -0.00015  -0.00000   2.30705
    R2       2.54863   0.00005   0.00039  -0.00025   0.00014   2.54877
    R3       2.54787   0.00006   0.00032  -0.00019   0.00013   2.54800
    R4       2.30704   0.00001   0.00015  -0.00014   0.00000   2.30704
    R5       2.30310   0.00002   0.00016  -0.00014   0.00003   2.30312
    R6       2.54792   0.00005   0.00030  -0.00019   0.00011   2.54804
    R7       2.55055   0.00003   0.00015  -0.00011   0.00004   2.55059
    R8       2.30308   0.00002   0.00017  -0.00013   0.00004   2.30311
    R9       2.29580   0.00002   0.00021  -0.00016   0.00005   2.29584
   R10       2.55059   0.00002   0.00014  -0.00011   0.00003   2.55062
   R11       2.61573   0.00002   0.00002  -0.00001   0.00001   2.61574
   R12       2.29579   0.00002   0.00020  -0.00015   0.00005   2.29584
   R13       2.64580  -0.00007  -0.00094   0.00021  -0.00073   2.64508
   R14       2.74039   0.00007   0.00151  -0.00065   0.00086   2.74125
   R15       2.61573   0.00002   0.00003  -0.00002   0.00001   2.61574
   R16       2.74040   0.00006   0.00151  -0.00068   0.00084   2.74124
   R17       2.73743   0.00009  -0.00140   0.00078  -0.00063   2.73680
    A1       2.61227   0.00005   0.00020   0.00016   0.00036   2.61263
    A2       2.64406  -0.00001  -0.00016  -0.00000  -0.00016   2.64389
    A3       2.61362   0.00003  -0.00025   0.00013  -0.00013   2.61350
    A4       2.71592  -0.00001   0.00007  -0.00010  -0.00003   2.71589
    A5       2.64284   0.00001   0.00024   0.00003   0.00028   2.64312
    A6       2.78155  -0.00007  -0.00014  -0.00024  -0.00038   2.78118
```

A7	2.71687	-0.00002	-0.00024	-0.00012	-0.00036	2.71651
A8	2.78088	-0.00006	0.00007	-0.00021	-0.00014	2.78074
A9	2.83141	-0.00004	-0.00055	0.00004	-0.00050	2.83090
A10	2.30583	0.00008	0.00071	-0.00001	0.00071	2.30654
A11	2.51966	-0.00011	-0.00053	-0.00013	-0.00066	2.51900
A12	1.45711	0.00002	-0.00018	0.00014	-0.00004	1.45707
A13	2.83109	-0.00004	-0.00045	0.00005	-0.00039	2.83070
A14	2.30597	0.00008	0.00066	-0.00000	0.00066	2.30663
A15	1.45705	0.00002	-0.00014	0.00012	-0.00002	1.45703
A16	2.51958	-0.00010	-0.00051	-0.00011	-0.00063	2.51895
A17	1.42774	-0.00003	0.00003	-0.00008	-0.00005	1.42769
A18	1.42779	-0.00002	-0.00001	-0.00004	-0.00005	1.42774
A19	2.87961	0.00000	-0.00023	0.00021	-0.00002	2.87959
A20	2.87999	-0.00000	-0.00034	0.00013	-0.00020	2.87979
A21	3.14134	0.00005	0.00137	0.00021	0.00158	3.14292
A22	3.14152	0.00004	0.00176	-0.00096	0.00080	3.14231
D1	0.08402	0.00004	0.00417	0.00040	0.00457	0.08859
D2	-0.07724	-0.00002	-0.00374	-0.00062	-0.00435	-0.08159
D3	-0.08021	-0.00003	-0.00455	-0.00048	-0.00503	-0.08524
D4	0.08406	0.00004	0.00419	0.00042	0.00461	0.08867
D5	0.11480	0.00002	0.00538	0.00026	0.00563	0.12043
D6	-0.08003	-0.00003	-0.00472	-0.00048	-0.00520	-0.08523
D7	0.09506	-0.00003	-0.00116	-0.00022	-0.00138	0.09368
D8	0.11458	0.00002	0.00563	0.00028	0.00592	0.12050
D9	0.09592	-0.00003	-0.00147	-0.00032	-0.00179	0.09413
D10	-0.64137	0.00002	-0.00178	0.00071	-0.00107	-0.64244
D11	2.55190	0.00000	-0.00203	0.00043	-0.00160	2.55030
D12	0.75102	-0.00000	-0.00052	-0.00007	-0.00059	0.75043
D13	-2.42069	0.00001	-0.00040	-0.00000	-0.00041	-2.42109
D14	-2.42086	0.00001	-0.00039	0.00009	-0.00031	-2.42117
D15	0.69061	0.00002	-0.00028	0.00015	-0.00012	0.69049
D16	2.40836	0.00001	-0.00038	0.00048	0.00010	2.40846
D17	-0.69466	-0.00001	-0.00059	0.00027	-0.00033	-0.69498
D18	-0.64269	0.00003	-0.00137	0.00062	-0.00075	-0.64344
D19	2.55027	0.00000	-0.00160	0.00049	-0.00111	2.54916
D20	-0.69465	-0.00002	-0.00059	0.00026	-0.00033	-0.69498
D21	2.40860	0.00000	-0.00040	0.00036	-0.00004	2.40856
D22	0.66921	-0.00002	-0.00017	0.00002	-0.00015	0.66907

Item	Value	Threshold	Converged?
Maximum Force	0.000108	0.000450	YES
RMS Force	0.000042	0.000300	YES
Maximum Displacement	0.001755	0.001800	YES
RMS Displacement	0.000606	0.001200	YES

Predicted change in Energy=-4.279991D-07
Optimization completed.
-- Stationary point found.

! Optimized Parameters !

Supporting Information file

! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.2208	-DE/DX = 0.0
R2	R(1,3)	1.3487	-DE/DX = 0.0001
R3	R(2,4)	1.3483	-DE/DX = 0.0001
R4	R(3,5)	1.2208	-DE/DX = 0.0
R5	R(4,6)	1.2187	-DE/DX = 0.0
R6	R(5,7)	1.3483	-DE/DX = 0.0001
R7	R(6,8)	1.3497	-DE/DX = 0.0
R8	R(7,9)	1.2187	-DE/DX = 0.0
R9	R(8,10)	1.2149	-DE/DX = 0.0
R10	R(9,11)	1.3497	-DE/DX = 0.0
R11	R(10,12)	1.3842	-DE/DX = 0.0
R12	R(11,13)	1.2149	-DE/DX = 0.0
R13	R(12,14)	1.4001	-DE/DX = -0.0001
R14	R(12,15)	1.4502	-DE/DX = 0.0001
R15	R(13,14)	1.3842	-DE/DX = 0.0
R16	R(14,16)	1.4502	-DE/DX = 0.0001
R17	R(15,16)	1.4486	-DE/DX = 0.0001
A1	A(2,1,3)	149.6721	-DE/DX = 0.0001
A2	A(1,2,4)	151.4933	-DE/DX = 0.0
A3	A(1,3,5)	149.7496	-DE/DX = 0.0
A4	A(2,4,6)	155.611	-DE/DX = 0.0
A5	A(3,5,7)	151.4236	-DE/DX = 0.0
A6	A(4,6,8)	159.3713	-DE/DX = -0.0001
A7	A(5,7,9)	155.6653	-DE/DX = 0.0
A8	A(7,9,11)	159.3325	-DE/DX = -0.0001
A9	A(8,10,12)	162.2277	-DE/DX = 0.0
A10	A(10,12,14)	132.1145	-DE/DX = 0.0001
A11	A(10,12,15)	144.366	-DE/DX = -0.0001
A12	A(14,12,15)	83.4862	-DE/DX = 0.0
A13	A(11,13,14)	162.2098	-DE/DX = 0.0
A14	A(12,14,13)	132.1225	-DE/DX = 0.0001
A15	A(12,14,16)	83.4831	-DE/DX = 0.0
A16	A(13,14,16)	144.3616	-DE/DX = -0.0001
A17	A(12,15,16)	81.8034	-DE/DX = 0.0
A18	A(14,16,15)	81.8061	-DE/DX = 0.0
A19	L(6,8,10,7,-1)	164.9895	-DE/DX = 0.0
A20	L(9,11,13,4,-1)	165.0111	-DE/DX = 0.0
A21	L(6,8,10,7,-2)	179.9856	-DE/DX = 0.0001
A22	L(9,11,13,4,-2)	179.9957	-DE/DX = 0.0
D1	D(3,1,2,4)	4.8138	-DE/DX = 0.0
D2	D(2,1,3,5)	-4.4253	-DE/DX = 0.0
D3	D(1,2,4,6)	-4.5956	-DE/DX = 0.0
D4	D(1,3,5,7)	4.8162	-DE/DX = 0.0
D5	D(2,4,6,8)	6.5774	-DE/DX = 0.0

```
! D6    D(3,5,7,9)           -4.5852        -DE/DX =    0.0              !
! D7    D(4,6,10,12)          5.4468         -DE/DX =    0.0              !
! D8    D(5,7,9,11)           6.5651        -DE/DX =    0.0              !
! D9    D(7,9,13,14)          5.496         -DE/DX =    0.0              !
! D10   D(8,10,12,14)        -36.7476        -DE/DX =    0.0              !
! D11   D(8,10,12,15)        146.2131        -DE/DX =    0.0              !
! D12   D(10,12,14,13)        43.0305        -DE/DX =    0.0              !
! D13   D(10,12,14,16)       -138.695         -DE/DX =    0.0              !
! D14   D(15,12,14,13)       -138.7051        -DE/DX =    0.0              !
! D15   D(15,12,14,16)        39.5693        -DE/DX =    0.0              !
! D16   D(10,12,15,16)        137.989         -DE/DX =    0.0              !
! D17   D(14,12,15,16)       -39.8008        -DE/DX =    0.0              !
! D18   D(11,13,14,12)       -36.8236        -DE/DX =    0.0              !
! D19   D(11,13,14,16)        146.1196        -DE/DX =    0.0              !
! D20   D(12,14,16,15)       -39.8006        -DE/DX =    0.0              !
! D21   D(13,14,16,15)        138.0026        -DE/DX =    0.0              !
! D22   D(12,15,16,14)         38.343         -DE/DX =    0.0              !
 ---------------------------------------------------------------------------
 Lowest energy point so far.  Saving SCF results.
 Largest change from initial coordinates is atom   15       0.102 Angstoms.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link  103 at Fri Aug 21 20:45:02 2026, MaxMem=    805306368 cpu:                  0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l202.exe)
                      Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.622838   -0.673225    0.011716
     2          6           0        3.007490   -1.726810    0.053562
     3          6           0        3.621999    0.675252   -0.011480
     4          6           0        1.854973   -2.426482    0.055949
     5          6           0        3.006776    1.728897   -0.053436
     6          6           0        0.645010   -2.572333    0.063750
     7          6           0        1.853460    2.427305   -0.055958
     8          6           0       -0.665950   -2.254040    0.022016
     9          6           0        0.643485    2.572960   -0.063840
    10          6           0       -1.731260   -1.671693   -0.021876
    11          6           0       -0.667229    2.253563   -0.022166
    12          6           0       -2.686802   -0.680760   -0.166639
    13          6           0       -1.732278    1.670718    0.021456
    14          6           0       -2.687114    0.679138    0.166459
    15          6           0       -4.042735   -0.405345   -0.600841
    16          6           0       -4.042663    0.402855    0.601329
 ---------------------------------------------------------------------
                      Distance matrix (angstroms):
```

Supporting Information file

		1	2	3	4	5
1	C	0.000000				
2	C	1.220838	0.000000			
3	C	1.348676	2.480273	0.000000		
4	C	2.490224	1.348274	3.570390	0.000000	
5	C	2.480719	3.457363	1.220831	4.313443	0.000000
6	C	3.532248	2.509248	4.406237	1.218746	4.908385
7	C	3.570513	4.312825	2.489860	4.855077	1.348302
8	C	4.570862	3.711216	5.193108	2.527041	5.418338
9	C	4.406809	4.908190	3.532079	5.145530	2.509521
10	C	5.446506	4.739671	5.845138	3.665628	5.832151
11	C	5.193449	5.417810	4.570411	5.316994	3.711410
12	C	6.312164	5.793762	6.454751	4.870812	6.183534
13	C	5.845633	5.831778	5.446129	5.445788	4.740002
14	C	6.455101	6.183030	6.311624	5.503421	5.794026
15	C	7.694673	7.202791	7.762937	6.268917	7.385814
16	C	7.763085	7.385133	7.693945	6.563893	7.202895

		6	7	8	9	10
6	C	0.000000				
7	C	5.145003	0.000000			
8	C	1.349692	5.316812	0.000000		
9	C	5.146875	1.218736	5.002191	0.000000	
10	C	2.542665	5.445472	1.214883	4.863975	0.000000
11	C	5.001861	2.526896	4.507819	1.349713	4.066914
12	C	3.838241	5.503299	2.568003	4.657046	1.384184
13	C	4.863822	3.665506	4.067035	2.542748	3.342692
14	C	4.656787	4.870562	3.565039	3.838293	2.544707
15	C	5.206964	6.563987	3.899782	5.578471	2.698473
16	C	5.578083	6.268548	4.335537	5.206899	3.167762

		11	12	13	14	15
11	C	0.000000				
12	C	3.565080	0.000000			
13	C	1.214882	2.544788	0.000000		
14	C	2.567942	1.400099	1.384185	0.000000	
15	C	4.335746	1.450152	3.167886	1.898041	0.000000
16	C	3.899669	1.897987	2.698446	1.450157	1.448586

		16
16	C	0.000000

Stoichiometry C16
Framework group C1[X(C16)]
Deg. of freedom 42
Full point group C1 NOp 1
RotChk: IX=0 Diff= 2.37D-16
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Supporting Information file

Number	Number	Type	X	Y	Z
1	6	0	3.622628	-0.674380	0.010077
2	6	0	3.006952	-1.727871	0.049402
3	6	0	3.622209	0.674148	-0.009889
4	6	0	1.854217	-2.427187	0.050122
5	6	0	3.007314	1.728083	-0.049316
6	6	0	0.644209	-2.572679	0.057583
7	6	0	1.854216	2.426854	-0.050156
8	6	0	-0.666652	-2.253878	0.016621
9	6	0	0.644287	2.572905	-0.057680
10	6	0	-1.731781	-1.671096	-0.025869
11	6	0	-0.666527	2.253817	-0.016762
12	6	0	-2.687015	-0.679522	-0.168250
13	6	0	-1.731757	1.671202	0.025471
14	6	0	-2.686902	0.679575	0.168105
15	6	0	-4.042865	-0.402644	-0.601781
16	6	0	-4.042533	0.402673	0.602322

Rotational constants (GHZ): 0.8474928 0.3941534 0.2718102
Leave Link 202 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

****

Population analysis using the SCF Density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Alpha virt. eigenvalues --	0.46495	0.46639	0.47553	0.47694	0.48811
Alpha virt. eigenvalues --	0.49117	0.50284	0.50725	0.50921	0.52249
Alpha virt. eigenvalues --	0.52732	0.52984	0.53200	0.54297	0.54536
Alpha virt. eigenvalues --	0.54926	0.55685	0.56069	0.56549	0.58161
Alpha virt. eigenvalues --	0.58302	0.59013	0.59185	0.59368	0.60396
Alpha virt. eigenvalues --	0.61116	0.63299	0.63574	0.63723	0.64293
Alpha virt. eigenvalues --	0.65210	0.67191	0.67561	0.67944	0.68624
Alpha virt. eigenvalues --	0.70914	0.71012	0.72044	0.72422	0.74301
Alpha virt. eigenvalues --	0.75848	0.76815	0.77208	0.78800	0.79808
Alpha virt. eigenvalues --	0.80557	0.84401	0.84818	0.85440	0.85915
Alpha virt. eigenvalues --	0.86699	0.90213	0.91512	0.92663	0.92870
Alpha virt. eigenvalues --	0.93592	0.95722	0.96684	0.98165	0.99140
Alpha virt. eigenvalues --	1.01137	1.01981	1.02368	1.05797	1.07381
Alpha virt. eigenvalues --	1.09301	1.09335	1.09879	1.12188	1.12432
Alpha virt. eigenvalues --	1.13358	1.15262	1.15994	1.16387	1.18464
Alpha virt. eigenvalues --	1.19675	1.22055	1.23127	1.23523	1.23875
Alpha virt. eigenvalues --	1.26222	1.27253	1.27711	1.27775	1.30100
Alpha virt. eigenvalues --	1.31458	1.33407	1.34466	1.35849	1.36137
Alpha virt. eigenvalues --	1.37502	1.38475	1.39202	1.39243	1.40757
Alpha virt. eigenvalues --	1.41670	1.42611	1.43166	1.43339	1.43747
Alpha virt. eigenvalues --	1.45417	1.46011	1.47089	1.48236	1.48834
Alpha virt. eigenvalues --	1.49155	1.49688	1.49957	1.50561	1.50861
Alpha virt. eigenvalues --	1.51264	1.53178	1.54048	1.54566	1.57963
Alpha virt. eigenvalues --	1.59431	1.61318	1.61735	1.62193	1.62991
Alpha virt. eigenvalues --	1.63954	1.64765	1.65752	1.67667	1.69594
Alpha virt. eigenvalues --	1.69727	1.71038	1.71633	1.72894	1.72985
Alpha virt. eigenvalues --	1.74463	1.76303	1.77824	1.77871	1.78794
Alpha virt. eigenvalues --	1.79143	1.81311	1.82715	1.84830	1.85724
Alpha virt. eigenvalues --	1.85892	1.86104	1.90730	1.92761	1.97301
Alpha virt. eigenvalues --	1.97394	1.98529	2.00087	2.00338	2.03215
Alpha virt. eigenvalues --	2.06572	2.10393	2.10749	2.11554	2.15349
Alpha virt. eigenvalues --	2.16006	2.16253	2.20506	2.22128	2.22994
Alpha virt. eigenvalues --	2.25084	2.26037	2.34826	2.36193	2.39105
Alpha virt. eigenvalues --	2.39541	2.40646	2.43305	2.43825	2.45271
Alpha virt. eigenvalues --	2.45641	2.46458	2.48206	2.48369	2.48652
Alpha virt. eigenvalues --	2.49877	2.49972	2.50630	2.52333	2.52909
Alpha virt. eigenvalues --	2.54337	2.55896	2.57415	2.59904	2.60059
Alpha virt. eigenvalues --	2.61447	2.62912	2.63001	2.63543	2.63877
Alpha virt. eigenvalues --	2.65023	2.65556	2.66665	2.69415	2.72825
Alpha virt. eigenvalues --	2.72966	2.73587	2.73969	2.74220	2.75500
Alpha virt. eigenvalues --	2.76290	2.78373	2.79430	2.80787	2.81160
Alpha virt. eigenvalues --	2.81927	2.82119	2.82687	2.83545	2.84161
Alpha virt. eigenvalues --	2.84257	2.85323	2.85747	2.86362	2.86737
Alpha virt. eigenvalues --	2.87626	2.87915	2.88434	2.89145	2.89823
Alpha virt. eigenvalues --	2.90026	2.90920	2.91331	2.92171	2.93036
Alpha virt. eigenvalues --	2.93049	2.96180	2.97117	2.97353	2.98234
Alpha virt. eigenvalues --	2.99198	2.99330	3.00503	3.01157	3.02464
Alpha virt. eigenvalues --	3.03691	3.04173	3.05115	3.05290	3.06112

Supporting Information file

Alpha virt. eigenvalues --	3.06968	3.09380	3.10536	3.11850	3.12890
Alpha virt. eigenvalues --	3.13088	3.14267	3.15253	3.15528	3.16162
Alpha virt. eigenvalues --	3.17364	3.19726	3.20239	3.20541	3.22443
Alpha virt. eigenvalues --	3.22585	3.25884	3.26203	3.26424	3.26889
Alpha virt. eigenvalues --	3.27539	3.28972	3.30006	3.31788	3.31805
Alpha virt. eigenvalues --	3.32125	3.34004	3.34047	3.35084	3.36171
Alpha virt. eigenvalues --	3.36488	3.36557	3.37888	3.40448	3.40497
Alpha virt. eigenvalues --	3.41377	3.42553	3.43457	3.43521	3.44323
Alpha virt. eigenvalues --	3.48510	3.48779	3.49564	3.49721	3.52594
Alpha virt. eigenvalues --	3.54345	3.54886	3.55158	3.55931	3.57777
Alpha virt. eigenvalues --	3.58282	3.63219	3.63308	3.64243	3.66162
Alpha virt. eigenvalues --	3.66642	3.70949	3.71954	3.75863	3.76958
Alpha virt. eigenvalues --	3.79693	3.82502	3.83022	3.86054	3.87574
Alpha virt. eigenvalues --	3.88441	3.89760	3.91625	3.94769	3.96338
Alpha virt. eigenvalues --	3.98359	4.04724	4.04935	4.06137	4.08851
Alpha virt. eigenvalues --	4.09491	4.10420	4.10655	4.16563	4.16906
Alpha virt. eigenvalues --	4.19249	4.21263	4.22009	4.25228	4.30376
Alpha virt. eigenvalues --	4.31725	4.38658	4.40094	4.41147	4.48289
Alpha virt. eigenvalues --	4.49793	4.51308	4.53702	4.57236	4.58556
Alpha virt. eigenvalues --	4.61495	4.67897	4.73076	4.75597	4.76838
Alpha virt. eigenvalues --	4.77724	4.78139	4.79230	4.89536	4.90163
Alpha virt. eigenvalues --	4.92645	4.96840	4.99803	5.03008	5.04347
Alpha virt. eigenvalues --	5.05594	5.06108	5.08303	5.12228	5.14609
Alpha virt. eigenvalues --	5.17477	5.18973	5.20311	5.21334	5.23774
Alpha virt. eigenvalues --	5.23822	5.25105	5.28525	5.30983	5.32793
Alpha virt. eigenvalues --	5.40418	5.40523	5.48109	5.55173	5.60214
Alpha virt. eigenvalues --	5.62385	5.76190	5.82830	5.99685	6.02968
Alpha virt. eigenvalues --	6.14446	6.22586	22.16659	22.23400	22.50352
Alpha virt. eigenvalues --	22.84888	23.09533	23.23080	23.31108	23.42168
Alpha virt. eigenvalues --	23.61197	23.69701	23.79969	23.83195	23.91931
Alpha virt. eigenvalues --	23.94694	24.23848	24.29259		

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.875929	0.884298	0.505163	-0.090050	-0.085682	-0.057731
2	C	0.884298	4.869911	-0.085968	0.525382	-0.051217	-0.093478
3	C	0.505163	-0.085968	4.877048	-0.013447	0.884280	-0.006946
4	C	-0.090050	0.525382	-0.013447	4.882921	-0.006879	0.919487
5	C	-0.085682	-0.051217	0.884280	-0.006879	4.868805	-0.002156
6	C	-0.057731	-0.093478	-0.006946	0.919487	-0.002156	4.996634
7	C	-0.013420	-0.006884	-0.090250	-0.001223	0.525000	-0.000513
8	C	-0.009837	-0.021991	-0.001051	-0.105374	-0.000494	0.513962
9	C	-0.006917	-0.002149	-0.057644	-0.000508	-0.093179	-0.000030
10	C	-0.002426	-0.009679	-0.000358	-0.077807	-0.000132	-0.206969
11	C	-0.001051	-0.000489	-0.009797	0.000209	-0.021911	0.001967
12	C	-0.000215	-0.000776	-0.000056	-0.007249	-0.000121	-0.031763
13	C	-0.000359	-0.000129	-0.002410	-0.000124	-0.009624	0.000372
14	C	-0.000057	-0.000121	-0.000213	-0.001250	-0.000770	-0.009122
15	C	-0.000002	-0.000016	0.000002	-0.000271	0.000006	-0.002747

16	C	0.000002	0.000006	-0.000002	0.000111	-0.000016	0.001037

		7	8	9	10	11	12
1	C	-0.013420	-0.009837	-0.006917	-0.002426	-0.001051	-0.000215
2	C	-0.006884	-0.021991	-0.002149	-0.009679	-0.000489	-0.000776
3	C	-0.090250	-0.001051	-0.057644	-0.000358	-0.009797	-0.000056
4	C	-0.001223	-0.105374	-0.000508	-0.077807	0.000209	-0.007249
5	C	0.525000	-0.000494	-0.093179	-0.000132	-0.021911	-0.000121
6	C	-0.000513	0.513962	-0.000030	-0.206969	0.001967	-0.031763
7	C	4.883748	0.000209	0.919368	-0.000122	-0.105232	-0.001243
8	C	0.000209	5.069291	0.001968	0.610821	0.013746	-0.159530
9	C	0.919368	0.001968	4.995279	0.000365	0.513482	-0.009099
10	C	-0.000122	0.610821	0.000365	5.493673	0.000349	0.491076
11	C	-0.105232	0.013746	0.513482	0.000349	5.068779	-0.075527
12	C	-0.001243	-0.159530	-0.009099	0.491076	-0.075527	5.217464
13	C	-0.077520	0.000351	-0.206536	0.003978	0.611039	-0.046164
14	C	-0.007204	-0.075562	-0.031555	-0.046324	-0.158943	0.364928
15	C	0.000111	-0.020940	0.001033	-0.093337	0.011950	0.036601
16	C	-0.000271	0.011952	-0.002738	0.010300	-0.020896	0.104612

		13	14	15	16
1	C	-0.000359	-0.000057	-0.000002	0.000002
2	C	-0.000129	-0.000121	-0.000016	0.000006
3	C	-0.002410	-0.000213	0.000002	-0.000002
4	C	-0.000124	-0.001250	-0.000271	0.000111
5	C	-0.009624	-0.000770	0.000006	-0.000016
6	C	0.000372	-0.009122	-0.002747	0.001037
7	C	-0.077520	-0.007204	0.000111	-0.000271
8	C	0.000351	-0.075562	-0.020940	0.011952
9	C	-0.206536	-0.031555	0.001033	-0.002738
10	C	0.003978	-0.046324	-0.093337	0.010300
11	C	0.611039	-0.158943	0.011950	-0.020896
12	C	-0.046164	0.364928	0.036601	0.104612
13	C	5.492106	0.490539	0.010203	-0.093142
14	C	0.490539	5.217036	0.104731	0.036670
15	C	0.010203	0.104731	5.913528	0.105640
16	C	-0.093142	0.036670	0.105640	5.913104

Mulliken charges:

		1
1	C	0.002356
2	C	-0.006702
3	C	0.001650
4	C	-0.023928
5	C	-0.005909
6	C	-0.022005
7	C	-0.024554
8	C	0.172479
9	C	-0.021142
10	C	-0.173407
11	C	0.172325

```
   12  C    0.117063
   13  C   -0.172581
   14  C    0.117217
   15  C   -0.066492
   16  C   -0.066370
 Sum of Mulliken charges =  -0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
                1
    1  C    0.002356
    2  C   -0.006702
    3  C    0.001650
    4  C   -0.023928
    5  C   -0.005909
    6  C   -0.022005
    7  C   -0.024554
    8  C    0.172479
    9  C   -0.021142
   10  C   -0.173407
   11  C    0.172325
   12  C    0.117063
   13  C   -0.172581
   14  C    0.117217
   15  C   -0.066492
   16  C   -0.066370
 Electronic spatial extent (au):  <R**2>=           3544.7415
 Charge=           -0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=            3.8545    Y=           -0.0035    Z=           -0.0003  Tot=            3.8545
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=         -103.3334   YY=          -85.1444   ZZ=          -90.9433
   XY=           -0.0031   XZ=            0.0018   YZ=           -1.6871
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=          -10.1930   YY=            7.9960   ZZ=            2.1971
   XY=           -0.0031   XZ=            0.0018   YZ=           -1.6871
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=          121.5883  YYY=           -0.0319  ZZZ=           -0.0049  XYY=            4.1229
  XXY=           -0.0097  XXZ=           -0.0023  XZZ=           17.3257  YZZ=           -0.0021
  YYZ=            0.0005  XYZ=            6.8734
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=         -4135.0365 YYYY=         -1695.6462 ZZZZ=          -137.2008 XXXY=           -
0.0650
 XXXZ=           -0.0015 YYYX=           -0.0240 YYYZ=           -3.3929 ZZZX=            0.0197
 ZZZY=           -4.0586 XXYY=          -878.9386 XXZZ=          -703.0480 YYZZ=           -
309.2486
 XXYZ=          -32.3114 YYXZ=            0.0000 ZZXY=            0.0033
 N-N= 7.176436409760D+02 E-N=-2.846286593279D+03  KE= 6.062420690731D+02
 No NMR shielding tensors so no spin-rotation constants.
```

Supporting Information file

Leave Link 601 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 2.2 elap: 0.4
(Enter /home/user/gauss16/g16/l9999.exe)
Unable to Open any file for archive entry.
1\1\GINC-MAKCLUS\FOpt\RwB97XD\def2TZVP\C16\USER\21-Aug-2026\0\\#p opt freq wb97xd/Def2TZVP\\title card\\0,1\C,3.6228376463,-0.6732249818,0.0117161678\C,3.0074903508,-1.7268103129,0.053561589\C,3.6219990344,0.6752517291,-0.0114804595\C,1.8549727576,-2.4264821233,0.0559489129\C,3.0067757714,1.7288968719,-0.053435984\C,0.6450102379,-2.5723325127,0.0637503509\C,1.8534597591,2.4273050814,-0.0559576911\C,-0.6659496215,-2.2540395139,0.0220162976\C,0.64348505,2.5729602883,-0.0638397256\C,-1.7312599731,-1.6716930394,-0.0218764649\C,-0.6672294743,2.2535625776,-0.0221657635\C,-2.6868018486,-0.6807603584,-0.1666389885\C,-1.7322778476,1.6707178542,0.0214559206\C,-2.6871144989,0.6791381312,0.1664592453\C,-4.0427351084,-0.4053452265,-0.6008413095\C,-4.0426632352,0.4028545352,0.6013289025\\Version=ES64L-G16RevC.01\State=1-A\HF=-608.9815402\RMSD=6.404e-09\RMSF=1.114e-04\Dipole=1.5164864,-0.0008938,-0.0001213\Quadrupole=-7.5782732,5.9387743,1.6394989,-0.0065292,0.0016962,-1.2646285\PG=C01 [X(C16)]\\@
The archive entry for this job was punched.

QUANTUM MECHANICS IS BOHRING -- M.S. GORDON
Leave Link 9999 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
Job cpu time: 0 days 17 hours 48 minutes 58.4 seconds.
Elapsed time: 0 days 2 hours 58 minutes 12.7 seconds.
File lengths (MBytes): RWF= 155 Int= 0 D2E= 0 Chk= 19 Scr= 1
Normal termination of Gaussian 16 at Fri Aug 21 20:45:02 2026.
(Enter /home/user/gauss16/g16/l1.exe)
Link1: Proceeding to internal job step number 2.

#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RwB97XD/def2TZVP Freq
---
1/10=4,29=7,30=1,38=1,40=1/1,3;
2/12=2,40=1/2;
3/5=44,7=101,11=2,14=-4,25=1,30=1,70=2,71=2,74=-58,116=1,140=1/1,2,3;
4/5=101/1;
5/5=2,38=6,98=1/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
Leave Link 1 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0

Supporting Information file

(Enter /home/user/gauss16/g16/l101.exe)
Structure from the checkpoint file: "cdca.chk"
---
title card

Charge = 0 Multiplicity = 1
Redundant internal coordinates found in file. (old form).
C,0,3.6228376463,-0.6732249818,0.0117161678
C,0,3.0074903508,-1.7268103129,0.053561589
C,0,3.6219990344,0.6752517291,-0.0114804595
C,0,1.8549727576,-2.4264821233,0.0559489129
C,0,3.0067757714,1.7288968719,-0.053435984
C,0,0.6450102379,-2.5723325127,0.0637503509
C,0,1.8534597591,2.4273050814,-0.0559576911
C,0,-0.6659496215,-2.2540395139,0.0220162976
C,0,0.64348505,2.5729602883,-0.0638397256
C,0,-1.7312599731,-1.6716930394,-0.0218764649
C,0,-0.6672294743,2.2535625776,-0.0221657635
C,0,-2.6868018486,-0.6807603584,-0.1666389885
C,0,-1.7322778476,1.6707178542,0.0214559206
C,0,-2.6871144989,0.6791381312,0.1664592453
C,0,-4.0427351084,-0.4053452265,-0.6008413095
C,0,-4.0426632352,0.4028545352,0.6013289025
Recover connectivity data from disk.
ITRead= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MicOpt= -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
NAtoms= 16 NQM= 16 NQMF= 0 NMMI= 0 NMMIF= 0
NMic= 0 NMicF= 0.
Isotopes and Nuclear Properties:
(Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic moments (NMagM)
in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10
IAtWgt= 12 12 12 12 12 12 12 12 12 12
AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000
12.0000000 12.0000000 12.0000000 12.0000000
NucSpn= 0 0 0 0 0 0 0 0 0 0
AtZEff= 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000
3.6000000 3.6000000 3.6000000
NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
0.0000000 0.0000000 0.0000000
NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
0.0000000 0.0000000 0.0000000
AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000
6.0000000 6.0000000 6.0000000

Atom 11 12 13 14 15 16
IAtWgt= 12 12 12 12 12 12

Supporting Information file

```
 AtmWgt=  12.0000000  12.0000000  12.0000000  12.0000000  12.0000000  12.0000000
 NucSpn=          0          0          0          0          0          0
 AtZEff=   3.6000000   3.6000000   3.6000000   3.6000000   3.6000000   3.6000000
 NQMom=    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
 NMagM=    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
 AtZNuc=   6.0000000   6.0000000   6.0000000   6.0000000   6.0000000   6.0000000
 Leave Link  101 at Fri Aug 21 20:45:03 2026, MaxMem=    805306368 cpu:                2.1 elap:
0.4
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
 --------------------------                          --------------------------
 ! Name  Definition              Value          Derivative Info.                !
 --------------------------------------------------------------------------------
 ! R1    R(1,2)                  1.2208         calculate D2E/DX2 analytically  !
 ! R2    R(1,3)                  1.3487         calculate D2E/DX2 analytically  !
 ! R3    R(2,4)                  1.3483         calculate D2E/DX2 analytically  !
 ! R4    R(3,5)                  1.2208         calculate D2E/DX2 analytically  !
 ! R5    R(4,6)                  1.2187         calculate D2E/DX2 analytically  !
 ! R6    R(5,7)                  1.3483         calculate D2E/DX2 analytically  !
 ! R7    R(6,8)                  1.3497         calculate D2E/DX2 analytically  !
 ! R8    R(7,9)                  1.2187         calculate D2E/DX2 analytically  !
 ! R9    R(8,10)                 1.2149         calculate D2E/DX2 analytically  !
 ! R10   R(9,11)                 1.3497         calculate D2E/DX2 analytically  !
 ! R11   R(10,12)                1.3842         calculate D2E/DX2 analytically  !
 ! R12   R(11,13)                1.2149         calculate D2E/DX2 analytically  !
 ! R13   R(12,14)                1.4001         calculate D2E/DX2 analytically  !
 ! R14   R(12,15)                1.4502         calculate D2E/DX2 analytically  !
 ! R15   R(13,14)                1.3842         calculate D2E/DX2 analytically  !
 ! R16   R(14,16)                1.4502         calculate D2E/DX2 analytically  !
 ! R17   R(15,16)                1.4486         calculate D2E/DX2 analytically  !
 ! A1    A(2,1,3)                149.6721       calculate D2E/DX2 analytically  !
 ! A2    A(1,2,4)                151.4933       calculate D2E/DX2 analytically  !
 ! A3    A(1,3,5)                149.7496       calculate D2E/DX2 analytically  !
 ! A4    A(2,4,6)                155.611        calculate D2E/DX2 analytically  !
 ! A5    A(3,5,7)                151.4236       calculate D2E/DX2 analytically  !
 ! A6    A(4,6,8)                159.3713       calculate D2E/DX2 analytically  !
 ! A7    A(5,7,9)                155.6653       calculate D2E/DX2 analytically  !
 ! A8    A(7,9,11)               159.3325       calculate D2E/DX2 analytically  !
 ! A9    A(8,10,12)              162.2277       calculate D2E/DX2 analytically  !
 ! A10   A(10,12,14)             132.1145       calculate D2E/DX2 analytically  !
 ! A11   A(10,12,15)             144.366        calculate D2E/DX2 analytically  !
 ! A12   A(14,12,15)             83.4862        calculate D2E/DX2 analytically  !
```

Supporting Information file

```
 ! A13   A(11,13,14)          162.2098         calculate D2E/DX2 analytically  !
 ! A14   A(12,14,13)          132.1225         calculate D2E/DX2 analytically  !
 ! A15   A(12,14,16)           83.4831         calculate D2E/DX2 analytically  !
 ! A16   A(13,14,16)          144.3616         calculate D2E/DX2 analytically  !
 ! A17   A(12,15,16)           81.8034         calculate D2E/DX2 analytically  !
 ! A18   A(14,16,15)           81.8061         calculate D2E/DX2 analytically  !
 ! A19   L(6,8,10,7,-1)       164.9895         calculate D2E/DX2 analytically  !
 ! A20   L(9,11,13,4,-1)      165.0111         calculate D2E/DX2 analytically  !
 ! A21   L(6,8,10,7,-2)       179.9856         calculate D2E/DX2 analytically  !
 ! A22   L(9,11,13,4,-2)      179.9957         calculate D2E/DX2 analytically  !
 ! D1    D(3,1,2,4)             4.8138         calculate D2E/DX2 analytically  !
 ! D2    D(2,1,3,5)            -4.4253         calculate D2E/DX2 analytically  !
 ! D3    D(1,2,4,6)            -4.5956         calculate D2E/DX2 analytically  !
 ! D4    D(1,3,5,7)             4.8162         calculate D2E/DX2 analytically  !
 ! D5    D(2,4,6,8)             6.5774         calculate D2E/DX2 analytically  !
 ! D6    D(3,5,7,9)            -4.5852         calculate D2E/DX2 analytically  !
 ! D7    D(4,6,10,12)           5.4468         calculate D2E/DX2 analytically  !
 ! D8    D(5,7,9,11)            6.5651         calculate D2E/DX2 analytically  !
 ! D9    D(7,9,13,14)           5.496          calculate D2E/DX2 analytically  !
 ! D10   D(8,10,12,14)        -36.7476         calculate D2E/DX2 analytically  !
 ! D11   D(8,10,12,15)        146.2131         calculate D2E/DX2 analytically  !
 ! D12   D(10,12,14,13)        43.0305         calculate D2E/DX2 analytically  !
 ! D13   D(10,12,14,16)      -138.695          calculate D2E/DX2 analytically  !
 ! D14   D(15,12,14,13)      -138.7051         calculate D2E/DX2 analytically  !
 ! D15   D(15,12,14,16)        39.5693         calculate D2E/DX2 analytically  !
 ! D16   D(10,12,15,16)       137.989          calculate D2E/DX2 analytically  !
 ! D17   D(14,12,15,16)       -39.8008         calculate D2E/DX2 analytically  !
 ! D18   D(11,13,14,12)       -36.8236         calculate D2E/DX2 analytically  !
 ! D19   D(11,13,14,16)       146.1196         calculate D2E/DX2 analytically  !
 ! D20   D(12,14,16,15)       -39.8006         calculate D2E/DX2 analytically  !
 ! D21   D(13,14,16,15)       138.0026         calculate D2E/DX2 analytically  !
 ! D22   D(12,15,16,14)        38.343          calculate D2E/DX2 analytically  !
 ---------------------------------------------------------------------------
  Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07 EigMax=2.50D+02 EigMin=1.00D-
04
 Number of steps in this run=      2 maximum allowed number of steps=      2.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

  Leave Link  103 at Fri Aug 21 20:45:03 2026, MaxMem=    805306368 cpu:                0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l202.exe)
                      Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.622838   -0.673225    0.011716
     2          6           0        3.007490   -1.726810    0.053562
```

3	6	0	3.621999	0.675252	-0.011480
4	6	0	1.854973	-2.426482	0.055949
5	6	0	3.006776	1.728897	-0.053436
6	6	0	0.645010	-2.572333	0.063750
7	6	0	1.853460	2.427305	-0.055958
8	6	0	-0.665950	-2.254040	0.022016
9	6	0	0.643485	2.572960	-0.063840
10	6	0	-1.731260	-1.671693	-0.021876
11	6	0	-0.667229	2.253563	-0.022166
12	6	0	-2.686802	-0.680760	-0.166639
13	6	0	-1.732278	1.670718	0.021456
14	6	0	-2.687114	0.679138	0.166459
15	6	0	-4.042735	-0.405345	-0.600841
16	6	0	-4.042663	0.402855	0.601329

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220838	0.000000			
3	C	1.348676	2.480273	0.000000		
4	C	2.490224	1.348274	3.570390	0.000000	
5	C	2.480719	3.457363	1.220831	4.313443	0.000000
6	C	3.532248	2.509248	4.406237	1.218746	4.908385
7	C	3.570513	4.312825	2.489860	4.855077	1.348302
8	C	4.570862	3.711216	5.193108	2.527041	5.418338
9	C	4.406809	4.908190	3.532079	5.145530	2.509521
10	C	5.446506	4.739671	5.845138	3.665628	5.832151
11	C	5.193449	5.417810	4.570411	5.316994	3.711410
12	C	6.312164	5.793762	6.454751	4.870812	6.183534
13	C	5.845633	5.831778	5.446129	5.445788	4.740002
14	C	6.455101	6.183030	6.311624	5.503421	5.794026
15	C	7.694673	7.202791	7.762937	6.268917	7.385814
16	C	7.763085	7.385133	7.693945	6.563893	7.202895

		6	7	8	9	10
6	C	0.000000				
7	C	5.145003	0.000000			
8	C	1.349692	5.316812	0.000000		
9	C	5.146875	1.218736	5.002191	0.000000	
10	C	2.542665	5.445472	1.214883	4.863975	0.000000
11	C	5.001861	2.526896	4.507819	1.349713	4.066914
12	C	3.838241	5.503299	2.568003	4.657046	1.384184
13	C	4.863822	3.665506	4.067035	2.542748	3.342692
14	C	4.656787	4.870562	3.565039	3.838293	2.544707
15	C	5.206964	6.563987	3.899782	5.578471	2.698473
16	C	5.578083	6.268548	4.335537	5.206899	3.167762

		11	12	13	14	15
11	C	0.000000				
12	C	3.565080	0.000000			

```
  13  C    1.214882   2.544788   0.000000
  14  C    2.567942   1.400099   1.384185   0.000000
  15  C    4.335746   1.450152   3.167886   1.898041   0.000000
  16  C    3.899669   1.897987   2.698446   1.450157   1.448586
            16
  16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 4.71D-16
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.622628   -0.674380    0.010077
     2          6           0        3.006952   -1.727871    0.049402
     3          6           0        3.622209    0.674148   -0.009889
     4          6           0        1.854217   -2.427187    0.050122
     5          6           0        3.007314    1.728083   -0.049316
     6          6           0        0.644209   -2.572679    0.057583
     7          6           0        1.854216    2.426854   -0.050156
     8          6           0       -0.666652   -2.253878    0.016621
     9          6           0        0.644287    2.572905   -0.057680
    10          6           0       -1.731781   -1.671096   -0.025869
    11          6           0       -0.666527    2.253817   -0.016762
    12          6           0       -2.687015   -0.679522   -0.168250
    13          6           0       -1.731757    1.671202    0.025471
    14          6           0       -2.686902    0.679575    0.168105
    15          6           0       -4.042865   -0.402644   -0.601781
    16          6           0       -4.042533    0.402673    0.602322
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8474928           0.3941534           0.2718102
 Leave Link  202 at Fri Aug 21 20:45:03 2026, MaxMem=    805306368 cpu:                 0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.6511336511 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
```

IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074926751 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.6436409760 Hartrees.
Leave Link 301 at Fri Aug 21 20:45:03 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.36D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 564 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 20:45:04 2026, MaxMem= 805306368 cpu: 3.9 elap: 0.7
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 20:45:04 2026, MaxMem= 805306368 cpu: 0.6 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000000 0.000000 -0.000000 Ang= 0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 20:45:04 2026, MaxMem= 805306368 cpu: 3.2 elap: 0.5
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.

Supporting Information file

```
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -608.981540194378
 DIIS: error= 1.54D-08 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -608.981540194378     IErMin= 1 ErrMin= 1.54D-08
 ErrMax= 1.54D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-14 BMatP= 4.16D-14
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.100D+01
 Coeff:      0.100D+01
 Gap=     0.247 Goal=   None    Shift=    0.000
 RMSDP=2.74D-09 MaxDP=9.39D-08              OVMax= 2.55D-07

 SCF Done:  E(RwB97XD) =  -608.981540194     A.U. after    1 cycles
          NFock=  1  Conv=0.27D-08     -V/T= 2.0045
 KE= 6.062420692550D+02 PE=-2.846286593461D+03 EE= 9.134193430358D+02
 Leave Link  502 at Fri Aug 21 20:46:20 2026, MaxMem=    805306368 cpu:               454.4 elap:
75.8
 (Enter /home/user/gauss16/g16/l801.exe)
 DoSCS=F DFT=T ScalE2(SS,OS)=  1.000000  1.000000
 Range of M.O.s used for correlation:     1   496
 NBasis=   496 NAE=    48 NBE=    48 NFC=     0 NFV=     0
 NROrb=    496 NOA=    48 NOB=    48 NVA=   448 NVB=   448

 **** Warning!!: The largest alpha MO coefficient is  0.62069364D+02

 Leave Link  801 at Fri Aug 21 20:46:20 2026, MaxMem=    805306368 cpu:                 0.4 elap:
0.1
 (Enter /home/user/gauss16/g16/l1101.exe)
 Using compressed storage, NAtomX=    16.
 Will process     17 centers per pass.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33580.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
 Leave Link 1101 at Fri Aug 21 20:46:22 2026, MaxMem=    805306368 cpu:                12.4 elap:
2.1
 (Enter /home/user/gauss16/g16/l1102.exe)
 Symmetrizing basis deriv contribution to polar:
```

IMax=3 JMax=2 DiffMx= 0.00D+00
Leave Link 1102 at Fri Aug 21 20:46:23 2026, MaxMem= 805306368 cpu: 0.8 elap: 0.2
(Enter /home/user/gauss16/g16/l1110.exe)
Forming Gx(P) for the SCF density, NAtomX= 16.
Integral derivatives from FoFJK, PRISM(SPDF).
Do as many integral derivatives as possible in FoFJK.
G2DrvN: MDV= 805304616.
G2DrvN: will do 17 centers at a time, making 1 passes.
Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.
FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 3507 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
End of G2Drv F.D. properties file 721 does not exist.
End of G2Drv F.D. properties file 722 does not exist.
End of G2Drv F.D. properties file 788 does not exist.
Leave Link 1110 at Fri Aug 21 21:01:07 2026, MaxMem= 805306368 cpu: 5305.4 elap: 884.4
(Enter /home/user/gauss16/g16/l1002.exe)
Minotr: Closed shell wavefunction.
IDoAtm=1111111111111111
Direct CPHF calculation.
Differentiating once with respect to electric field.
with respect to dipole field.
Differentiating once with respect to nuclear coordinates.
Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.
Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.
NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.
4769 words used for storage of precomputed grid.
Two-electron integrals replicated using symmetry.
MDV= 805306368 using IRadAn= 1.
Solving linear equations simultaneously, MaxMat= 384.
FoF2E skips out because all densities are zero.
CalDSu exits because no D1Ps are significant.
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 48 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2 IDoP0=3 IntGTp=3.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 48 NMatS0= 48 NMatT0= 0 NMatD0= 48 NMtDS0= 0 NMtDT0= 0
Integrals replicated using symmetry in FoFCou.
There are 51 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.
48 vectors produced by pass 0 Test12= 4.22D-14 1.96D-09 XBig12= 4.14D+02 1.03D+01.
AX will form 48 AO Fock derivatives at one time.

48 vectors produced by pass 1 Test12= 4.22D-14 1.96D-09 XBig12= 7.35D+01 1.52D+00.
48 vectors produced by pass 2 Test12= 4.22D-14 1.96D-09 XBig12= 5.91D+00 5.19D-01.
48 vectors produced by pass 3 Test12= 4.22D-14 1.96D-09 XBig12= 2.41D-01 9.54D-02.
48 vectors produced by pass 4 Test12= 4.22D-14 1.96D-09 XBig12= 4.53D-03 1.33D-02.
48 vectors produced by pass 5 Test12= 4.22D-14 1.96D-09 XBig12= 5.55D-05 8.86D-04.
48 vectors produced by pass 6 Test12= 4.22D-14 1.96D-09 XBig12= 5.43D-07 8.46D-05.
48 vectors produced by pass 7 Test12= 4.22D-14 1.96D-09 XBig12= 4.09D-09 9.80D-06.
21 vectors produced by pass 8 Test12= 4.22D-14 1.96D-09 XBig12= 3.74D-11 1.05D-06.
3 vectors produced by pass 9 Test12= 4.22D-14 1.96D-09 XBig12= 3.42D-13 8.25D-08.
3 vectors produced by pass 10 Test12= 4.22D-14 1.96D-09 XBig12= 7.80D-15 1.17D-08.
3 vectors produced by pass 11 Test12= 4.22D-14 1.96D-09 XBig12= 2.77D-14 3.04D-08.
2 vectors produced by pass 12 Test12= 4.22D-14 1.96D-09 XBig12= 6.72D-15 1.31D-08.
InvSVY: IOpt=1 It= 1 EMax= 8.88D-15
Solved reduced A of dimension 416 with 51 vectors.
FullF1: Do perturbations 1 to 3.
Isotropic polarizability for W= 0.000000 217.59 Bohr**3.
End of Minotr F.D. properties file 721 does not exist.
End of Minotr F.D. properties file 722 does not exist.
End of Minotr F.D. properties file 788 does not exist.
Leave Link 1002 at Fri Aug 21 21:42:01 2026, MaxMem= 805306368 cpu: 14720.2 elap: 2453.7
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

****

Population analysis using the SCF Density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Alpha virt. eigenvalues --	0.49117	0.50284	0.50725	0.50921	0.52249
Alpha virt. eigenvalues --	0.52732	0.52984	0.53200	0.54297	0.54536
Alpha virt. eigenvalues --	0.54926	0.55685	0.56069	0.56549	0.58161
Alpha virt. eigenvalues --	0.58302	0.59013	0.59185	0.59368	0.60396
Alpha virt. eigenvalues --	0.61116	0.63299	0.63574	0.63723	0.64293
Alpha virt. eigenvalues --	0.65210	0.67191	0.67561	0.67944	0.68624
Alpha virt. eigenvalues --	0.70914	0.71012	0.72044	0.72422	0.74301
Alpha virt. eigenvalues --	0.75848	0.76815	0.77208	0.78800	0.79808
Alpha virt. eigenvalues --	0.80557	0.84401	0.84818	0.85440	0.85915
Alpha virt. eigenvalues --	0.86699	0.90213	0.91512	0.92663	0.92870
Alpha virt. eigenvalues --	0.93592	0.95722	0.96684	0.98165	0.99140
Alpha virt. eigenvalues --	1.01137	1.01981	1.02368	1.05797	1.07381
Alpha virt. eigenvalues --	1.09301	1.09335	1.09879	1.12188	1.12432
Alpha virt. eigenvalues --	1.13358	1.15262	1.15994	1.16387	1.18464
Alpha virt. eigenvalues --	1.19675	1.22055	1.23127	1.23523	1.23875
Alpha virt. eigenvalues --	1.26222	1.27253	1.27711	1.27775	1.30100
Alpha virt. eigenvalues --	1.31458	1.33407	1.34466	1.35849	1.36137
Alpha virt. eigenvalues --	1.37502	1.38475	1.39202	1.39243	1.40757
Alpha virt. eigenvalues --	1.41670	1.42611	1.43166	1.43339	1.43747
Alpha virt. eigenvalues --	1.45417	1.46011	1.47089	1.48236	1.48834
Alpha virt. eigenvalues --	1.49155	1.49688	1.49957	1.50561	1.50861
Alpha virt. eigenvalues --	1.51264	1.53178	1.54048	1.54566	1.57963
Alpha virt. eigenvalues --	1.59431	1.61318	1.61735	1.62193	1.62991
Alpha virt. eigenvalues --	1.63954	1.64765	1.65752	1.67667	1.69594
Alpha virt. eigenvalues --	1.69727	1.71038	1.71633	1.72894	1.72985
Alpha virt. eigenvalues --	1.74463	1.76303	1.77824	1.77871	1.78794
Alpha virt. eigenvalues --	1.79143	1.81311	1.82715	1.84830	1.85724
Alpha virt. eigenvalues --	1.85892	1.86104	1.90730	1.92761	1.97301
Alpha virt. eigenvalues --	1.97394	1.98529	2.00087	2.00338	2.03215
Alpha virt. eigenvalues --	2.06572	2.10393	2.10749	2.11554	2.15349
Alpha virt. eigenvalues --	2.16006	2.16253	2.20506	2.22128	2.22994
Alpha virt. eigenvalues --	2.25084	2.26037	2.34826	2.36193	2.39105
Alpha virt. eigenvalues --	2.39541	2.40646	2.43305	2.43825	2.45271
Alpha virt. eigenvalues --	2.45641	2.46458	2.48206	2.48369	2.48652
Alpha virt. eigenvalues --	2.49877	2.49972	2.50630	2.52333	2.52909
Alpha virt. eigenvalues --	2.54337	2.55896	2.57415	2.59904	2.60059
Alpha virt. eigenvalues --	2.61447	2.62912	2.63001	2.63543	2.63877
Alpha virt. eigenvalues --	2.65023	2.65556	2.66665	2.69415	2.72825
Alpha virt. eigenvalues --	2.72966	2.73587	2.73969	2.74220	2.75500
Alpha virt. eigenvalues --	2.76290	2.78373	2.79430	2.80787	2.81160
Alpha virt. eigenvalues --	2.81927	2.82119	2.82687	2.83545	2.84161
Alpha virt. eigenvalues --	2.84257	2.85323	2.85747	2.86362	2.86737
Alpha virt. eigenvalues --	2.87626	2.87915	2.88434	2.89145	2.89823
Alpha virt. eigenvalues --	2.90026	2.90920	2.91331	2.92171	2.93036
Alpha virt. eigenvalues --	2.93049	2.96180	2.97117	2.97353	2.98234
Alpha virt. eigenvalues --	2.99198	2.99330	3.00503	3.01157	3.02464
Alpha virt. eigenvalues --	3.03691	3.04173	3.05115	3.05290	3.06112
Alpha virt. eigenvalues --	3.06968	3.09380	3.10536	3.11850	3.12890

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Alpha virt. eigenvalues --	3.13088	3.14267	3.15253	3.15528	3.16162
Alpha virt. eigenvalues --	3.17364	3.19726	3.20239	3.20541	3.22443
Alpha virt. eigenvalues --	3.22585	3.25884	3.26203	3.26424	3.26889
Alpha virt. eigenvalues --	3.27539	3.28972	3.30006	3.31788	3.31805
Alpha virt. eigenvalues --	3.32125	3.34004	3.34047	3.35084	3.36171
Alpha virt. eigenvalues --	3.36488	3.36557	3.37888	3.40448	3.40497
Alpha virt. eigenvalues --	3.41377	3.42553	3.43457	3.43521	3.44323
Alpha virt. eigenvalues --	3.48510	3.48779	3.49564	3.49721	3.52594
Alpha virt. eigenvalues --	3.54345	3.54886	3.55158	3.55931	3.57777
Alpha virt. eigenvalues --	3.58282	3.63219	3.63308	3.64243	3.66162
Alpha virt. eigenvalues --	3.66642	3.70949	3.71954	3.75863	3.76958
Alpha virt. eigenvalues --	3.79693	3.82502	3.83022	3.86054	3.87574
Alpha virt. eigenvalues --	3.88441	3.89760	3.91625	3.94769	3.96338
Alpha virt. eigenvalues --	3.98359	4.04724	4.04935	4.06137	4.08851
Alpha virt. eigenvalues --	4.09491	4.10420	4.10655	4.16563	4.16906
Alpha virt. eigenvalues --	4.19249	4.21263	4.22009	4.25228	4.30376
Alpha virt. eigenvalues --	4.31725	4.38658	4.40094	4.41147	4.48289
Alpha virt. eigenvalues --	4.49793	4.51308	4.53702	4.57236	4.58556
Alpha virt. eigenvalues --	4.61495	4.67897	4.73076	4.75597	4.76838
Alpha virt. eigenvalues --	4.77724	4.78139	4.79230	4.89536	4.90163
Alpha virt. eigenvalues --	4.92645	4.96840	4.99803	5.03008	5.04347
Alpha virt. eigenvalues --	5.05594	5.06108	5.08303	5.12228	5.14609
Alpha virt. eigenvalues --	5.17477	5.18973	5.20311	5.21334	5.23774
Alpha virt. eigenvalues --	5.23822	5.25105	5.28525	5.30983	5.32793
Alpha virt. eigenvalues --	5.40418	5.40523	5.48109	5.55173	5.60214
Alpha virt. eigenvalues --	5.62385	5.76190	5.82830	5.99685	6.02968
Alpha virt. eigenvalues --	6.14446	6.22586	22.16659	22.23400	22.50352
Alpha virt. eigenvalues --	22.84888	23.09533	23.23080	23.31108	23.42168
Alpha virt. eigenvalues --	23.61197	23.69701	23.79969	23.83195	23.91931
Alpha virt. eigenvalues --	23.94694	24.23848	24.29259		

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.875929	0.884298	0.505163	-0.090050	-0.085682	-0.057731
2	C	0.884298	4.869912	-0.085968	0.525382	-0.051217	-0.093478
3	C	0.505163	-0.085968	4.877048	-0.013447	0.884280	-0.006946
4	C	-0.090050	0.525382	-0.013447	4.882921	-0.006879	0.919487
5	C	-0.085682	-0.051217	0.884280	-0.006879	4.868805	-0.002156
6	C	-0.057731	-0.093478	-0.006946	0.919487	-0.002156	4.996634
7	C	-0.013420	-0.006884	-0.090250	-0.001223	0.525000	-0.000513
8	C	-0.009837	-0.021991	-0.001051	-0.105374	-0.000494	0.513962
9	C	-0.006917	-0.002149	-0.057644	-0.000508	-0.093179	-0.000030
10	C	-0.002426	-0.009679	-0.000358	-0.077807	-0.000132	-0.206969
11	C	-0.001051	-0.000489	-0.009797	0.000209	-0.021911	0.001967
12	C	-0.000215	-0.000776	-0.000056	-0.007249	-0.000121	-0.031763
13	C	-0.000359	-0.000129	-0.002410	-0.000124	-0.009624	0.000372
14	C	-0.000057	-0.000121	-0.000213	-0.001250	-0.000770	-0.009122
15	C	-0.000002	-0.000016	0.000002	-0.000271	0.000006	-0.002747
16	C	0.000002	0.000006	-0.000002	0.000111	-0.000016	0.001037

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		7	8	9	10	11	12
1	C	-0.013420	-0.009837	-0.006917	-0.002426	-0.001051	-0.000215
2	C	-0.006884	-0.021991	-0.002149	-0.009679	-0.000489	-0.000776
3	C	-0.090250	-0.001051	-0.057644	-0.000358	-0.009797	-0.000056
4	C	-0.001223	-0.105374	-0.000508	-0.077807	0.000209	-0.007249
5	C	0.525000	-0.000494	-0.093179	-0.000132	-0.021911	-0.000121
6	C	-0.000513	0.513962	-0.000030	-0.206969	0.001967	-0.031763
7	C	4.883748	0.000209	0.919368	-0.000122	-0.105232	-0.001243
8	C	0.000209	5.069291	0.001968	0.610821	0.013746	-0.159530
9	C	0.919368	0.001968	4.995279	0.000365	0.513482	-0.009099
10	C	-0.000122	0.610821	0.000365	5.493673	0.000349	0.491076
11	C	-0.105232	0.013746	0.513482	0.000349	5.068779	-0.075527
12	C	-0.001243	-0.159530	-0.009099	0.491076	-0.075527	5.217465
13	C	-0.077520	0.000351	-0.206536	0.003978	0.611039	-0.046164
14	C	-0.007204	-0.075562	-0.031555	-0.046324	-0.158943	0.364928
15	C	0.000111	-0.020940	0.001033	-0.093337	0.011950	0.036601
16	C	-0.000271	0.011952	-0.002738	0.010300	-0.020896	0.104612

		13	14	15	16
1	C	-0.000359	-0.000057	-0.000002	0.000002
2	C	-0.000129	-0.000121	-0.000016	0.000006
3	C	-0.002410	-0.000213	0.000002	-0.000002
4	C	-0.000124	-0.001250	-0.000271	0.000111
5	C	-0.009624	-0.000770	0.000006	-0.000016
6	C	0.000372	-0.009122	-0.002747	0.001037
7	C	-0.077520	-0.007204	0.000111	-0.000271
8	C	0.000351	-0.075562	-0.020940	0.011952
9	C	-0.206536	-0.031555	0.001033	-0.002738
10	C	0.003978	-0.046324	-0.093337	0.010300
11	C	0.611039	-0.158943	0.011950	-0.020896
12	C	-0.046164	0.364928	0.036601	0.104612
13	C	5.492106	0.490539	0.010203	-0.093142
14	C	0.490539	5.217036	0.104731	0.036670
15	C	0.010203	0.104731	5.913528	0.105640
16	C	-0.093142	0.036670	0.105640	5.913104

Mulliken charges:

		1
1	C	0.002356
2	C	-0.006702
3	C	0.001650
4	C	-0.023928
5	C	-0.005909
6	C	-0.022005
7	C	-0.024554
8	C	0.172479
9	C	-0.021142
10	C	-0.173407
11	C	0.172325
12	C	0.117063

13 C -0.172581
14 C 0.117217
15 C -0.066492
16 C -0.066369
Sum of Mulliken charges = -0.00000
Mulliken charges with hydrogens summed into heavy atoms:
1
1 C 0.002356
2 C -0.006702
3 C 0.001650
4 C -0.023928
5 C -0.005909
6 C -0.022005
7 C -0.024554
8 C 0.172479
9 C -0.021142
10 C -0.173407
11 C 0.172325
12 C 0.117063
13 C -0.172581
14 C 0.117217
15 C -0.066492
16 C -0.066369
APT charges:
1
1 C 0.013827
2 C -0.045402
3 C 0.015993
4 C 0.084501
5 C -0.047409
6 C -0.081372
7 C 0.086202
8 C 0.137229
9 C -0.082796
10 C -0.185599
11 C 0.138393
12 C 0.207257
13 C -0.186590
14 C 0.208124
15 C -0.131092
16 C -0.131265
Sum of APT charges = 0.00000
APT charges with hydrogens summed into heavy atoms:
1
1 C 0.013827
2 C -0.045402
3 C 0.015993
4 C 0.084501

```
     5  C   -0.047409
     6  C   -0.081372
     7  C    0.086202
     8  C    0.137229
     9  C   -0.082796
    10  C   -0.185599
    11  C    0.138393
    12  C    0.207257
    13  C   -0.186590
    14  C    0.208124
    15  C   -0.131092
    16  C   -0.131265
 Electronic spatial extent (au):  <R**2>=           3544.7415
 Charge=           0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=            3.8545    Y=           -0.0035    Z=           -0.0003  Tot=            3.8545
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=         -103.3333   YY=          -85.1444   ZZ=          -90.9433
   XY=           -0.0031   XZ=            0.0018   YZ=           -1.6871
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=          -10.1930   YY=            7.9960   ZZ=            2.1971
   XY=           -0.0031   XZ=            0.0018   YZ=           -1.6871
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=          121.5883  YYY=           -0.0319  ZZZ=           -0.0049  XYY=            4.1229
  XXY=           -0.0097  XXZ=           -0.0023  XZZ=           17.3257  YZZ=           -0.0021
  YYZ=            0.0005  XYZ=            6.8734
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=         -4135.0360 YYYY=         -1695.6463 ZZZZ=          -137.2008 XXXY=           -
0.0652
 XXXZ=           -0.0016 YYYX=           -0.0240 YYYZ=           -3.3929 ZZZX=            0.0197
 ZZZY=           -4.0586 XXYY=          -878.9386 XXZZ=          -703.0480 YYZZ=           -
309.2486
 XXYZ=          -32.3114 YYXZ=            0.0000 ZZXY=            0.0032
 N-N= 7.176436409760D+02 E-N=-2.846286594380D+03  KE= 6.062420692550D+02
  Exact polarizability:     354.639       0.004     213.576      -0.001       3.808      84.567
 Approx polarizability:     510.448       0.003     312.109       0.005       6.877     106.046
 No NMR shielding tensors so no spin-rotation constants.
 Leave Link  601 at Fri Aug 21 21:42:02 2026, MaxMem=    805306368 cpu:                4.3 elap:
0.8
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral second derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 2nd derivatives to the Hessian.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33580.
 LDataN:  DoStor=T MaxTD1= 8 Len=  415
 Leave Link  701 at Fri Aug 21 21:42:03 2026, MaxMem=    805306368 cpu:                6.8 elap:
1.1
```

Supporting Information file

(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 21:42:03 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral second derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 100527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 22:47:47 2026, MaxMem= 805306368 cpu: 23660.1 elap: 3943.7
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.51648676D+00-1.36431139D-03-1.33960126D-04
Polarizability= 3.54638790D+02 4.05366868D-03 2.13575586D+02
-6.35958186D-04 3.80770050D+00 8.45666968D+01
Full mass-weighted force constant matrix:
Low frequencies --- -4.6599 -3.5184 -0.0007 0.0004 0.0008 1.3316
Low frequencies --- 61.9248 92.9960 93.5658
Diagonal vibrational polarizability:
19.8734280 54.8697081 15.6163733
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	61.9196	92.9959	93.5656
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.0271	0.0611	0.0619
IR Inten --	1.9521	0.0757	0.1042

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	0.01	0.27	0.29	-0.00	-0.02	0.11	-0.16	0.04
2	6	-0.03	0.03	0.14	0.15	0.08	-0.05	0.22	-0.23	0.02
3	6	-0.01	0.01	0.27	0.29	0.00	0.02	-0.11	-0.16	0.04
4	6	-0.01	0.00	-0.06	0.04	0.26	-0.04	0.18	-0.18	-0.02
5	6	0.03	0.03	0.14	0.15	-0.08	0.05	-0.22	-0.23	0.02
6	6	-0.02	0.02	-0.22	0.03	0.37	-0.02	0.16	0.02	-0.04
7	6	0.01	0.00	-0.06	0.04	-0.26	0.04	-0.19	-0.18	-0.02
8	6	-0.02	-0.01	-0.28	0.00	0.28	0.03	0.20	0.20	-0.04
9	6	0.02	0.02	-0.22	0.02	-0.37	0.02	-0.16	0.02	-0.04
10	6	-0.02	-0.01	-0.23	-0.10	0.09	0.05	0.24	0.27	-0.01

11	6	0.02	-0.01	-0.28	0.00	-0.27	-0.03	-0.20	0.20	-0.04
12	6	-0.06	-0.01	-0.04	-0.20	-0.01	0.03	0.12	0.15	0.02
13	6	0.02	-0.01	-0.23	-0.11	-0.08	-0.05	-0.24	0.27	-0.01
14	6	0.06	-0.01	-0.04	-0.20	0.01	-0.03	-0.12	0.15	0.02
15	6	-0.21	-0.03	0.42	-0.20	-0.04	0.02	0.06	-0.08	0.04
16	6	0.22	-0.03	0.42	-0.20	0.04	-0.02	-0.06	-0.08	0.04

	4	5	6
	A	A	A
Frequencies --	111.5699	152.8709	226.1202
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.0880	0.1652	0.3615
IR Inten --	0.0004	1.4329	0.1768

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.04	0.00	0.15	0.03	-0.04	-0.29	0.13	-0.12	0.00
2	6	0.02	0.02	0.34	-0.01	-0.01	-0.01	0.28	-0.20	0.01
3	6	0.04	-0.00	-0.15	-0.03	-0.04	-0.29	-0.13	-0.12	0.00
4	6	-0.01	0.06	0.28	-0.01	-0.01	0.27	0.08	0.11	-0.01
5	6	0.02	-0.02	-0.34	0.01	-0.01	-0.01	-0.28	-0.20	0.01
6	6	-0.01	0.07	0.03	-0.01	0.05	0.31	0.06	0.33	-0.01
7	6	-0.01	-0.06	-0.28	0.01	-0.01	0.27	-0.08	0.11	-0.01
8	6	-0.00	0.05	-0.23	-0.00	0.05	0.08	0.01	0.15	0.02
9	6	-0.01	-0.07	-0.03	0.01	0.05	0.31	-0.06	0.33	-0.01
10	6	-0.01	0.03	-0.37	0.01	0.06	-0.23	-0.22	-0.26	0.01
11	6	-0.00	-0.05	0.23	0.00	0.05	0.08	-0.01	0.15	0.02
12	6	-0.02	0.04	-0.19	-0.03	0.01	-0.29	-0.15	-0.18	0.00
13	6	-0.01	-0.02	0.37	-0.01	0.06	-0.23	0.22	-0.26	0.01
14	6	-0.02	-0.04	0.19	0.03	0.01	-0.29	0.15	-0.18	0.00
15	6	-0.00	0.17	-0.12	-0.22	-0.12	0.16	-0.07	0.16	-0.03
16	6	-0.00	-0.17	0.12	0.22	-0.12	0.16	0.07	0.16	-0.03

	7	8	9
	A	A	A
Frequencies --	233.2281	259.1251	270.4374
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.3846	0.4747	0.5171
IR Inten --	0.0095	0.0483	9.9603

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	0.00	0.18	-0.29	0.01	-0.04	-0.15	0.08	-0.24
2	6	0.03	-0.04	0.32	0.06	-0.20	-0.07	0.13	-0.07	0.16
3	6	-0.06	-0.00	-0.18	-0.29	-0.01	0.04	0.15	0.08	-0.24
4	6	0.05	-0.09	0.00	0.12	-0.32	-0.00	0.02	0.08	0.28
5	6	0.03	0.04	-0.32	0.06	0.20	0.07	-0.13	-0.07	0.16
6	6	0.04	-0.03	-0.34	0.08	0.05	0.09	0.05	-0.17	-0.02
7	6	0.05	0.09	-0.00	0.12	0.32	0.00	-0.02	0.08	0.28
8	6	0.05	0.02	-0.22	0.16	0.35	0.05	0.07	-0.05	-0.27
9	6	0.04	0.03	0.34	0.08	-0.05	-0.09	-0.05	-0.17	-0.02
10	6	0.03	0.03	0.18	0.09	0.21	-0.09	0.05	-0.07	-0.16
11	6	0.05	-0.02	0.22	0.16	-0.35	-0.05	-0.07	-0.06	-0.27
12	6	-0.04	-0.04	0.22	-0.11	0.02	-0.04	0.02	-0.03	0.22

13	6	0.03	-0.03	-0.18	0.09	-0.21	0.09	-0.05	-0.07	-0.16
14	6	-0.04	0.04	-0.22	-0.11	-0.02	0.04	-0.02	-0.03	0.22
15	6	-0.11	-0.23	0.17	-0.12	0.02	-0.02	0.17	0.24	0.02
16	6	-0.11	0.23	-0.17	-0.12	-0.02	0.02	-0.17	0.24	0.02

	10	11	12
	A	A	A
Frequencies --	298.5004	351.0421	359.5839
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.6300	0.8713	0.9142
IR Inten --	140.6285	18.8782	0.0994

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.42	0.14	0.12	0.04	0.07	0.18	0.14	-0.01	-0.17
2	6	0.22	-0.23	-0.09	-0.03	0.09	-0.21	-0.04	0.09	-0.17
3	6	0.42	0.14	0.12	-0.04	0.07	0.18	0.14	0.01	0.18
4	6	-0.08	0.21	-0.13	0.13	-0.19	-0.14	0.00	0.02	0.19
5	6	-0.21	-0.23	-0.09	0.03	0.09	-0.22	-0.04	-0.09	0.17
6	6	-0.02	-0.21	0.06	0.11	-0.11	0.24	0.02	-0.21	0.18
7	6	0.08	0.21	-0.13	-0.13	-0.19	-0.14	0.00	-0.02	-0.19
8	6	0.04	0.13	0.12	0.10	-0.04	0.13	0.04	-0.10	-0.19
9	6	0.02	-0.21	0.06	-0.11	-0.11	0.24	0.02	0.21	-0.18
10	6	-0.02	-0.00	-0.01	0.08	-0.07	-0.25	0.14	0.11	-0.22
11	6	-0.04	0.13	0.12	-0.10	-0.04	0.12	0.04	0.09	0.19
12	6	0.02	0.02	-0.12	-0.05	-0.10	0.01	-0.06	-0.01	0.12
13	6	0.02	-0.00	-0.01	-0.08	-0.07	-0.26	0.14	-0.11	0.22
14	6	-0.02	0.02	-0.12	0.05	-0.10	0.02	-0.06	0.01	-0.12
15	6	-0.07	-0.05	0.05	0.03	0.36	0.05	-0.23	-0.24	0.20
16	6	0.07	-0.05	0.05	-0.02	0.36	0.05	-0.23	0.24	-0.20

	13	14	15
	A	A	A
Frequencies --	402.3573	411.0813	434.8547
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.1446	1.1948	1.3370
IR Inten --	0.1682	2.7035	1.5677

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.25	-0.12	0.11	-0.18	0.01	-0.16	0.05	-0.01	0.54
2	6	0.16	-0.08	-0.14	0.22	-0.23	-0.11	0.06	-0.04	-0.32
3	6	-0.25	-0.12	0.11	-0.18	-0.01	0.16	0.05	0.01	-0.54
4	6	-0.10	0.37	-0.04	0.07	-0.02	0.20	0.04	-0.07	0.12
5	6	-0.16	-0.08	-0.15	0.22	0.23	0.11	0.06	0.04	0.32
6	6	-0.05	0.01	0.15	0.03	0.28	0.04	0.03	-0.00	-0.09
7	6	0.10	0.37	-0.04	0.07	0.02	-0.20	0.04	0.07	-0.12
8	6	-0.13	-0.31	-0.02	-0.07	-0.14	-0.17	-0.04	-0.09	0.14
9	6	0.05	0.01	0.15	0.03	-0.28	-0.04	0.03	0.00	0.09
10	6	0.09	0.08	-0.14	-0.18	-0.30	-0.02	-0.02	-0.06	-0.13
11	6	0.14	-0.31	-0.02	-0.07	0.14	0.17	-0.04	0.09	-0.14
12	6	0.10	0.10	0.06	0.05	-0.04	0.06	-0.06	-0.02	-0.02
13	6	-0.09	0.08	-0.14	-0.18	0.30	0.02	-0.02	0.06	0.13
14	6	-0.10	0.10	0.06	0.05	0.04	-0.06	-0.06	0.02	0.02

15	6	0.12	-0.04	0.03	0.05	-0.09	0.07	-0.06	-0.06	0.02
16	6	-0.12	-0.04	0.04	0.05	0.09	-0.07	-0.06	0.06	-0.02

	16	17	18
	A	A	A
Frequencies --	451.6357	455.3021	482.6042
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.4421	1.4657	1.6467
IR Inten --	0.8725	1.5609	67.0569

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.17	0.00	-0.13	0.02	-0.00	-0.08	0.20	-0.03	-0.02
2	6	0.12	0.03	0.25	-0.16	0.11	-0.24	-0.27	0.25	0.04
3	6	-0.17	0.00	-0.13	0.02	0.00	0.08	0.20	0.03	0.02
4	6	0.05	0.10	-0.08	-0.04	-0.03	0.43	0.13	-0.44	-0.06
5	6	-0.12	0.03	0.25	-0.16	-0.11	0.24	-0.27	-0.25	-0.04
6	6	0.08	-0.23	-0.21	-0.04	0.00	-0.22	0.04	0.22	0.07
7	6	-0.05	0.10	-0.08	-0.04	0.03	-0.42	0.14	0.44	0.06
8	6	0.01	-0.17	0.23	0.04	0.17	-0.14	-0.01	-0.02	-0.03
9	6	-0.08	-0.23	-0.21	-0.04	-0.00	0.22	0.04	-0.22	-0.07
10	6	0.09	0.04	0.14	0.01	0.10	0.24	-0.11	-0.17	-0.04
11	6	-0.01	-0.17	0.23	0.04	-0.17	0.14	-0.01	0.02	0.03
12	6	-0.02	-0.01	-0.23	0.02	-0.00	0.01	-0.00	-0.03	-0.00
13	6	-0.09	0.04	0.14	0.01	-0.10	-0.24	-0.11	0.17	0.04
14	6	0.02	-0.01	-0.23	0.02	0.00	-0.01	-0.00	0.03	0.00
15	6	-0.18	0.24	0.03	0.16	0.09	-0.11	0.01	-0.05	0.02
16	6	0.18	0.24	0.03	0.16	-0.09	0.11	0.01	0.05	-0.02

	19	20	21
	A	A	A
Frequencies --	496.3280	498.9982	502.6511
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.7417	1.7605	1.7863
IR Inten --	9.1949	1.2747	0.8005

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.28	0.11	-0.07	-0.05	0.07	0.15	0.17	-0.04	-0.21
2	6	0.08	-0.08	0.15	0.09	-0.02	-0.37	0.18	-0.07	0.07
3	6	0.28	0.11	-0.07	0.05	0.07	0.15	0.17	0.04	0.21
4	6	0.10	-0.18	-0.12	0.08	-0.07	0.38	0.11	-0.15	0.13
5	6	-0.09	-0.09	0.15	-0.09	-0.02	-0.37	0.18	0.07	-0.07
6	6	0.03	0.36	0.00	0.05	0.03	-0.14	0.08	-0.24	-0.24
7	6	-0.10	-0.18	-0.12	-0.08	-0.07	0.38	0.11	0.15	-0.13
8	6	-0.16	-0.35	0.10	-0.04	-0.17	-0.11	-0.03	-0.10	0.21
9	6	-0.03	0.36	-0.00	-0.05	0.03	-0.14	0.08	0.24	0.24
10	6	0.07	0.06	-0.07	0.03	0.05	0.23	-0.10	-0.13	0.02
11	6	0.16	-0.35	0.10	0.05	-0.17	-0.11	-0.03	0.10	-0.21
12	6	0.06	0.06	-0.02	-0.02	0.02	-0.12	-0.18	-0.01	-0.08
13	6	-0.07	0.06	-0.07	-0.04	0.05	0.23	-0.10	0.13	-0.02
14	6	-0.06	0.06	-0.02	0.02	0.02	-0.12	-0.18	0.01	0.09
15	6	0.04	0.02	0.03	-0.14	0.10	-0.02	-0.23	0.17	-0.09
16	6	-0.03	0.02	0.03	0.14	0.10	-0.02	-0.24	-0.17	0.09

Supporting Information file

		22			23			24		
		A			A			A		
Frequencies --		511.1834			531.6258			532.9193		
Red. masses --		12.0000			12.0000			12.0000		
Frc consts --		1.8475			1.9982			2.0080		
IR Inten --		94.3506			0.4710			0.5998		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	0.01	0.06	-0.01	-0.02	0.02	0.09	-0.02	0.16
2	6	-0.02	0.03	-0.01	-0.04	-0.00	-0.09	0.11	-0.06	-0.06
3	6	0.03	-0.01	-0.06	0.00	-0.02	0.03	0.09	0.02	-0.16
4	6	-0.03	0.09	-0.04	-0.04	0.02	0.22	0.05	-0.07	-0.10
5	6	-0.02	-0.03	0.02	0.03	-0.00	-0.09	0.11	0.06	0.06
6	6	0.01	-0.31	0.07	-0.02	0.03	-0.38	0.03	-0.11	0.28
7	6	-0.03	-0.09	0.04	0.03	0.01	0.22	0.05	0.08	0.11
8	6	0.18	0.38	-0.05	-0.02	0.06	0.42	-0.02	-0.08	-0.35
9	6	0.01	0.31	-0.07	0.02	0.02	-0.36	0.03	0.11	-0.30
10	6	-0.24	-0.37	-0.05	-0.01	-0.02	-0.32	-0.04	0.01	0.30
11	6	0.18	-0.38	0.05	0.02	0.06	0.40	-0.02	0.08	0.37
12	6	0.03	-0.03	0.02	0.01	0.01	0.10	-0.09	0.01	0.02
13	6	-0.24	0.37	0.05	0.01	-0.02	-0.30	-0.04	-0.01	-0.31
14	6	0.04	0.03	-0.02	-0.00	0.01	0.10	-0.09	-0.01	-0.02
15	6	0.05	-0.06	0.05	0.12	-0.07	0.01	-0.12	0.25	-0.11
16	6	0.05	0.06	-0.05	-0.11	-0.06	0.01	-0.13	-0.25	0.11

		25			26			27		
		A			A			A		
Frequencies --		619.8844			678.7639			702.9138		
Red. masses --		12.0000			12.0000			12.0000		
Frc consts --		2.7168			3.2574			3.4933		
IR Inten --		4.9908			0.4912			2.1400		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.09	-0.05	-0.02	0.09	0.07	-0.00	-0.00	-0.00	0.01
2	6	0.10	-0.07	0.03	0.09	0.05	-0.00	0.00	-0.00	-0.01
3	6	0.09	0.05	0.02	-0.09	0.07	-0.00	-0.00	0.00	-0.01
4	6	-0.02	-0.06	-0.04	0.10	-0.11	0.01	-0.00	0.00	0.01
5	6	0.10	0.07	-0.03	-0.09	0.05	-0.00	0.00	0.00	0.01
6	6	-0.02	-0.09	0.05	0.05	-0.09	0.00	-0.00	-0.00	-0.00
7	6	-0.02	0.06	0.04	-0.10	-0.11	0.01	-0.00	-0.00	-0.01
8	6	-0.09	-0.01	-0.05	-0.04	0.01	0.00	0.00	0.00	-0.05
9	6	-0.02	0.09	-0.05	-0.05	-0.09	0.00	-0.00	0.00	0.00
10	6	-0.03	0.08	0.01	-0.28	-0.30	0.02	-0.01	0.01	0.19
11	6	-0.09	0.01	0.05	0.04	0.01	0.00	0.00	-0.00	0.05
12	6	-0.31	-0.14	-0.13	0.28	0.38	-0.14	0.16	0.09	-0.58
13	6	-0.03	-0.08	-0.01	0.28	-0.30	0.01	-0.01	-0.01	-0.19
14	6	-0.31	0.14	0.13	-0.28	0.38	-0.14	0.16	-0.09	0.58
15	6	0.29	-0.38	-0.28	0.15	-0.02	0.12	-0.15	-0.20	0.17
16	6	0.29	0.38	0.28	-0.15	-0.02	0.12	-0.15	0.20	-0.17

	28	29	30
	A	A	A

Supporting Information file

Frequencies --		749.9623			774.6939			977.9677		
Red. masses --		12.0000			12.0000			12.0000		
Frc consts --		3.9766			4.2432			6.7621		
IR Inten --		53.5471			4.4243			5.8715		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.08	-0.14	0.01	0.26	-0.17	-0.01	0.12	0.17	-0.01
2	6	-0.21	-0.03	-0.02	0.14	-0.23	0.02	0.21	0.03	0.00
3	6	0.08	-0.14	0.01	0.26	0.17	0.01	-0.12	0.17	-0.01
4	6	-0.10	0.12	0.02	-0.17	-0.20	0.00	-0.03	-0.16	0.00
5	6	0.21	-0.03	-0.02	0.14	0.23	-0.02	-0.21	0.03	0.00
6	6	-0.02	0.16	-0.04	-0.24	-0.04	-0.00	-0.15	-0.08	-0.00
7	6	0.10	0.12	0.02	-0.17	0.20	-0.00	0.03	-0.16	0.00
8	6	0.17	0.03	-0.01	-0.20	0.13	0.00	-0.23	0.08	-0.01
9	6	0.02	0.17	-0.04	-0.24	0.04	0.00	0.15	-0.08	-0.00
10	6	0.16	-0.09	0.11	-0.12	0.16	-0.05	-0.10	0.22	0.04
11	6	-0.17	0.03	-0.01	-0.20	-0.13	-0.00	0.23	0.08	-0.01
12	6	0.28	-0.19	-0.26	0.20	0.14	0.08	-0.11	-0.24	-0.17
13	6	-0.16	-0.09	0.11	-0.12	-0.16	0.05	0.10	0.22	0.04
14	6	-0.28	-0.19	-0.26	0.20	-0.14	-0.08	0.11	-0.24	-0.17
15	6	0.25	0.14	0.18	0.12	0.02	0.17	0.35	-0.02	0.14
16	6	-0.25	0.14	0.18	0.11	-0.02	-0.17	-0.35	-0.02	0.14
		31			32			33		
		A			A			A		
Frequencies --		1110.1688			1211.8512			1227.8555		
Red. masses --		12.0000			12.0000			12.0000		
Frc consts --		8.7138			10.3832			10.6592		
IR Inten --		1.9878			1.4432			2.4680		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.12	-0.25	0.00	-0.02	0.02	0.00	0.12	0.18	-0.01
2	6	-0.14	-0.25	0.01	0.03	0.04	-0.00	0.18	-0.01	0.00
3	6	0.12	0.25	-0.00	-0.02	-0.02	-0.00	-0.12	0.18	-0.01
4	6	-0.25	-0.01	0.00	0.01	-0.01	0.00	-0.23	-0.16	0.00
5	6	-0.14	0.25	-0.01	0.03	-0.04	0.00	-0.18	-0.01	0.00
6	6	-0.13	0.12	-0.01	0.01	-0.00	-0.00	-0.30	0.04	-0.01
7	6	-0.25	0.01	-0.00	0.01	0.01	-0.00	0.23	-0.16	0.00
8	6	0.28	-0.03	0.01	-0.05	0.02	0.00	0.04	0.06	0.00
9	6	-0.13	-0.12	0.01	0.01	0.00	0.00	0.30	0.04	-0.01
10	6	0.26	-0.19	0.02	-0.04	-0.02	0.00	0.12	-0.06	-0.03
11	6	0.28	0.03	-0.01	-0.05	-0.02	-0.00	-0.04	0.06	0.00
12	6	0.01	-0.16	-0.02	0.27	0.33	0.13	0.37	-0.11	0.11
13	6	0.26	0.19	-0.02	-0.04	0.02	-0.00	-0.12	-0.06	-0.03
14	6	0.01	0.16	0.02	0.27	-0.33	-0.13	-0.37	-0.11	0.11
15	6	-0.14	-0.02	-0.14	-0.21	-0.23	-0.44	-0.24	0.06	-0.08
16	6	-0.14	0.02	0.14	-0.22	0.23	0.44	0.23	0.06	-0.08
		34			35			36		
		A			A			A		
Frequencies --		1442.2673			1452.5346			1608.5413		
Red. masses --		12.0000			12.0000			12.0000		

Frc consts --		14.7070			14.9171			18.2935		
IR Inten --		0.2587			14.0776			7.2492		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.37	-0.01	-0.07	-0.11	0.00	0.01	-0.08	0.00
2	6	0.29	0.21	-0.00	-0.08	0.03	-0.00	-0.11	-0.09	-0.00
3	6	-0.01	-0.37	0.01	0.07	-0.11	0.00	0.01	0.08	-0.00
4	6	-0.15	-0.15	0.00	0.24	0.09	0.00	0.18	0.07	0.00
5	6	0.29	-0.21	0.00	0.08	0.03	-0.00	-0.11	0.09	0.00
6	6	-0.30	0.01	-0.00	0.17	-0.07	0.01	0.07	-0.04	0.00
7	6	-0.15	0.15	-0.00	-0.24	0.09	0.00	0.18	-0.07	-0.00
8	6	0.03	0.04	-0.00	-0.27	0.08	-0.01	-0.17	0.05	-0.01
9	6	-0.30	-0.01	0.00	-0.17	-0.07	0.01	0.07	0.04	-0.00
10	6	0.11	-0.05	0.00	-0.20	0.19	-0.04	-0.13	0.14	-0.03
11	6	0.03	-0.04	0.00	0.27	0.08	-0.01	-0.17	-0.05	0.01
12	6	0.10	-0.24	-0.01	0.37	-0.24	0.08	0.29	-0.50	0.00
13	6	0.11	0.05	-0.00	0.20	0.19	-0.04	-0.13	-0.14	0.03
14	6	0.10	0.24	0.01	-0.37	-0.24	0.08	0.29	0.50	-0.00
15	6	-0.08	0.00	-0.05	-0.12	0.03	-0.04	-0.13	-0.01	-0.11
16	6	-0.08	-0.00	0.05	0.12	0.03	-0.04	-0.13	0.01	0.11
		37			38			39		
		A			A			A		
Frequencies --		2060.0743			2145.9350			2216.3405		
Red. masses --		12.0000			12.0000			12.0000		
Frc consts --		30.0052			32.5585			34.7300		
IR Inten --		0.0033			0.1842			6.7119		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.15	0.36	-0.00	-0.18	-0.32	0.01	-0.05	-0.16	0.00
2	6	-0.21	-0.29	0.00	0.22	0.34	-0.01	-0.01	0.03	-0.00
3	6	0.15	-0.36	0.00	0.18	-0.32	0.01	-0.05	0.16	-0.00
4	6	0.22	0.05	0.00	0.21	0.01	-0.00	0.42	0.09	-0.00
5	6	-0.21	0.29	-0.00	-0.22	0.34	-0.01	-0.01	-0.03	0.00
6	6	-0.23	0.00	-0.00	-0.29	-0.02	-0.00	-0.38	-0.03	-0.00
7	6	0.22	-0.05	-0.00	-0.21	0.01	-0.00	0.42	-0.09	0.00
8	6	0.25	-0.12	0.01	-0.10	0.07	-0.00	-0.18	0.10	-0.01
9	6	-0.23	-0.00	0.00	0.29	-0.02	-0.00	-0.38	0.03	0.00
10	6	-0.17	0.10	-0.01	0.18	-0.11	0.01	0.26	-0.16	0.02
11	6	0.25	0.12	-0.01	0.10	0.07	-0.00	-0.18	-0.10	0.01
12	6	-0.02	0.06	0.00	-0.03	0.03	-0.01	-0.05	0.06	-0.01
13	6	-0.17	-0.10	0.01	-0.18	-0.11	0.01	0.26	0.16	-0.02
14	6	-0.02	-0.06	-0.00	0.03	0.03	-0.01	-0.05	-0.06	0.01
15	6	0.02	-0.02	-0.01	0.00	0.00	0.00	0.01	0.00	0.01
16	6	0.02	0.02	0.01	-0.00	0.00	0.00	0.01	-0.00	-0.01
		40			41			42		
		A			A			A		
Frequencies --		2261.1337			2277.1383			2278.7681		
Red. masses --		12.0000			12.0000			12.0000		
Frc consts --		36.1480			36.6615			36.7140		
IR Inten --		25.0541			53.7806			3.3255		

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Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.10	-0.20	0.01	-0.13	-0.33	0.01	0.04	0.06	-0.00
2	6	0.22	0.27	-0.01	0.16	0.22	-0.01	-0.05	-0.07	0.00
3	6	0.10	-0.20	0.01	-0.13	0.33	-0.01	-0.04	0.07	-0.00
4	6	-0.42	-0.11	-0.00	0.08	0.01	0.00	-0.10	-0.01	-0.00
5	6	-0.22	0.27	-0.01	0.16	-0.22	0.01	0.05	-0.07	0.00
6	6	0.35	0.02	0.00	-0.22	0.00	-0.00	0.23	-0.01	0.01
7	6	0.42	-0.11	-0.00	0.08	-0.01	0.00	0.10	-0.01	-0.00
8	6	0.04	-0.03	0.00	0.35	-0.16	0.01	-0.44	0.20	-0.02
9	6	-0.35	0.02	0.00	-0.21	-0.00	0.00	-0.23	-0.01	0.01
10	6	-0.10	0.06	-0.01	-0.27	0.17	-0.02	0.37	-0.23	0.02
11	6	-0.04	-0.03	0.00	0.34	0.16	-0.01	0.44	0.21	-0.02
12	6	0.03	-0.02	0.00	0.03	-0.02	0.01	-0.03	0.04	-0.01
13	6	0.10	0.06	-0.01	-0.27	-0.17	0.02	-0.37	-0.23	0.02
14	6	-0.03	-0.02	0.00	0.03	0.02	-0.01	0.03	0.04	-0.01
15	6	-0.00	0.00	-0.00	0.00	-0.01	-0.01	0.00	0.01	0.00
16	6	0.00	0.00	-0.00	0.00	0.01	0.01	0.00	0.01	0.00

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 6 and mass 12.00000
Atom 2 has atomic number 6 and mass 12.00000
Atom 3 has atomic number 6 and mass 12.00000
Atom 4 has atomic number 6 and mass 12.00000
Atom 5 has atomic number 6 and mass 12.00000
Atom 6 has atomic number 6 and mass 12.00000
Atom 7 has atomic number 6 and mass 12.00000
Atom 8 has atomic number 6 and mass 12.00000
Atom 9 has atomic number 6 and mass 12.00000
Atom 10 has atomic number 6 and mass 12.00000
Atom 11 has atomic number 6 and mass 12.00000
Atom 12 has atomic number 6 and mass 12.00000
Atom 13 has atomic number 6 and mass 12.00000
Atom 14 has atomic number 6 and mass 12.00000
Atom 15 has atomic number 6 and mass 12.00000
Atom 16 has atomic number 6 and mass 12.00000
Molecular mass: 192.00000 amu.
Principal axes and moments of inertia in atomic units:

	1	2	3
Eigenvalues --	2129.50630	4578.77873	6639.71053
X	1.00000	0.00000	0.00000
Y	-0.00000	1.00000	0.00000
Z	0.00000	-0.00000	1.00000

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation

may cause significant error
Rotational temperatures (Kelvin) 0.04067 0.01892 0.01304
Rotational constants (GHZ): 0.84749 0.39415 0.27181
Zero-point vibrational energy 203480.6 (Joules/Mol)
48.63302 (Kcal/Mol)
Warning -- explicit consideration of 25 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 89.09 133.80 134.62 160.52 219.95
(Kelvin) 325.34 335.56 372.82 389.10 429.48
505.07 517.36 578.90 591.45 625.66
649.80 655.08 694.36 714.11 717.95
723.20 735.48 764.89 766.75 891.88
976.59 1011.34 1079.03 1114.61 1407.08
1597.29 1743.58 1766.61 2075.10 2089.87
2314.33 2963.99 3087.52 3188.82 3253.27
3276.29 3278.64

Zero-point correction= 0.077502 (Hartree/Particle)
Thermal correction to Energy= 0.090696
Thermal correction to Enthalpy= 0.091640
Thermal correction to Gibbs Free Energy= 0.037966
Sum of electronic and zero-point Energies= -608.904039
Sum of electronic and thermal Energies= -608.890844
Sum of electronic and thermal Enthalpies= -608.889900
Sum of electronic and thermal Free Energies= -608.943575

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.912	48.627	112.967
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	41.662
Rotational	0.889	2.981	32.537
Vibrational	55.135	42.665	38.767
Vibration 1	0.597	1.972	4.395
Vibration 2	0.602	1.954	3.596
Vibration 3	0.603	1.954	3.584
Vibration 4	0.607	1.940	3.241
Vibration 5	0.619	1.899	2.636
Vibration 6	0.650	1.801	1.910
Vibration 7	0.654	1.790	1.854
Vibration 8	0.668	1.747	1.668
Vibration 9	0.674	1.728	1.593
Vibration 10	0.692	1.677	1.425
Vibration 11	0.728	1.573	1.162
Vibration 12	0.734	1.556	1.124
Vibration 13	0.768	1.465	0.954
Vibration 14	0.775	1.446	0.923
Vibration 15	0.795	1.394	0.843

Vibration	16	0.810	1.357	0.791
Vibration	17	0.814	1.349	0.780
Vibration	18	0.839	1.289	0.703
Vibration	19	0.852	1.258	0.667
Vibration	20	0.854	1.252	0.661
Vibration	21	0.858	1.244	0.652
Vibration	22	0.866	1.225	0.631
Vibration	23	0.887	1.180	0.584
Vibration	24	0.888	1.177	0.581
Vibration	25	0.980	0.990	0.417

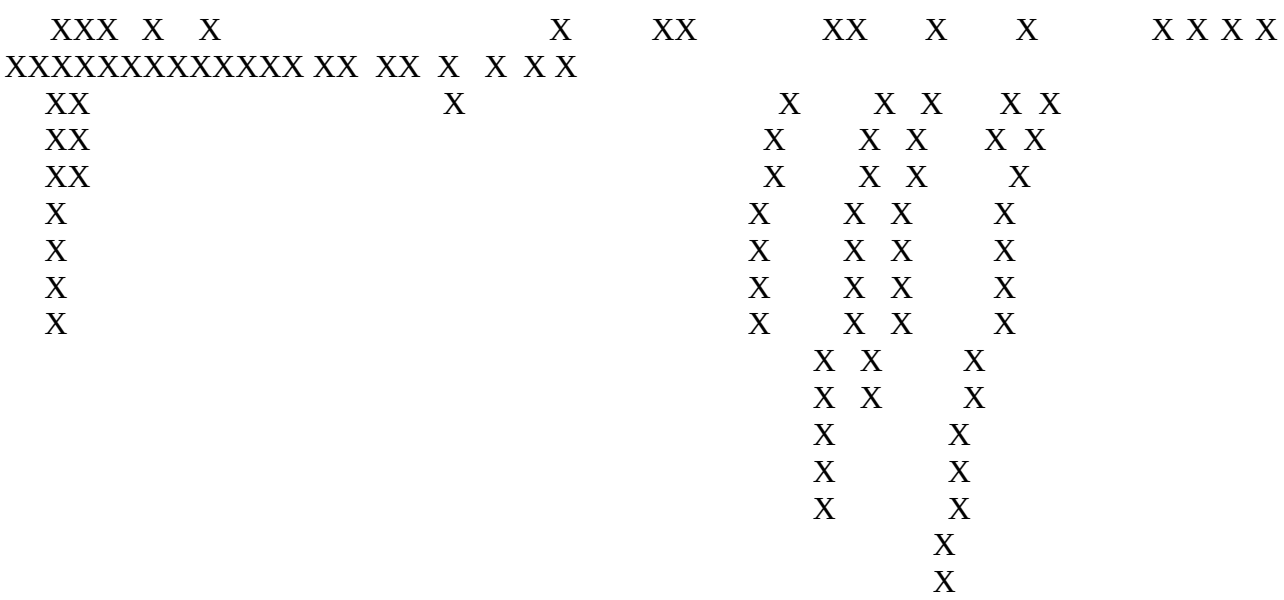
		Q	Log10(Q)	Ln(Q)
Total Bot		0.344399D-17	-17.462938	-40.209900
Total V=0		0.153221D+19	18.185318	41.873242
Vib (Bot)		0.114346D-31	-31.941778	-73.548662
Vib (Bot)	1	0.333425D+01	0.522998	1.204248
Vib (Bot)	2	0.220973D+01	0.344339	0.792870
Vib (Bot)	3	0.219605D+01	0.341642	0.786660
Vib (Bot)	4	0.183511D+01	0.263661	0.607103
Vib (Bot)	5	0.132530D+01	0.122313	0.281636
Vib (Bot)	6	0.872501D+00	-0.059234	-0.136392
Vib (Bot)	7	0.843288D+00	-0.074024	-0.170447
Vib (Bot)	8	0.749888D+00	-0.125003	-0.287831
Vib (Bot)	9	0.714465D+00	-0.146019	-0.336221
Vib (Bot)	10	0.637643D+00	-0.195422	-0.449977
Vib (Bot)	11	0.525220D+00	-0.279659	-0.643938
Vib (Bot)	12	0.509870D+00	-0.292540	-0.673599
Vib (Bot)	13	0.442214D+00	-0.354368	-0.815961
Vib (Bot)	14	0.430033D+00	-0.366498	-0.843892
Vib (Bot)	15	0.399160D+00	-0.398853	-0.918393
Vib (Bot)	16	0.379198D+00	-0.421134	-0.969698
Vib (Bot)	17	0.375019D+00	-0.425947	-0.980778
Vib (Bot)	18	0.345775D+00	-0.461207	-1.061968
Vib (Bot)	19	0.332215D+00	-0.478581	-1.101972
Vib (Bot)	20	0.329658D+00	-0.481936	-1.109699
Vib (Bot)	21	0.326202D+00	-0.486514	-1.120239
Vib (Bot)	22	0.318310D+00	-0.497150	-1.144731
Vib (Bot)	23	0.300374D+00	-0.522338	-1.202728
Vib (Bot)	24	0.299283D+00	-0.523919	-1.206367
Vib (Bot)	25	0.235945D+00	-0.627190	-1.444159
Vib (V=0)		0.508719D+04	3.706478	8.534481
Vib (V=0)	1	0.387153D+01	0.587883	1.353651
Vib (V=0)	2	0.276559D+01	0.441788	1.017255
Vib (V=0)	3	0.275225D+01	0.439688	1.012419
Vib (V=0)	4	0.240200D+01	0.380574	0.876303
Vib (V=0)	5	0.191648D+01	0.282504	0.650489
Vib (V=0)	6	0.150561D+01	0.177713	0.409200
Vib (V=0)	7	0.148037D+01	0.170372	0.392295
Vib (V=0)	8	0.140129D+01	0.146530	0.337397

Supporting Information file

Vib (V=0)	9	0.137204D+01	0.137368	0.316302
Vib (V=0)	10	0.131030D+01	0.117371	0.270257
Vib (V=0)	11	0.122516D+01	0.088193	0.203071
Vib (V=0)	12	0.121412D+01	0.084262	0.194020
Vib (V=0)	13	0.116750D+01	0.067256	0.154863
Vib (V=0)	14	0.115949D+01	0.064267	0.147981
Vib (V=0)	15	0.113979D+01	0.056824	0.130842
Vib (V=0)	16	0.112753D+01	0.052127	0.120027
Vib (V=0)	17	0.112501D+01	0.051157	0.117793
Vib (V=0)	18	0.110791D+01	0.044506	0.102480
Vib (V=0)	19	0.110031D+01	0.041513	0.095588
Vib (V=0)	20	0.109889D+01	0.040956	0.094305
Vib (V=0)	21	0.109700D+01	0.040206	0.092578
Vib (V=0)	22	0.109272D+01	0.038510	0.088673
Vib (V=0)	23	0.108329D+01	0.034744	0.080000
Vib (V=0)	24	0.108273D+01	0.034519	0.079482
Vib (V=0)	25	0.105287D+01	0.022376	0.051524
Electronic		0.100000D+01	0.000000	0.000000
Translational		0.104570D+09	8.019406	18.465364
Rotational		0.288028D+07	6.459434	14.873398

title card
IR Spectrum

222 2 2 2 1 11 11 1
222 2 1 0 6 44 22 1 9 7 7 7 6 6555544444444 33 22222 1 1
776 1 4 6 0 54 21 1 7 7 5 0 7 2331099855310 65 97532 5 19 6
971 6 6 0 9 32 82 0 8 5 0 3 9 0321396352512 01 90936 3 23 2



X
X
X
X
X

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000026742	-0.000040611	-0.000199520
2	6	0.000064859	0.000017183	0.000201419
3	6	0.000005187	0.000048474	0.000198639
4	6	-0.000028936	-0.000005904	-0.000184805
5	6	0.000041066	-0.000035119	-0.000201666
6	6	0.000000976	-0.000053270	0.000163739
7	6	-0.000017691	0.000026573	0.000189349
8	6	0.000014151	0.000044729	-0.000031424
9	6	-0.000002066	0.000037143	-0.000162688
10	6	-0.000075355	-0.000105387	-0.000118614
11	6	0.000014127	-0.000038154	0.000013721
12	6	0.000110762	0.000188922	0.000193861
13	6	-0.000074882	0.000102586	0.000136524
14	6	0.000105298	-0.000185016	-0.000193031
15	6	-0.000070752	-0.000082656	-0.000131268
16	6	-0.000060001	0.000080507	0.000125764

Cartesian Forces: Max 0.000201666 RMS 0.000111412
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Leave Link 716 at Fri Aug 21 22:47:47 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Red2BG is reusing G-inverse.
Internal Forces: Max 0.000108474 RMS 0.000041763
Search for a local minimum.
Step number 1 out of a maximum of 2
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
ITU= 0
Eigenvalues --- 0.00193 0.00207 0.00288 0.00298 0.00470
Eigenvalues --- 0.00684 0.00989 0.01227 0.01569 0.01612
Eigenvalues --- 0.02528 0.04620 0.05086 0.05343 0.06241
Eigenvalues --- 0.06663 0.06989 0.07334 0.08641 0.08700
Eigenvalues --- 0.09441 0.09790 0.09900 0.10735 0.11714

Eigenvalues --- 0.15191 0.21168 0.26179 0.33581 0.40931
Eigenvalues --- 0.44213 0.45351 0.48684 0.51551 0.53549
Eigenvalues --- 0.55101 0.94020 0.94665 0.99374 1.01760
Eigenvalues --- 1.03111 1.03334
Angle between quadratic step and forces= 70.18 degrees.
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.00133676 RMS(Int)= 0.00000737
Iteration 2 RMS(Cart)= 0.00000391 RMS(Int)= 0.00000449
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000449
ITry= 1 IFail=0 DXMaxC= 3.58D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.30705	0.00001	0.00000	0.00004	0.00004	2.30709
R2	2.54863	0.00005	0.00000	0.00000	0.00000	2.54863
R3	2.54787	0.00006	0.00000	0.00008	0.00008	2.54795
R4	2.30704	0.00001	0.00000	0.00006	0.00005	2.30709
R5	2.30310	0.00002	0.00000	0.00006	0.00006	2.30316
R6	2.54792	0.00005	0.00000	0.00003	0.00003	2.54795
R7	2.55055	0.00003	0.00000	0.00005	0.00005	2.55060
R8	2.30308	0.00002	0.00000	0.00008	0.00008	2.30316
R9	2.29580	0.00002	0.00000	0.00004	0.00004	2.29583
R10	2.55059	0.00002	0.00000	0.00001	0.00001	2.55060
R11	2.61573	0.00002	0.00000	0.00006	0.00006	2.61579
R12	2.29579	0.00002	0.00000	0.00004	0.00004	2.29583
R13	2.64580	-0.00007	0.00000	-0.00078	-0.00078	2.64502
R14	2.74039	0.00007	0.00000	0.00068	0.00068	2.74107
R15	2.61573	0.00002	0.00000	0.00006	0.00006	2.61579
R16	2.74040	0.00006	0.00000	0.00067	0.00067	2.74107
R17	2.73743	0.00009	0.00000	-0.00011	-0.00011	2.73732
A1	2.61227	0.00005	0.00000	0.00105	0.00104	2.61331
A2	2.64406	-0.00001	0.00000	-0.00095	-0.00096	2.64310
A3	2.61362	0.00003	0.00000	-0.00030	-0.00031	2.61331
A4	2.71592	-0.00001	0.00000	0.00055	0.00054	2.71646
A5	2.64284	0.00001	0.00000	0.00027	0.00026	2.64310
A6	2.78155	-0.00007	0.00000	-0.00158	-0.00158	2.77997
A7	2.71687	-0.00002	0.00000	-0.00040	-0.00041	2.71646
A8	2.78088	-0.00006	0.00000	-0.00090	-0.00091	2.77997
A9	2.83141	-0.00004	0.00000	-0.00060	-0.00060	2.83080
A10	2.30583	0.00008	0.00000	0.00117	0.00117	2.30700
A11	2.51966	-0.00011	0.00000	-0.00118	-0.00118	2.51848
A12	1.45711	0.00002	0.00000	0.00003	0.00003	1.45714
A13	2.83109	-0.00004	0.00000	-0.00029	-0.00030	2.83080
A14	2.30597	0.00008	0.00000	0.00103	0.00103	2.30700
A15	1.45705	0.00002	0.00000	0.00009	0.00009	1.45714
A16	2.51958	-0.00010	0.00000	-0.00110	-0.00110	2.51848
A17	1.42774	-0.00003	0.00000	-0.00012	-0.00012	1.42762
A18	1.42779	-0.00002	0.00000	-0.00017	-0.00017	1.42762

A19	2.87961	0.00000	0.00000	0.00063	0.00063	2.88024
A20	2.87999	-0.00000	0.00000	0.00026	0.00025	2.88024
A21	3.14134	0.00005	0.00000	0.00081	0.00081	3.14216
A22	3.14152	0.00004	0.00000	0.00064	0.00064	3.14216
D1	0.08402	0.00004	0.00000	0.01461	0.01460	0.09862
D2	-0.07724	-0.00002	0.00000	-0.01438	-0.01438	-0.09162
D3	-0.08021	-0.00003	0.00000	-0.01433	-0.01433	-0.09454
D4	0.08406	0.00004	0.00000	0.01456	0.01456	0.09862
D5	0.11480	0.00002	0.00000	0.01372	0.01372	0.12851
D6	-0.08003	-0.00003	0.00000	-0.01450	-0.01451	-0.09453
D7	0.09506	-0.00003	0.00000	-0.00902	-0.00902	0.08604
D8	0.11458	0.00002	0.00000	0.01393	0.01393	0.12851
D9	0.09592	-0.00003	0.00000	-0.00987	-0.00987	0.08605
D10	-0.64137	0.00002	0.00000	0.00529	0.00529	-0.63608
D11	2.55190	0.00000	0.00000	0.00424	0.00424	2.55614
D12	0.75102	-0.00000	0.00000	-0.00094	-0.00094	0.75008
D13	-2.42069	0.00001	0.00000	-0.00055	-0.00055	-2.42124
D14	-2.42086	0.00001	0.00000	-0.00038	-0.00038	-2.42124
D15	0.69061	0.00002	0.00000	0.00001	0.00001	0.69063
D16	2.40836	0.00001	0.00000	0.00055	0.00055	2.40891
D17	-0.69466	-0.00001	0.00000	-0.00027	-0.00027	-0.69493
D18	-0.64269	0.00003	0.00000	0.00660	0.00660	-0.63609
D19	2.55027	0.00000	0.00000	0.00586	0.00586	2.55613
D20	-0.69465	-0.00002	0.00000	-0.00028	-0.00028	-0.69493
D21	2.40860	0.00000	0.00000	0.00031	0.00031	2.40891
D22	0.66921	-0.00002	0.00000	-0.00014	-0.00014	0.66907

Item	Value	Threshold	Converged?
Maximum Force	0.000108	0.000450	YES
RMS Force	0.000042	0.000300	YES
Maximum Displacement	0.003576	0.001800	NO
RMS Displacement	0.001337	0.001200	NO

Predicted change in Energy=-2.312353D-06

Non-Optimized Parameters !
(Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.
! R1	R(1,2)	1.2209	-DE/DX = 0.0 !
! R2	R(1,3)	1.3487	-DE/DX = 0.0001 !
! R3	R(2,4)	1.3483	-DE/DX = 0.0001 !
! R4	R(3,5)	1.2209	-DE/DX = 0.0 !
! R5	R(4,6)	1.2188	-DE/DX = 0.0 !
! R6	R(5,7)	1.3483	-DE/DX = 0.0001 !
! R7	R(6,8)	1.3497	-DE/DX = 0.0 !
! R8	R(7,9)	1.2188	-DE/DX = 0.0 !
! R9	R(8,10)	1.2149	-DE/DX = 0.0 !
! R10	R(9,11)	1.3497	-DE/DX = 0.0 !

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! R11   R(10,12)            1.3842       -DE/DX =    0.0             !
! R12   R(11,13)            1.2149       -DE/DX =    0.0             !
! R13   R(12,14)            1.3997       -DE/DX =   -0.0001          !
! R14   R(12,15)            1.4505       -DE/DX =    0.0001          !
! R15   R(13,14)            1.3842       -DE/DX =    0.0             !
! R16   R(14,16)            1.4505       -DE/DX =    0.0001          !
! R17   R(15,16)            1.4485       -DE/DX =    0.0001          !
! A1    A(2,1,3)           149.7316      -DE/DX =    0.0001          !
! A2    A(1,2,4)           151.4383      -DE/DX =    0.0             !
! A3    A(1,3,5)           149.7316      -DE/DX =    0.0             !
! A4    A(2,4,6)           155.6416      -DE/DX =    0.0             !
! A5    A(3,5,7)           151.4384      -DE/DX =    0.0             !
! A6    A(4,6,8)           159.2805      -DE/DX =   -0.0001          !
! A7    A(5,7,9)           155.6417      -DE/DX =    0.0             !
! A8    A(7,9,11)          159.2805       -DE/DX =   -0.0001          !
! A9    A(8,10,12)         162.1931       -DE/DX =    0.0             !
! A10   A(10,12,14)        132.1816       -DE/DX =    0.0001          !
! A11   A(10,12,15)        144.2984       -DE/DX =   -0.0001          !
! A12   A(14,12,15)         83.4881       -DE/DX =    0.0             !
! A13   A(11,13,14)        162.1928       -DE/DX =    0.0             !
! A14   A(12,14,13)        132.1816       -DE/DX =    0.0001          !
! A15   A(12,14,16)         83.4881       -DE/DX =    0.0             !
! A16   A(13,14,16)        144.2984       -DE/DX =   -0.0001          !
! A17   A(12,15,16)         81.7965       -DE/DX =    0.0             !
! A18   A(14,16,15)         81.7965       -DE/DX =    0.0             !
! A19   L(6,8,10,7,-1)      165.0255       -DE/DX =    0.0             !
! A20   L(9,11,13,4,-1)     165.0256       -DE/DX =    0.0             !
! A21   L(6,8,10,7,-2)      180.0323       -DE/DX =    0.0001          !
! A22   L(9,11,13,4,-2)     180.0323       -DE/DX =    0.0             !
! D1    D(3,1,2,4)            5.6505      -DE/DX =    0.0             !
! D2    D(2,1,3,5)           -5.2492      -DE/DX =    0.0             !
! D3    D(1,2,4,6)           -5.4165      -DE/DX =    0.0             !
! D4    D(1,3,5,7)            5.6503      -DE/DX =    0.0             !
! D5    D(2,4,6,8)            7.3633      -DE/DX =    0.0             !
! D6    D(3,5,7,9)           -5.4163      -DE/DX =    0.0             !
! D7    D(4,6,10,12)          4.9298       -DE/DX =    0.0             !
! D8    D(5,7,9,11)           7.3631      -DE/DX =    0.0             !
! D9    D(7,9,13,14)          4.9302       -DE/DX =    0.0             !
! D10   D(8,10,12,14)       -36.4448       -DE/DX =    0.0             !
! D11   D(8,10,12,15)       146.4559       -DE/DX =    0.0             !
! D12   D(10,12,14,13)       42.9765       -DE/DX =    0.0             !
! D13   D(10,12,14,16)     -138.7266       -DE/DX =    0.0             !
! D14   D(15,12,14,13)     -138.7267       -DE/DX =    0.0             !
! D15   D(15,12,14,16)       39.5701       -DE/DX =    0.0             !
! D16   D(10,12,15,16)      138.0205       -DE/DX =    0.0             !
! D17   D(14,12,15,16)      -39.8165       -DE/DX =    0.0             !
! D18   D(11,13,14,12)      -36.4454       -DE/DX =    0.0             !
! D19   D(11,13,14,16)      146.4552       -DE/DX =    0.0             !
```

Supporting Information file

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 ! D20   D(12,14,16,15)       -39.8165        -DE/DX =    0.0              !
 ! D21   D(13,14,16,15)       138.0205        -DE/DX =    0.0              !
 ! D22   D(12,15,16,14)       38.3348         -DE/DX =    0.0              !
 ------------------------------------------------------------------------------
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link  103 at Fri Aug 21 22:47:47 2026, MaxMem=    805306368 cpu:                0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l9999.exe)

 ----------------------------------------------------------------------

 Electric dipole moment (input orientation):
 (Debye = 10**-18 statcoulomb cm , SI units = C m)
               (au)          (Debye)        (10**-30 SI)
  Tot       0.151649D+01     0.385453D+01     0.128573D+02
  x         0.151649D+01     0.385453D+01     0.128573D+02
  y        -0.891933D-03    -0.226707D-02    -0.756213D-02
  z        -0.120768D-03    -0.306961D-03    -0.102391D-02

 Dipole polarizability, Alpha (input orientation).
 (esu units = cm**3 , SI units = C**2 m**2 J**-1)
 Alpha(0;0):
             (au)          (10**-24 esu)      (10**-40 SI)
  iso       0.217594D+03     0.322441D+02     0.358764D+02
  aniso     0.234060D+03     0.346841D+02     0.385913D+02
  xx        0.354639D+03     0.525520D+02     0.584720D+02
  yx        0.479937D-01     0.711194D-02     0.791310D-02
  yy        0.213593D+03     0.316512D+02     0.352167D+02
  zx        0.312236D-04     0.462686D-05     0.514807D-05
  zy        0.349858D+01     0.518437D+00     0.576839D+00
  zz        0.845492D+02     0.125289D+02     0.139403D+02

 ----------------------------------------------------------------------

 Dipole orientation:
     6        -0.02343150       -1.26817043        6.84691624
     6        -0.10358678       -3.25979494        5.68524330
     6         0.02190278        1.28005365        6.84383621
     6        -0.10870319       -4.58326100        3.50807837
     6         0.10245058        3.27042323        5.68006817
     6        -0.12342659       -4.86021446        1.22174192
     6         0.10816503        4.58893825        3.49984129
     6        -0.04401045       -4.26023164       -1.25596022
     6         0.12340312        4.86283290        1.21316017
     6         0.03974177       -3.16098960       -3.26974532
     6         0.04449213        4.25784831       -1.26338215
     6         0.31454788       -1.28962190       -5.07653704
```

6	-0.03842917	3.15529643	-3.27539029
6	-0.31340481	1.28058279	-5.07868946
6	1.13558051	-0.77115269	-7.63911986
6	-1.13529320	0.75745923	-7.64006323

Electric dipole moment (dipole orientation):
(Debye = 10**-18 statcoulomb cm , SI units = C m)

	(au)	(Debye)	(10**-30 SI)
Tot	0.151649D+01	0.385453D+01	0.128573D+02
x	0.000000D+00	0.000000D+00	0.000000D+00
y	0.000000D+00	0.000000D+00	0.000000D+00
z	0.151649D+01	0.385453D+01	0.128573D+02

Dipole polarizability, Alpha (dipole orientation).
(esu units = cm**3 , SI units = C**2 m**2 J**-1)
Alpha(0;0):

	(au)	(10**-24 esu)	(10**-40 SI)
iso	0.217594D+03	0.322441D+02	0.358764D+02
aniso	0.234060D+03	0.346841D+02	0.385913D+02
xx	0.845451D+02	0.125283D+02	0.139396D+02
yx	-0.342269D+01	-0.507191D+00	-0.564326D+00
yy	0.213597D+03	0.316519D+02	0.352174D+02
zx	-0.194056D-01	-0.287561D-02	-0.319955D-02
zy	0.130684D+00	0.193653D-01	0.215468D-01
zz	0.354639D+03	0.525520D+02	0.584720D+02

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,0.00060644,0.00000931,-0.00224887,0.00449262,-0.00129336,-0.00687705,
0.00155399,-0.00091551,0.00453614,-0.00334087,0.00169471,0.01003863,-0
.00684800,-0.00122113,-0.00674889,0.00068157,-0.00274063,-0.02235669,0
.01403315,0.00616757,0.00840918,0.00199789,0.00137761,-0.18948495,0.06
672953,-0.06668775,-0.00780525,-0.00740296,0.01625618,-0.00716340,-0.0
4512337,-0.06300634,0.24398238,-0.00039565,-0.00652842,0.00079839,0.00
428301,0.00598751,-0.00088391,-0.00244071,0.00547533,-0.00053209,-0.00
787156,-0.00413677,0.00111198,0.00455752,-0.00338539,0.00029077,0.0113
0141,-0.00035712,-0.00139801,-0.00546070,0.00145184,-0.00008281,-0.014
27462,0.00509679,0.00070625,0.00548190,0.00058376,0.00005445,0.0382196
6,-0.01447993,0.01062938,-0.00517253,-0.00184777,-0.00002743,-0.003118
61,-0.05737341,0.00529490,0.00512595,0.00131638,-0.00272449,-0.0685189
6,0.01676168,-0.01628805,0.00695662,0.11456242,-0.00076314,-0.00616845
,0.00034356,0.00418243,0.00518113,-0.00042179,-0.00209390,0.00568927,-
0.00015033,-0.00677333,-0.00323675,0.00046530,0.00462424,-0.00398389,0
.00005252,0.00882126,-0.00010589,-0.00067892,-0.00638475,0.00205743,0.
00032632,-0.01091685,0.00276945,0.00075042,0.00720326,0.00081183,-0.00
144906,0.01387339,-0.00728406,0.00588899,-0.00843151,-0.00312988,0.000
52569,-0.11140302,0.00780324,-0.08143414,0.01632961,0.00215774,0.01209
393,-0.06872541,-0.00564536,0.00911126,0.13498292,0.07320590,0.2226058
2,-0.00069606,0.00466432,-0.00112452,-0.00225040,-0.00449624,0.0012939
7,0.00271306,-0.00374537,0.00076915,0.00453635,0.00334157,-0.00169464,
-0.00423755,0.00206823,-0.00052951,-0.00674987,-0.00068387,0.00274115,

Supporting Information file

0.00562175,-0.00060484,-0.00001046,0.00840533,-0.00199158,-0.00137762,
-0.00688276,-0.00155889,0.00091490,-0.00780995,0.00739293,-0.01625000,
0.01003823,0.00685448,0.00122076,-0.00718171,0.04512590,0.06303386,-0.
02234036,-0.01404098,-0.00615351,-0.18933345,-0.06682239,0.06671041,-0
.02767504,0.03132727,0.02547480,0.24384242,0.00243527,0.00547636,-0.00
053223,-0.00455431,-0.00338783,0.00029207,0.00039998,-0.00653113,0.000
79835,0.00545643,0.00145648,-0.00008467,-0.00428900,0.00598677,-0.0008
8340,-0.00548035,0.00057934,0.00005619,0.00788099,-0.00413572,0.001111
43,0.00517464,-0.00184326,-0.00002898,-0.01130897,-0.00036387,-0.00139
725,-0.00512983,0.00131872,-0.00273099,0.01428203,0.00511158,0.0007072
9,0.06849882,0.01682881,-0.01628815,-0.03822544,-0.01451101,0.01063738
,0.00304077,-0.05742544,0.00534297,-0.03135051,-0.06312689,-0.07012171
,-0.00683053,0.11456708,0.00208831,0.00568287,-0.00014942,-0.00461670,
-0.00398073,0.00005192,0.00076429,-0.00616371,0.00034300,0.00637382,0.
00205847,0.00032692,-0.00418075,0.00517499,-0.00042168,-0.00719386,0.0
0080667,-0.00145157,0.00677140,-0.00323264,0.00046575,0.00842959,-0.00
312159,0.00052638,-0.00881613,-0.00010999,-0.00067927,-0.01632402,0.00
214481,0.01211313,0.01091044,0.00277310,0.00074993,0.06872972,-0.00562
867,0.00903876,-0.01385832,-0.00728614,0.00589667,0.11145038,0.0079161
0,-0.08151932,-0.02550941,-0.07015524,-0.16802957,-0.13501874,0.073121
71,0.22273839\\0.00002674,0.00004061,0.00019952,-0.00006486,-0.0000171
8,-0.00020142,-0.00000519,-0.00004847,-0.00019864,0.00002894,0.0000059
0,0.00018481,-0.00004107,0.00003512,0.00020167,-0.00000098,0.00005327,
-0.00016374,0.00001769,-0.00002657,-0.00018935,-0.00001415,-0.00004473
,0.00003142,0.00000207,-0.00003714,0.00016269,0.00007536,0.00010539,0.
00011861,-0.00001413,0.00003815,-0.00001372,-0.00011076,-0.00018892,-0
.00019386,0.00007488,-0.00010259,-0.00013652,-0.00010530,0.00018502,0.
00019303,0.00007075,0.00008266,0.00013127,0.00006000,-0.00008051,-0.00
012576\\\@
The archive entry for this job was punched.

Statistics are no substitute for judgment.
-- Henry Clay
Job cpu time: 0 days 12 hours 16 minutes 17.2 seconds.
Elapsed time: 0 days 2 hours 2 minutes 43.8 seconds.
File lengths (MBytes): RWF= 340 Int= 0 D2E= 0 Chk= 21 Scr= 1
Normal termination of Gaussian 16 at Fri Aug 21 22:47:47 2026.

Supporting Information file

S2.2 CDCA: Triplet

Entering Gaussian System, Link 0=g16
Input=cdca.gjf
Output=cdca.log
Initial command:
/home/user/gauss16/g16/l1.exe "/home/user/paper/rahul/grun/Gau-3362053.inp" -scrdir="/home/user/paper/rahul/grun/"
Entering Link 1 = /home/user/gauss16/g16/l1.exe PID= 3362055.

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Gaussian 16, Revision C.01,
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J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas,
J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

****
Gaussian 16: ES64L-G16RevC.01 3-Jul-2019
21-Aug-2026
****
%chk=cdca.chk
%nprocshared=6
Will use up to 6 processors via shared memory.
%mem=6GB

#p opt freq wb97xd/Def2TZVP

1/18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=44,7=101,11=2,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;

Supporting Information file

7//1,2,3,16;
1/18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=44,7=101,11=2,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
Leave Link 1 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l101.exe)
---
title card

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	3.67178	-0.66747	0.01221
C	3.03521	-1.75659	0.04517
C	3.66925	0.66854	-0.01135
C	1.89228	-2.44682	0.05319
C	3.03459	1.75871	-0.04399
C	0.64369	-2.60207	0.05369
C	1.88967	2.44586	-0.05351
C	-0.65305	-2.27941	0.02653
C	0.64146	2.60353	-0.05465
C	-1.75483	-1.68767	-0.02951
C	-0.65508	2.27946	-0.02801
C	-2.70062	-0.70814	-0.15496
C	-1.75691	1.68774	0.0279
C	-2.70096	0.70705	0.1552
C	-4.12795	-0.45453	-0.57652
C	-4.12853	0.4518	0.5786

ITRead= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MicOpt= -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
NAtoms= 16 NQM= 16 NQMF= 0 NMMI= 0 NMMIF= 0
NMic= 0 NMicF= 0.
Isotopes and Nuclear Properties:
(Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic moments (NMagM) in nuclear magnetons)

Atom	1	2	3	4	5	6	7	8	9	10
IAtWgt=	12	12	12	12	12	12	12	12	12	12

Supporting Information file

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000
NucSpn= 0 0 0 0 0 0 0 0 0 0
AtZEff= -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000
NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 11 12 13 14 15 16
IAtWgt= 12 12 12 12 12 12
AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000
NucSpn= 0 0 0 0 0 0
AtZEff= -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000
NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000
Leave Link 101 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 1.7 elap: 0.3
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.2619	estimate D2E/DX2
R2	R(1,3)	1.3362	estimate D2E/DX2
R3	R(2,4)	1.3352	estimate D2E/DX2
R4	R(3,5)	1.2619	estimate D2E/DX2
R5	R(4,6)	1.2582	estimate D2E/DX2
R6	R(5,7)	1.3353	estimate D2E/DX2
R7	R(6,8)	1.3366	estimate D2E/DX2
R8	R(7,9)	1.2581	estimate D2E/DX2
R9	R(8,10)	1.2519	estimate D2E/DX2
R10	R(9,11)	1.3367	estimate D2E/DX2
R11	R(10,12)	1.3674	estimate D2E/DX2
R12	R(11,13)	1.2519	estimate D2E/DX2
R13	R(12,14)	1.4488	estimate D2E/DX2
R14	R(12,15)	1.5097	estimate D2E/DX2
R15	R(13,14)	1.3672	estimate D2E/DX2

```
! R16   R(14,16)            1.5108       estimate D2E/DX2            !
! R17   R(15,16)            1.4682       estimate D2E/DX2            !
! A1    A(2,1,3)           149.59         estimate D2E/DX2           !
! A2    A(1,2,4)           151.4146       estimate D2E/DX2            !
! A3    A(1,3,5)           149.9053       estimate D2E/DX2            !
! A4    A(2,4,6)           155.9579       estimate D2E/DX2            !
! A5    A(3,5,7)           151.1622       estimate D2E/DX2            !
! A6    A(4,6,8)           158.9071       estimate D2E/DX2            !
! A7    A(5,7,9)           156.2257       estimate D2E/DX2            !
! A8    A(7,9,11)          158.7351       estimate D2E/DX2             !
! A9    A(8,10,12)         162.0748       estimate D2E/DX2              !
! A10   A(10,12,14)        132.8646       estimate D2E/DX2               !
! A11   A(10,12,15)        143.1181       estimate D2E/DX2               !
! A12   A(14,12,15)         84.0          estimate D2E/DX2             !
! A13   A(11,13,14)        161.9754       estimate D2E/DX2               !
! A14   A(12,14,13)        132.889        estimate D2E/DX2              !
! A15   A(12,14,16)         83.9833       estimate D2E/DX2              !
! A16   A(13,14,16)        143.1088       estimate D2E/DX2               !
! A17   A(12,15,16)         83.3609       estimate D2E/DX2              !
! A18   A(14,16,15)         83.306        estimate D2E/DX2             !
! A19   L(6,8,10,7,-1)     165.7176       estimate D2E/DX2              !
! A20   L(9,11,13,4,-1)    165.7795       estimate D2E/DX2               !
! A21   L(6,8,10,7,-2)     178.8531       estimate D2E/DX2               !
! A22   L(9,11,13,4,-2)    178.8388       estimate D2E/DX2               !
! D1    D(3,1,2,4)          2.5816       estimate D2E/DX2             !
! D2    D(2,1,3,5)         -2.4473       estimate D2E/DX2             !
! D3    D(1,2,4,6)         -1.7812       estimate D2E/DX2             !
! D4    D(1,3,5,7)          2.3877       estimate D2E/DX2             !
! D5    D(2,4,6,8)          2.5026       estimate D2E/DX2             !
! D6    D(3,5,7,9)         -1.5325       estimate D2E/DX2             !
! D7    D(4,6,10,12)        4.8617       estimate D2E/DX2              !
! D8    D(5,7,9,11)         2.3885       estimate D2E/DX2             !
! D9    D(7,9,13,14)        5.0483       estimate D2E/DX2              !
! D10   D(8,10,12,14)     -30.2344       estimate D2E/DX2               !
! D11   D(8,10,12,15)     151.8784       estimate D2E/DX2               !
! D12   D(10,12,14,13)     38.8549       estimate D2E/DX2               !
! D13   D(10,12,14,16)   -142.4823       estimate D2E/DX2                !
! D14   D(15,12,14,13)   -142.4199       estimate D2E/DX2                !
! D15   D(15,12,14,16)     36.2428       estimate D2E/DX2               !
! D16   D(10,12,15,16)     140.9213       estimate D2E/DX2               !
! D17   D(14,12,15,16)     -37.5217       estimate D2E/DX2               !
! D18   D(11,13,14,12)     -30.5456       estimate D2E/DX2               !
! D19   D(11,13,14,16)     151.6702       estimate D2E/DX2               !
! D20   D(12,14,16,15)     -37.4983       estimate D2E/DX2               !
! D21   D(13,14,16,15)     140.8695       estimate D2E/DX2               !
! D22   D(12,15,16,14)      35.7931       estimate D2E/DX2              !
--------------------------------------------------------------------------------
```

Supporting Information file

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06 EigMax=2.50D+02 EigMin=1.00D-04
Number of steps in this run= 71 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.671775	-0.667468	0.012214
2	6	0	3.035208	-1.756588	0.045172
3	6	0	3.669250	0.668543	-0.011351
4	6	0	1.892277	-2.446817	0.053192
5	6	0	3.034586	1.758714	-0.043991
6	6	0	0.643693	-2.602073	0.053693
7	6	0	1.889669	2.445864	-0.053513
8	6	0	-0.653046	-2.279414	0.026533
9	6	0	0.641461	2.603532	-0.054652
10	6	0	-1.754827	-1.687667	-0.029514
11	6	0	-0.655081	2.279462	-0.028006
12	6	0	-2.700618	-0.708137	-0.154955
13	6	0	-1.756907	1.687737	0.027896
14	6	0	-2.700958	0.707047	0.155202
15	6	0	-4.127951	-0.454532	-0.576519
16	6	0	-4.128532	0.451796	0.578600

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.261937	0.000000			
3	C	1.336221	2.507282	0.000000		
4	C	2.516818	1.335205	3.587097	0.000000	
5	C	2.509089	3.516433	1.261878	4.358991	0.000000
6	C	3.593563	2.536585	4.455912	1.258200	4.974171
7	C	3.587904	4.356903	2.515463	4.893845	1.335328
8	C	4.615480	3.725173	5.232029	2.550961	5.469011
9	C	4.459452	4.975001	3.593545	5.204056	2.537889
10	C	5.521825	4.791113	5.913769	3.726193	5.900528
11	C	5.235236	5.469304	4.614670	5.369668	3.726268
12	C	6.374715	5.834295	6.518519	4.915386	6.244216
13	C	5.917586	5.901529	5.521184	5.514682	4.792558
14	C	6.520848	6.243813	6.372501	5.572708	5.834565
15	C	7.824811	7.307031	7.897915	6.372510	7.515582
16	C	7.900527	7.515363	7.823070	6.702847	7.307935

Supporting Information file

		6	7	8	9	10
6	C	0.000000				
7	C	5.200540	0.000000			
8	C	1.336555	5.366569	0.000000		
9	C	5.206733	1.258127	5.052277	0.000000	
10	C	2.568260	5.510808	1.251889	4.914999	0.000000
11	C	5.052017	2.550312	4.559203	1.336695	4.116741
12	C	3.849019	5.570345	2.587354	4.706029	1.367383
13	C	4.915894	3.725440	4.117863	2.568592	3.375893
14	C	4.706089	4.913339	3.623458	3.848696	2.581461
15	C	5.270454	6.700566	3.970999	5.689586	2.729753
16	C	5.689971	6.371391	4.454581	5.271035	3.252934

		11	12	13	14	15
11	C	0.000000				
12	C	3.622994	0.000000			
13	C	1.251912	2.581518	0.000000		
14	C	2.586826	1.448773	1.367184	0.000000	
15	C	4.453809	1.509739	3.252151	1.980149	0.000000
16	C	3.971548	1.980527	2.730463	1.510757	1.468241

		16
16	C	0.000000

Stoichiometry C16
Framework group C1[X(C16)]
Deg. of freedom 42
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.671775	-0.667468	0.012214
2	6	0	3.035208	-1.756588	0.045172
3	6	0	3.669250	0.668543	-0.011351
4	6	0	1.892277	-2.446817	0.053192
5	6	0	3.034586	1.758714	-0.043991
6	6	0	0.643693	-2.602073	0.053693
7	6	0	1.889669	2.445864	-0.053513
8	6	0	-0.653046	-2.279414	0.026533
9	6	0	0.641461	2.603532	-0.054652
10	6	0	-1.754827	-1.687667	-0.029514
11	6	0	-0.655081	2.279462	-0.028006
12	6	0	-2.700618	-0.708137	-0.154955
13	6	0	-1.756907	1.687737	0.027896
14	6	0	-2.700958	0.707047	0.155202
15	6	0	-4.127951	-0.454532	-0.576519
16	6	0	-4.128532	0.451796	0.578600

Supporting Information file

Rotational constants (GHZ): 0.8286404 0.3836542 0.2646593
Leave Link 202 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 707.7593326469 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0073441590 Hartrees.
Nuclear repulsion after empirical dispersion term = 707.7519884879 Hartrees.
Leave Link 301 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14162 LenP2D= 33380.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.11D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 564 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 2.4 elap: 0.4
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 17:46:48 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)

Supporting Information file

ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.889454862564
JPrj=0 DoOrth=F DoCkMO=F.
Leave Link 401 at Fri Aug 21 17:46:51 2026, MaxMem= 805306368 cpu: 13.5 elap: 2.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.785467573105
DIIS: error= 5.21D-02 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.785467573105 IErMin= 1 ErrMin= 5.21D-02
ErrMax= 5.21D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D+00 BMatP= 1.38D+00
IDIUse=3 WtCom= 4.79D-01 WtEn= 5.21D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.245 Goal= None Shift= 0.000
GapD= 0.245 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.
Damping current iteration by 5.00D-01
RMSDP=8.53D-03 MaxDP=4.45D-01 OVMax= 1.06D-01

Cycle 2 Pass 0 IDiag 1:

RMSU= 2.66D-03 CP: 7.62D-01
E= -608.869789276275 Delta-E= -0.084321703170 Rises=F Damp=T
DIIS: error= 2.44D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.869789276275 IErMin= 2 ErrMin= 2.44D-02
ErrMax= 2.44D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.97D-01 BMatP= 1.38D+00
IDIUse=3 WtCom= 7.56D-01 WtEn= 2.44D-01
Coeff-Com: -0.793D+00 0.179D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.600D+00 0.160D+01
Gap= 0.275 Goal= None Shift= 0.000
RMSDP=4.94D-03 MaxDP=1.93D-01 DE=-8.43D-02 OVMax= 1.27D-01

Cycle 3 Pass 0 IDiag 1:
RMSU= 2.33D-03 CP: 5.45D-01 2.18D+00
E= -608.900230311374 Delta-E= -0.030441035099 Rises=F Damp=F
DIIS: error= 1.59D-02 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.900230311374 IErMin= 3 ErrMin= 1.59D-02
ErrMax= 1.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.18D-02 BMatP= 2.97D-01
IDIUse=3 WtCom= 8.41D-01 WtEn= 1.59D-01
Coeff-Com: -0.468D+00 0.101D+01 0.453D+00
Coeff-En: 0.000D+00 0.213D+00 0.787D+00
Coeff: -0.394D+00 0.888D+00 0.506D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.21D-02 MaxDP=9.49D-01 DE=-3.04D-02 OVMax= 1.09D-01

Cycle 4 Pass 0 IDiag 1:
RMSU= 1.89D-02 CP: 8.68D-01 3.00D+00 3.00D+00
E= -608.956879908755 Delta-E= -0.056649597382 Rises=F Damp=F
DIIS: error= 7.80D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.956879908755 IErMin= 4 ErrMin= 7.80D-03
ErrMax= 7.80D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-02 BMatP= 5.18D-02
IDIUse=3 WtCom= 9.22D-01 WtEn= 7.80D-02
Coeff-Com: -0.305D+00 0.660D+00 0.366D+00 0.279D+00
Coeff-En: 0.000D+00 0.000D+00 0.702D-01 0.930D+00
Coeff: -0.281D+00 0.609D+00 0.343D+00 0.329D+00
Gap= 0.224 Goal= None Shift= 0.000
RMSDP=3.20D+02 MaxDP=1.30D+04 DE=-5.66D-02 OVMax= 9.69D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 5 Pass 1 IDiag 1:
E= -608.956027483243 Delta-E= 0.000852425513 Rises=F Damp=F
DIIS: error= 6.26D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.956027483243 IErMin= 1 ErrMin= 6.26D-03
ErrMax= 6.26D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.49D-03 BMatP= 6.49D-03
IDIUse=3 WtCom= 9.37D-01 WtEn= 6.26D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01

Coeff: 0.100D+01
Gap= 0.233 Goal= None Shift= 0.000
GapD= 0.233 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=2.39D-02 MaxDP=1.03D+00 DE= 8.52D-04 OVMax= 6.51D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 7.10D-03 CP: 1.80D-01
E= -608.939729452319 Delta-E= 0.016298030924 Rises=F Damp=F
DIIS: error= 1.08D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -608.956027483243 IErMin= 1 ErrMin= 6.26D-03
ErrMax= 1.08D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-02 BMatP= 6.49D-03
IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00
Coeff-En: 0.726D+00 0.274D+00
Coeff: 0.726D+00 0.274D+00
Gap= 0.225 Goal= None Shift= 0.000
RMSDP=4.19D-04 MaxDP=1.43D-02 DE= 1.63D-02 OVMax= 3.12D-02

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.61D-04 CP: 1.68D-01 1.01D+00
E= -608.962489653777 Delta-E= -0.022760201458 Rises=F Damp=F
DIIS: error= 2.26D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.962489653777 IErMin= 3 ErrMin= 2.26D-03
ErrMax= 2.26D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.42D-04 BMatP= 6.49D-03
IDIUse=3 WtCom= 9.77D-01 WtEn= 2.26D-02
Coeff-Com: 0.437D-01-0.222D+00 0.118D+01
Coeff-En: 0.105D+00 0.000D+00 0.895D+00
Coeff: 0.451D-01-0.217D+00 0.117D+01
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=8.08D-04 MaxDP=2.42D-02 DE=-2.28D-02 OVMax= 1.13D-02

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.17D-04 CP: 1.43D-01 1.02D+00 1.94D+00
E= -608.963594944859 Delta-E= -0.001105291082 Rises=F Damp=F
DIIS: error= 4.52D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.963594944859 IErMin= 4 ErrMin= 4.52D-04
ErrMax= 4.52D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.35D-05 BMatP= 9.42D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.52D-03
Coeff-Com: -0.351D-01-0.158D+00 0.672D+00 0.521D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.350D-01-0.157D+00 0.669D+00 0.523D+00
Gap= 0.226 Goal= None Shift= 0.000
RMSDP=1.32D-04 MaxDP=3.52D-03 DE=-1.11D-03 OVMax= 2.50D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 1.96D-05 CP: 1.40D-01 1.03D+00 2.08D+00 1.21D+00
E= -608.963650020709 Delta-E= -0.000055075850 Rises=F Damp=F
DIIS: error= 2.36D-04 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.963650020709 IErMin= 5 ErrMin= 2.36D-04

ErrMax= 2.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.13D-06 BMatP= 3.35D-05
IDIUse=3 WtCom= 9.98D-01 WtEn= 2.36D-03
Coeff-Com: -0.209D-01 0.207D-02-0.680D-01 0.147D+00 0.939D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.209D-01 0.207D-02-0.678D-01 0.147D+00 0.939D+00
Gap= 0.226 Goal= None Shift= 0.000
RMSDP=5.13D-05 MaxDP=1.33D-03 DE=-5.51D-05 OVMax= 3.12D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.54D-05 CP: 1.38D-01 1.03D+00 2.14D+00 1.29D+00 1.30D+00
E= -608.963673070358 Delta-E= -0.000023049649 Rises=F Damp=F
DIIS: error= 1.75D-04 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.963673070358 IErMin= 6 ErrMin= 1.75D-04
ErrMax= 1.75D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.24D-06 BMatP= 4.13D-06
IDIUse=3 WtCom= 9.98D-01 WtEn= 1.75D-03
Coeff-Com: 0.187D-02 0.704D-01-0.338D+00-0.152D+00 0.594D+00 0.824D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.186D-02 0.703D-01-0.338D+00-0.152D+00 0.593D+00 0.824D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.53D-05 MaxDP=5.31D-04 DE=-2.30D-05 OVMax= 2.82D-03

Cycle 11 Pass 1 IDiag 1:
RMSU= 6.93D-06 CP: 1.38D-01 1.03D+00 2.16D+00 1.29D+00 1.59D+00
CP: 1.75D+00
E= -608.963683721066 Delta-E= -0.000010650708 Rises=F Damp=F
DIIS: error= 7.43D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.963683721066 IErMin= 7 ErrMin= 7.43D-05
ErrMax= 7.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.08D-07 BMatP= 2.24D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.349D-02 0.280D-01-0.126D+00-0.911D-01 0.884D-01 0.355D+00
Coeff-Com: 0.742D+00
Coeff: 0.349D-02 0.280D-01-0.126D+00-0.911D-01 0.884D-01 0.355D+00
Coeff: 0.742D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=2.28D-05 MaxDP=7.10D-04 DE=-1.07D-05 OVMax= 1.06D-03

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.24D-06 CP: 1.39D-01 1.03D+00 2.13D+00 1.26D+00 1.72D+00
CP: 1.98D+00 1.22D+00
E= -608.963685106964 Delta-E= -0.000001385898 Rises=F Damp=F
DIIS: error= 3.25D-05 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.963685106964 IErMin= 8 ErrMin= 3.25D-05
ErrMax= 3.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.23D-08 BMatP= 3.08D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.129D-02-0.291D-02 0.185D-01-0.135D-01-0.101D+00-0.417D-02
Coeff-Com: 0.373D+00 0.729D+00
Coeff: 0.129D-02-0.291D-02 0.185D-01-0.135D-01-0.101D+00-0.417D-02
Coeff: 0.373D+00 0.729D+00

Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.57D-05 MaxDP=4.89D-04 DE=-1.39D-06 OVMax= 4.51D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.29D-06 CP: 1.40D-01 1.03D+00 2.12D+00 1.24D+00 1.77D+00
CP: 2.06D+00 1.38D+00 1.57D+00
E= -608.963685528414 Delta-E= -0.000000421449 Rises=F Damp=F
DIIS: error= 1.63D-05 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.963685528414 IErMin= 9 ErrMin= 1.63D-05
ErrMax= 1.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-08 BMatP= 9.23D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.478D-03-0.104D-01 0.492D-01 0.206D-01-0.699D-01-0.107D+00
Coeff-Com: -0.958D-01 0.312D+00 0.902D+00
Coeff: -0.478D-03-0.104D-01 0.492D-01 0.206D-01-0.699D-01-0.107D+00
Coeff: -0.958D-01 0.312D+00 0.902D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=7.32D-06 MaxDP=2.44D-04 DE=-4.21D-07 OVMax= 3.27D-04

Cycle 14 Pass 1 IDiag 1:
RMSU= 7.53D-07 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.79D+00
CP: 2.08D+00 1.46D+00 1.96D+00 1.62D+00
E= -608.963685699409 Delta-E= -0.000000170995 Rises=F Damp=F
DIIS: error= 8.61D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.963685699409 IErMin=10 ErrMin= 8.61D-06
ErrMax= 8.61D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.98D-09 BMatP= 2.46D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.392D-03-0.234D-02 0.989D-02 0.822D-02 0.650D-02-0.284D-01
Coeff-Com: -0.156D+00-0.118D+00 0.367D+00 0.913D+00
Coeff: -0.392D-03-0.234D-02 0.989D-02 0.822D-02 0.650D-02-0.284D-01
Coeff: -0.156D+00-0.118D+00 0.367D+00 0.913D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.40D-06 MaxDP=3.78D-05 DE=-1.71D-07 OVMax= 2.23D-04

Cycle 15 Pass 1 IDiag 1:
RMSU= 5.68D-07 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.09D+00 1.48D+00 2.12D+00 1.86D+00 1.58D+00
E= -608.963685749107 Delta-E= -0.000000049698 Rises=F Damp=F
DIIS: error= 3.12D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.963685749107 IErMin=11 ErrMin= 3.12D-06
ErrMax= 3.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-09 BMatP= 6.98D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.325D-04 0.145D-02-0.746D-02-0.206D-02 0.183D-01 0.147D-01
Coeff-Com: -0.346D-01-0.114D+00-0.692D-01 0.313D+00 0.880D+00
Coeff: -0.325D-04 0.145D-02-0.746D-02-0.206D-02 0.183D-01 0.147D-01
Coeff: -0.346D-01-0.114D+00-0.692D-01 0.313D+00 0.880D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.96D-06 MaxDP=6.48D-05 DE=-4.97D-08 OVMax= 8.40D-05

Supporting Information file

Cycle 16 Pass 1 IDiag 1:
RMSU= 2.76D-07 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.09D+00 1.48D+00 2.08D+00 1.94D+00 1.92D+00
CP: 1.41D+00
E= -608.963685757433 Delta-E= -0.000000008326 Rises=F Damp=F
DIIS: error= 9.21D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.963685757433 IErMin=12 ErrMin= 9.21D-07
ErrMax= 9.21D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-10 BMatP= 1.20D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.440D-04 0.665D-03-0.311D-02-0.189D-02 0.207D-02 0.761D-02
Coeff-Com: 0.221D-01 0.165D-02-0.789D-01-0.120D+00 0.138D+00 0.103D+01
Coeff: 0.440D-04 0.665D-03-0.311D-02-0.189D-02 0.207D-02 0.761D-02
Coeff: 0.221D-01 0.165D-02-0.789D-01-0.120D+00 0.138D+00 0.103D+01
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=7.72D-07 MaxDP=3.06D-05 DE=-8.33D-09 OVMax= 3.26D-05

Cycle 17 Pass 1 IDiag 1:
RMSU= 9.25D-08 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.09D+00 1.49D+00 2.05D+00 1.93D+00 2.05D+00
CP: 1.62D+00 1.52D+00
E= -608.963685758613 Delta-E= -0.000000001179 Rises=F Damp=F
DIIS: error= 4.18D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.963685758613 IErMin=13 ErrMin= 4.18D-07
ErrMax= 4.18D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.16D-11 BMatP= 1.49D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.163D-04 0.549D-05 0.662D-04-0.240D-03-0.192D-02 0.435D-03
Coeff-Com: 0.125D-01 0.173D-01-0.175D-01-0.844D-01-0.791D-01 0.367D+00
Coeff-Com: 0.786D+00
Coeff: 0.163D-04 0.549D-05 0.662D-04-0.240D-03-0.192D-02 0.435D-03
Coeff: 0.125D-01 0.173D-01-0.175D-01-0.844D-01-0.791D-01 0.367D+00
Coeff: 0.786D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.39D-07 MaxDP=5.47D-06 DE=-1.18D-09 OVMax= 9.16D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 2.60D-08 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.81D+00
CP: 2.10D+00 1.49D+00 2.04D+00 1.93D+00 2.06D+00
CP: 1.63D+00 1.71D+00 1.38D+00
E= -608.963685758719 Delta-E= -0.000000000106 Rises=F Damp=F
DIIS: error= 1.72D-07 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.963685758719 IErMin=14 ErrMin= 1.72D-07
ErrMax= 1.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.71D-12 BMatP= 3.16D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.283D-07-0.748D-04 0.358D-03 0.204D-03-0.429D-03-0.101D-02
Coeff-Com: -0.564D-03 0.221D-02 0.681D-02 0.408D-02-0.361D-01-0.810D-01
Coeff-Com: 0.141D+00 0.965D+00
Coeff: 0.283D-07-0.748D-04 0.358D-03 0.204D-03-0.429D-03-0.101D-02
Coeff: -0.564D-03 0.221D-02 0.681D-02 0.408D-02-0.361D-01-0.810D-01

Coeff: 0.141D+00 0.965D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=1.58D-07 MaxDP=4.64D-06 DE=-1.06D-10 OVMax= 3.53D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.24D-08 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.80D+00
CP: 2.10D+00 1.49D+00 2.04D+00 1.94D+00 2.06D+00
CP: 1.62D+00 1.76D+00 1.56D+00 1.43D+00
E= -608.963685758752 Delta-E= -0.000000000033 Rises=F Damp=F
DIIS: error= 7.16D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -608.963685758752 IErMin=15 ErrMin= 7.16D-08
ErrMax= 7.16D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.89D-13 BMatP= 3.71D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.186D-05-0.190D-04 0.779D-04 0.902D-04 0.145D-03-0.396D-03
Coeff-Com: -0.174D-02-0.183D-02 0.387D-02 0.127D-01 0.211D-02-0.688D-01
Coeff-Com: -0.845D-01 0.246D+00 0.892D+00
Coeff: -0.186D-05-0.190D-04 0.779D-04 0.902D-04 0.145D-03-0.396D-03
Coeff: -0.174D-02-0.183D-02 0.387D-02 0.127D-01 0.211D-02-0.688D-01
Coeff: -0.845D-01 0.246D+00 0.892D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=4.25D-08 MaxDP=1.29D-06 DE=-3.32D-11 OVMax= 1.61D-06

Cycle 20 Pass 1 IDiag 1:
RMSU= 5.70D-09 CP: 1.40D-01 1.03D+00 2.11D+00 1.23D+00 1.80D+00
CP: 2.10D+00 1.49D+00 2.04D+00 1.94D+00 2.05D+00
CP: 1.61D+00 1.77D+00 1.59D+00 1.64D+00 1.29D+00
E= -608.963685758750 Delta-E= 0.000000000002 Rises=F Damp=F
DIIS: error= 3.75D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -608.963685758752 IErMin=16 ErrMin= 3.75D-08
ErrMax= 3.75D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.18D-13 BMatP= 7.89D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.114D-05 0.607D-05-0.343D-04 0.697D-05 0.143D-03 0.148D-04
Coeff-Com: -0.746D-03-0.128D-02 0.384D-03 0.518D-02 0.955D-02-0.152D-01
Coeff-Com: -0.774D-01-0.103D+00 0.448D+00 0.734D+00
Coeff: -0.114D-05 0.607D-05-0.343D-04 0.697D-05 0.143D-03 0.148D-04
Coeff: -0.746D-03-0.128D-02 0.384D-03 0.518D-02 0.955D-02-0.152D-01
Coeff: -0.774D-01-0.103D+00 0.448D+00 0.734D+00
Gap= 0.227 Goal= None Shift= 0.000
RMSDP=6.28D-09 MaxDP=2.53D-07 DE= 1.82D-12 OVMax= 8.53D-07

SCF Done: E(RwB97XD) = -608.963685759 A.U. after 20 cycles
NFock= 20 Conv=0.63D-08 -V/T= 2.0063
KE= 6.051483865749D+02 PE=-2.825487511843D+03 EE= 9.036234510209D+02
Leave Link 502 at Fri Aug 21 17:54:15 2026, MaxMem= 805306368 cpu: 2663.8 elap: 444.1
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

Supporting Information file

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Population analysis using the SCF Density.

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Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(

Supporting Information file

(A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -10.40690 -10.40650 -10.37744 -10.37670 -10.37584
Alpha occ. eigenvalues -- -10.37576 -10.37458 -10.37430 -10.37264 -10.37251
Alpha occ. eigenvalues -- -10.37144 -10.37109 -10.36674 -10.36633 -10.36232
Alpha occ. eigenvalues -- -10.36197 -1.05999 -0.98288 -0.96768 -0.94986
Alpha occ. eigenvalues -- -0.93120 -0.90373 -0.87806 -0.83889 -0.81446
Alpha occ. eigenvalues -- -0.78413 -0.75080 -0.72252 -0.69470 -0.67314
Alpha occ. eigenvalues -- -0.63827 -0.63640 -0.53512 -0.52920 -0.52039
Alpha occ. eigenvalues -- -0.51608 -0.50673 -0.50080 -0.46376 -0.46351
Alpha occ. eigenvalues -- -0.44330 -0.42870 -0.38788 -0.38377 -0.34736
Alpha occ. eigenvalues -- -0.32480 -0.31924 -0.31769
Alpha virt. eigenvalues -- -0.09094 -0.08811 -0.06639 -0.03779 -0.00340
Alpha virt. eigenvalues -- 0.02605 0.03715 0.04468 0.07072 0.08937
Alpha virt. eigenvalues -- 0.10070 0.10970 0.11335 0.12055 0.12673
Alpha virt. eigenvalues -- 0.15689 0.17021 0.18884 0.21138 0.21609
Alpha virt. eigenvalues -- 0.21664 0.22970 0.23058 0.23674 0.24865
Alpha virt. eigenvalues -- 0.26244 0.26700 0.27094 0.27999 0.28249
Alpha virt. eigenvalues -- 0.29255 0.29978 0.30712 0.30917 0.31334
Alpha virt. eigenvalues -- 0.31880 0.32712 0.33636 0.34526 0.34775
Alpha virt. eigenvalues -- 0.35562 0.36990 0.37088 0.37740 0.37765
Alpha virt. eigenvalues -- 0.38925 0.38996 0.39287 0.40559 0.41526
Alpha virt. eigenvalues -- 0.41557 0.42309 0.42360 0.43859 0.45261
Alpha virt. eigenvalues -- 0.46054 0.46117 0.46674 0.47397 0.48721
Alpha virt. eigenvalues -- 0.48922 0.49763 0.50159 0.50358 0.52303
Alpha virt. eigenvalues -- 0.52541 0.52664 0.52964 0.53837 0.54204
Alpha virt. eigenvalues -- 0.54382 0.54511 0.55485 0.55857 0.57073
Alpha virt. eigenvalues -- 0.58165 0.58417 0.58482 0.59196 0.59423
Alpha virt. eigenvalues -- 0.60685 0.62545 0.62873 0.63279 0.63667
Alpha virt. eigenvalues -- 0.64966 0.67206 0.67571 0.67633 0.68150
Alpha virt. eigenvalues -- 0.70217 0.70541 0.71511 0.72082 0.73953
Alpha virt. eigenvalues -- 0.74744 0.76060 0.76622 0.78011 0.78954
Alpha virt. eigenvalues -- 0.80927 0.82709 0.83458 0.84356 0.85052
Alpha virt. eigenvalues -- 0.86608 0.88275 0.89661 0.91027 0.91241
Alpha virt. eigenvalues -- 0.92390 0.94524 0.95100 0.97186 0.98545
Alpha virt. eigenvalues -- 0.98956 1.01019 1.01125 1.03659 1.05979
Alpha virt. eigenvalues -- 1.07190 1.08687 1.08747 1.11288 1.11587
Alpha virt. eigenvalues -- 1.12023 1.13912 1.14107 1.15482 1.16947
Alpha virt. eigenvalues -- 1.17791 1.20372 1.21786 1.22279 1.22977
Alpha virt. eigenvalues -- 1.25713 1.26192 1.26203 1.27377 1.29578
Alpha virt. eigenvalues -- 1.31965 1.33063 1.33682 1.34257 1.35299
Alpha virt. eigenvalues -- 1.36631 1.37452 1.37792 1.39236 1.39619
Alpha virt. eigenvalues -- 1.41936 1.42298 1.42439 1.42907 1.44085
Alpha virt. eigenvalues -- 1.45158 1.45496 1.46790 1.46943 1.48193
Alpha virt. eigenvalues -- 1.48537 1.49287 1.49483 1.50997 1.51694
Alpha virt. eigenvalues -- 1.52713 1.52832 1.54902 1.55318 1.57879
Alpha virt. eigenvalues -- 1.59154 1.59282 1.61352 1.61398 1.62952
Alpha virt. eigenvalues -- 1.64029 1.65346 1.67030 1.68233 1.69343

Alpha virt. eigenvalues --	1.69748	1.69957	1.71333	1.73328	1.73951
Alpha virt. eigenvalues --	1.75280	1.75578	1.76219	1.77549	1.77627
Alpha virt. eigenvalues --	1.78157	1.80551	1.82226	1.82561	1.83393
Alpha virt. eigenvalues --	1.84430	1.85205	1.88923	1.92130	1.94462
Alpha virt. eigenvalues --	1.94904	1.96375	1.97236	2.00359	2.03126
Alpha virt. eigenvalues --	2.06640	2.08108	2.11388	2.15317	2.15590
Alpha virt. eigenvalues --	2.17916	2.19108	2.19672	2.23329	2.25035
Alpha virt. eigenvalues --	2.26368	2.29808	2.33103	2.37580	2.37798
Alpha virt. eigenvalues --	2.40023	2.40672	2.43296	2.43425	2.44461
Alpha virt. eigenvalues --	2.45671	2.45890	2.45978	2.47767	2.49563
Alpha virt. eigenvalues --	2.49612	2.49851	2.52076	2.53038	2.54048
Alpha virt. eigenvalues --	2.54298	2.56845	2.57158	2.60039	2.60116
Alpha virt. eigenvalues --	2.60394	2.61715	2.62096	2.62743	2.63814
Alpha virt. eigenvalues --	2.64732	2.65694	2.68557	2.68700	2.71686
Alpha virt. eigenvalues --	2.71766	2.73222	2.73486	2.74591	2.75966
Alpha virt. eigenvalues --	2.76207	2.76590	2.77597	2.79378	2.79493
Alpha virt. eigenvalues --	2.80529	2.82441	2.82794	2.83480	2.83989
Alpha virt. eigenvalues --	2.84800	2.85391	2.85714	2.85963	2.86711
Alpha virt. eigenvalues --	2.87619	2.87852	2.87888	2.88309	2.88628
Alpha virt. eigenvalues --	2.89525	2.90250	2.90532	2.90623	2.92189
Alpha virt. eigenvalues --	2.94205	2.95921	2.95949	2.96448	2.98521
Alpha virt. eigenvalues --	2.98816	2.99596	2.99859	3.00374	3.00873
Alpha virt. eigenvalues --	3.01977	3.02713	3.03550	3.04517	3.04853
Alpha virt. eigenvalues --	3.05890	3.08265	3.08794	3.10400	3.11433
Alpha virt. eigenvalues --	3.11699	3.12798	3.13657	3.14714	3.14829
Alpha virt. eigenvalues --	3.16620	3.17281	3.17575	3.18364	3.19966
Alpha virt. eigenvalues --	3.20524	3.23800	3.24583	3.24916	3.25283
Alpha virt. eigenvalues --	3.25441	3.27026	3.28262	3.29475	3.29551
Alpha virt. eigenvalues --	3.30339	3.30824	3.31428	3.33555	3.34132
Alpha virt. eigenvalues --	3.34382	3.35017	3.35381	3.36979	3.38246
Alpha virt. eigenvalues --	3.38800	3.40529	3.41383	3.42282	3.42552
Alpha virt. eigenvalues --	3.45853	3.46699	3.46818	3.48387	3.49029
Alpha virt. eigenvalues --	3.51456	3.51949	3.52918	3.53396	3.54830
Alpha virt. eigenvalues --	3.55909	3.58944	3.59871	3.60189	3.61996
Alpha virt. eigenvalues --	3.62781	3.68637	3.70325	3.70769	3.71758
Alpha virt. eigenvalues --	3.74026	3.78299	3.78508	3.81650	3.82991
Alpha virt. eigenvalues --	3.83287	3.83695	3.86912	3.89434	3.93028
Alpha virt. eigenvalues --	3.95765	3.99046	3.99927	4.02474	4.02659
Alpha virt. eigenvalues --	4.03871	4.04149	4.05597	4.11559	4.12337
Alpha virt. eigenvalues --	4.13711	4.17586	4.18341	4.20836	4.24842
Alpha virt. eigenvalues --	4.26572	4.31431	4.31810	4.35208	4.42212
Alpha virt. eigenvalues --	4.43172	4.46315	4.51087	4.52254	4.53026
Alpha virt. eigenvalues --	4.58309	4.62117	4.65883	4.71192	4.72864
Alpha virt. eigenvalues --	4.72888	4.74977	4.75142	4.81502	4.83137
Alpha virt. eigenvalues --	4.91778	4.91817	4.96066	5.00123	5.02929
Alpha virt. eigenvalues --	5.03424	5.07235	5.08528	5.09052	5.10261
Alpha virt. eigenvalues --	5.14230	5.16411	5.17161	5.17904	5.19066
Alpha virt. eigenvalues --	5.20071	5.23538	5.24358	5.27545	5.27626

Supporting Information file

Alpha virt. eigenvalues -- 5.35726 5.36158 5.42819 5.51883 5.54656
Alpha virt. eigenvalues -- 5.57667 5.67572 5.74351 5.92913 5.97855
Alpha virt. eigenvalues -- 6.03944 6.11064 22.06007 22.13458 22.48653
Alpha virt. eigenvalues -- 22.84147 23.07746 23.19356 23.19409 23.33661
Alpha virt. eigenvalues -- 23.45384 23.53563 23.62173 23.64950 23.86424
Alpha virt. eigenvalues -- 23.91611 24.14183 24.17979

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.798194	0.869986	0.557626	-0.077954	-0.075579	-0.043476
2	C	0.869986	4.801135	-0.076715	0.579704	-0.038944	-0.072960
3	C	0.557626	-0.076715	4.801360	-0.020958	0.869855	-0.007302
4	C	-0.077954	0.579704	-0.020958	4.788184	-0.006792	0.928531
5	C	-0.075579	-0.038944	0.869855	-0.006792	4.797278	-0.001774
6	C	-0.043476	-0.072960	-0.007302	0.928531	-0.001774	4.906160
7	C	-0.020761	-0.006765	-0.078473	-0.001895	0.578494	-0.000550
8	C	-0.010157	-0.030783	-0.001644	-0.091806	-0.000422	0.557387
9	C	-0.007204	-0.001748	-0.043144	-0.000532	-0.071634	-0.000118
10	C	-0.002127	-0.010642	-0.000351	-0.058597	-0.000139	-0.194905
11	C	-0.001620	-0.000396	-0.009915	-0.000171	-0.030036	0.001821
12	C	-0.000193	-0.001115	-0.000071	-0.007119	-0.000079	-0.037944
13	C	-0.000351	-0.000124	-0.002062	-0.000001	-0.010366	0.000303
14	C	-0.000074	-0.000079	-0.000185	-0.000951	-0.001083	-0.009891
15	C	-0.000001	-0.000014	0.000001	-0.000176	0.000006	-0.002319
16	C	0.000001	0.000007	-0.000001	0.000081	-0.000013	0.001085

		7	8	9	10	11	12
1	C	-0.020761	-0.010157	-0.007204	-0.002127	-0.001620	-0.000193
2	C	-0.006765	-0.030783	-0.001748	-0.010642	-0.000396	-0.001115
3	C	-0.078473	-0.001644	-0.043144	-0.000351	-0.009915	-0.000071
4	C	-0.001895	-0.091806	-0.000532	-0.058597	-0.000171	-0.007119
5	C	0.578494	-0.000422	-0.071634	-0.000139	-0.030036	-0.000079
6	C	-0.000550	0.557387	-0.000118	-0.194905	0.001821	-0.037944
7	C	4.789911	-0.000170	0.927763	0.000004	-0.090791	-0.000924
8	C	-0.000170	4.987906	0.001839	0.695979	0.009464	-0.138798
9	C	0.927763	0.001839	4.901054	0.000275	0.555253	-0.009800
10	C	0.000004	0.695979	0.000275	5.323346	0.001827	0.485613
11	C	-0.090791	0.009464	0.555253	0.001827	4.984459	-0.071505
12	C	-0.000924	-0.138798	-0.009800	0.485613	-0.071505	5.221782
13	C	-0.057351	0.001848	-0.192632	0.003765	0.696320	-0.058251
14	C	-0.006915	-0.071611	-0.036821	-0.059047	-0.136077	0.344902
15	C	0.000081	-0.017111	0.001072	-0.096879	0.010431	0.076592
16	C	-0.000174	0.010454	-0.002262	0.015512	-0.016753	0.090437

		13	14	15	16
1	C	-0.000351	-0.000074	-0.000001	0.000001
2	C	-0.000124	-0.000079	-0.000014	0.000007
3	C	-0.002062	-0.000185	0.000001	-0.000001
4	C	-0.000001	-0.000951	-0.000176	0.000081
5	C	-0.010366	-0.001083	0.000006	-0.000013
6	C	0.000303	-0.009891	-0.002319	0.001085

7	C	-0.057351	-0.006915	0.000081	-0.000174
8	C	0.001848	-0.071611	-0.017111	0.010454
9	C	-0.192632	-0.036821	0.001072	-0.002262
10	C	0.003765	-0.059047	-0.096879	0.015512
11	C	0.696320	-0.136077	0.010431	-0.016753
12	C	-0.058251	0.344902	0.076592	0.090437
13	C	5.317366	0.483984	0.015153	-0.096080
14	C	0.483984	5.219283	0.090908	0.076797
15	C	0.015153	0.090908	5.848828	0.125363
16	C	-0.096080	0.076797	0.125363	5.847013

Mulliken charges:

		1
1	C	0.013688
2	C	-0.010546
3	C	0.011979
4	C	-0.029547
5	C	-0.008772
6	C	-0.024046
7	C	-0.031484
8	C	0.097625
9	C	-0.021361
10	C	-0.103635
11	C	0.097689
12	C	0.106474
13	C	-0.101521
14	C	0.106860
15	C	-0.051937
16	C	-0.051467

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.013688
2	C	-0.010546
3	C	0.011979
4	C	-0.029547
5	C	-0.008772
6	C	-0.024046
7	C	-0.031484
8	C	0.097625
9	C	-0.021361
10	C	-0.103635
11	C	0.097689
12	C	0.106474
13	C	-0.101521
14	C	0.106860
15	C	-0.051937
16	C	-0.051467

Electronic spatial extent (au): <R**2>= 3633.9794

Supporting Information file

Charge= 0.0000 electrons
Dipole moment (field-independent basis, Debye):
X= 3.9839 Y= -0.0140 Z= -0.0009 Tot= 3.9840
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -103.2801 YY= -85.8090 ZZ= -91.6089
XY= -0.0179 XZ= 0.0087 YZ= -1.8712
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= -9.7141 YY= 7.7570 ZZ= 1.9571
XY= -0.0179 XZ= 0.0087 YZ= -1.8712
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= 122.6799 YYY= -0.1474 ZZZ= -0.0153 XYY= 5.8268
XXY= -0.0116 XXZ= -0.0257 XZZ= 16.9118 YZZ= -0.0017
YYZ= 0.0053 XYZ= 7.8055
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -4254.0953 YYYY= -1748.8643 ZZZZ= -136.0370 XXXY= -0.4368
XXXZ= 0.1687 YYYX= -0.1109 YYYZ= -3.9202 ZZZX= 0.0689
ZZZY= -4.3561 XXYY= -912.8794 XXZZ= -723.8826 YYZZ= -318.8057
XXYZ= -37.4656 YYXZ= -0.0124 ZZXY= -0.0086
N-N= 7.077519884879D+02 E-N=-2.825487509729D+03 KE= 6.051483865749D+02
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Fri Aug 21 17:54:15 2026, MaxMem= 805306368 cpu: 1.4 elap: 0.3
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14162 LenP2D= 33380.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 17:54:15 2026, MaxMem= 805306368 cpu: 1.6 elap: 0.3
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 17:54:15 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Supporting Information file

Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 17:58:24 2026, MaxMem= 805306368 cpu: 1493.2 elap: 248.9
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.56740265D+00-5.50370036D-03-3.53603128D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.026122176	-0.036561762	-0.000459688
2	6	0.020024419	0.041312129	0.000389164
3	6	-0.026032801	0.036570504	0.000513453
4	6	-0.044293150	-0.003071849	-0.001763152
5	6	0.019917331	-0.041323625	-0.000485336
6	6	0.045465917	0.008118935	0.001614338
7	6	-0.044226127	0.003192823	0.001792536
8	6	-0.038935528	0.022249724	-0.004235468
9	6	0.045393096	-0.008223820	-0.001605159
10	6	0.043299844	-0.022273147	0.005391363
11	6	-0.038907177	-0.022287175	0.004223549
12	6	-0.024409829	0.033896526	0.003264056
13	6	0.043446609	0.022421201	-0.005361667
14	6	-0.024772636	-0.034074442	-0.003147689
15	6	0.024900316	0.016211880	0.021354089
16	6	0.025251893	-0.016157902	-0.021484389

Cartesian Forces: Max 0.045465917 RMS 0.025647041
Leave Link 716 at Fri Aug 21 17:58:24 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.051858148 RMS 0.017618546
Search for a local minimum.
Step number 1 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .17619D-01 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Second derivative matrix not updated -- first step.
ITU= 0
Eigenvalues --- 0.01281 0.01313 0.01666 0.01726 0.02624
Eigenvalues --- 0.02870 0.03117 0.03421 0.03429 0.03926
Eigenvalues --- 0.03950 0.03968 0.04046 0.08416 0.09136
Eigenvalues --- 0.24506 0.24597 0.24996 0.24997 0.24999
Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.27993 0.28436 0.32297 0.36130 0.51317
Eigenvalues --- 0.51368 0.57396 0.57823 0.57982 0.58172
Eigenvalues --- 0.58238 0.78591 0.78681 0.79707 0.80286
Eigenvalues --- 0.82175 0.82428
RFO step: Lambda=-2.86399074D-02 EMin= 1.28103738D-02
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.05417072 RMS(Int)= 0.00133444
Iteration 2 RMS(Cart)= 0.00085692 RMS(Int)= 0.00032466
Iteration 3 RMS(Cart)= 0.00000115 RMS(Int)= 0.00032466
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00032466
ITry= 1 IFail=0 DXMaxC= 1.61D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.38472	-0.05186	0.00000	-0.06336	-0.06334	2.32138
R2	2.52509	-0.00827	0.00000	-0.01356	-0.01354	2.51156
R3	2.52317	-0.00702	0.00000	-0.01148	-0.01147	2.51170
R4	2.38460	-0.05183	0.00000	-0.06331	-0.06329	2.32131
R5	2.37765	-0.05081	0.00000	-0.06110	-0.06110	2.31655
R6	2.52340	-0.00706	0.00000	-0.01155	-0.01154	2.51187
R7	2.52572	-0.00513	0.00000	-0.00842	-0.00843	2.51729
R8	2.37752	-0.05079	0.00000	-0.06108	-0.06107	2.31644
R9	2.36573	-0.05000	0.00000	-0.05854	-0.05855	2.30718
R10	2.52599	-0.00517	0.00000	-0.00851	-0.00851	2.51748
R11	2.58398	-0.00131	0.00000	-0.00240	-0.00242	2.58156
R12	2.36577	-0.05003	0.00000	-0.05858	-0.05859	2.30718
R13	2.73778	-0.03318	0.00000	-0.08427	-0.08437	2.65342
R14	2.85299	-0.02535	0.00000	-0.07305	-0.07299	2.78000
R15	2.58360	-0.00113	0.00000	-0.00207	-0.00209	2.58151
R16	2.85492	-0.02560	0.00000	-0.07401	-0.07395	2.78096
R17	2.77457	-0.02566	0.00000	-0.06389	-0.06393	2.71064
A1	2.61084	0.00041	0.00000	0.00024	0.00030	2.61114
A2	2.64268	0.00053	0.00000	0.00070	0.00074	2.64342
A3	2.61634	0.00042	0.00000	0.00025	0.00032	2.61666
A4	2.72198	0.00022	0.00000	-0.00042	-0.00044	2.72154
A5	2.63828	0.00048	0.00000	0.00046	0.00049	2.63877
A6	2.77345	0.00081	0.00000	0.00175	0.00166	2.77512
A7	2.72665	0.00016	0.00000	-0.00073	-0.00075	2.72590
A8	2.77045	0.00080	0.00000	0.00162	0.00153	2.77198
A9	2.82874	-0.00088	0.00000	-0.00418	-0.00439	2.82435
A10	2.31893	-0.00140	0.00000	0.00294	0.00318	2.32211
A11	2.49788	0.00160	0.00000	0.01535	0.01579	2.51368
A12	1.46608	-0.00015	0.00000	-0.01767	-0.01868	1.44740
A13	2.82700	-0.00086	0.00000	-0.00415	-0.00436	2.82264
A14	2.31935	-0.00140	0.00000	0.00293	0.00317	2.32252
A15	1.46578	-0.00013	0.00000	-0.01756	-0.01858	1.44721
A16	2.49772	0.00158	0.00000	0.01529	0.01573	2.51345
A17	1.45492	-0.00264	0.00000	-0.02428	-0.02532	1.42960

A18	1.45396	-0.00250	0.00000	-0.02376	-0.02480	1.42916
A19	2.89232	0.00024	0.00000	-0.00220	-0.00234	2.88997
A20	2.89340	0.00030	0.00000	-0.00158	-0.00172	2.89168
A21	3.12157	0.00014	0.00000	0.00670	0.00662	3.12819
A22	3.12133	0.00015	0.00000	0.00688	0.00680	3.12813
D1	0.04506	0.00043	0.00000	0.00761	0.00762	0.05267
D2	-0.04271	-0.00003	0.00000	0.00055	0.00056	-0.04216
D3	-0.03109	-0.00034	0.00000	-0.00296	-0.00298	-0.03407
D4	0.04167	0.00045	0.00000	0.00790	0.00790	0.04957
D5	0.04368	-0.00014	0.00000	0.00171	0.00166	0.04534
D6	-0.02675	-0.00035	0.00000	-0.00317	-0.00319	-0.02994
D7	0.08485	-0.00105	0.00000	-0.01948	-0.01956	0.06529
D8	0.04169	-0.00014	0.00000	0.00170	0.00165	0.04334
D9	0.08811	-0.00105	0.00000	-0.01952	-0.01961	0.06850
D10	-0.52769	0.00084	0.00000	0.00831	0.00830	-0.51939
D11	2.65078	-0.00239	0.00000	-0.02937	-0.02943	2.62135
D12	0.67815	-0.00023	0.00000	0.01031	0.01070	0.68885
D13	-2.48679	0.00178	0.00000	0.03360	0.03361	-2.45318
D14	-2.48570	0.00176	0.00000	0.03346	0.03346	-2.45224
D15	0.63256	0.00377	0.00000	0.05674	0.05636	0.68892
D16	2.45954	-0.00205	0.00000	-0.03018	-0.02982	2.42972
D17	-0.65488	-0.00439	0.00000	-0.05797	-0.05762	-0.71250
D18	-0.53312	0.00086	0.00000	0.00849	0.00848	-0.52464
D19	2.64714	-0.00240	0.00000	-0.02939	-0.02946	2.61768
D20	-0.65447	-0.00444	0.00000	-0.05813	-0.05780	-0.71227
D21	2.45864	-0.00208	0.00000	-0.03021	-0.02985	2.42878
D22	0.62471	0.00205	0.00000	0.05160	0.05076	0.67547

Item	Value	Threshold	Converged?
Maximum Force	0.051858	0.000450	NO
RMS Force	0.017619	0.000300	NO
Maximum Displacement	0.161422	0.001800	NO
RMS Displacement	0.054278	0.001200	NO

Predicted change in Energy=-1.525237D-02
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 17:58:24 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.611949	-0.663657	0.016690
2	6	0	2.992478	-1.723722	0.055889
3	6	0	3.609597	0.664999	-0.015917
4	6	0	1.855475	-2.412032	0.063476

5	6	0	2.992237	1.726263	-0.054861
6	6	0	0.639091	-2.564149	0.058743
7	6	0	1.853282	2.411490	-0.063765
8	6	0	-0.653894	-2.245910	0.021513
9	6	0	0.637205	2.565589	-0.059549
10	6	0	-1.728368	-1.668931	-0.035128
11	6	0	-0.655409	2.245393	-0.022712
12	6	0	-2.668593	-0.685235	-0.155797
13	6	0	-1.730023	1.668645	0.033644
14	6	0	-2.668828	0.683839	0.155988
15	6	0	-4.043089	-0.399623	-0.595523
16	6	0	-4.043111	0.397041	0.597311

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.228420	0.000000			
3	C	1.329058	2.468193	0.000000		
4	C	2.478750	1.329137	3.542791	0.000000	
5	C	2.469996	3.451762	1.228386	4.293218	0.000000
6	C	3.528671	2.498951	4.388265	1.225867	4.894674
7	C	3.543432	4.290928	2.477330	4.825201	1.329223
8	C	4.549831	3.683734	5.162572	2.515212	5.392427
9	C	4.391235	4.894775	3.528351	5.126015	2.500134
10	C	5.434358	4.722041	5.825930	3.661401	5.814795
11	C	5.164733	5.391393	4.548402	5.291840	3.684542
12	C	6.282947	5.759426	6.423267	4.847381	6.153902
13	C	5.828943	5.814693	5.433351	5.432183	4.723441
14	C	6.425209	6.152784	6.280806	5.482910	5.760101
15	C	7.684017	7.188656	7.748094	6.267147	7.369364
16	C	7.749977	7.368194	7.681913	6.555089	7.189457

		6	7	8	9	10
6	C	0.000000				
7	C	5.123109	0.000000			
8	C	1.332094	5.290046	0.000000		
9	C	5.131101	1.225809	4.982372	0.000000	
10	C	2.532803	5.429445	1.220905	4.850535	0.000000
11	C	4.981371	2.514518	4.491521	1.332190	4.058734
12	C	3.810134	5.481380	2.554634	4.637393	1.366104
13	C	4.850760	3.660790	4.059796	2.533172	3.338284
14	C	4.636940	4.845879	3.558297	3.810156	2.540968
15	C	5.199620	6.553801	3.908472	5.566408	2.698725
16	C	5.566123	6.265978	4.336304	5.199944	3.166426

		11	12	13	14	15
11	C	0.000000				
12	C	3.557978	0.000000			
13	C	1.220906	2.541172	0.000000		
14	C	2.554259	1.404128	1.366076	0.000000	

```
   15  C    4.335966   1.471113   3.166048   1.904535   0.000000
   16  C    3.908626   1.904677   2.699087   1.471623   1.434408
              16
   16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 3.53D-03
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.611845   -0.664263    0.015013
     2          6           0        2.992208   -1.724324    0.051575
     3          6           0        3.609701    0.664471   -0.014284
     4          6           0        1.855098   -2.412474    0.057455
     5          6           0        2.992507    1.725925   -0.050580
     6          6           0        0.638690   -2.564387    0.052350
     7          6           0        1.853659    2.411351   -0.057769
     8          6           0       -0.654246   -2.245855    0.015922
     9          6           0        0.637606    2.565629   -0.053161
    10          6           0       -1.728630   -1.668567   -0.039275
    11          6           0       -0.655057    2.245545   -0.017114
    12          6           0       -2.668701   -0.684427   -0.157486
    13          6           0       -1.729761    1.668827    0.037812
    14          6           0       -2.668720    0.683867    0.157708
    15          6           0       -4.043155   -0.397505   -0.596491
    16          6           0       -4.043045    0.396186    0.598324
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8539217           0.3964308           0.2735002
 Leave Link  202 at Fri Aug 21 17:58:24 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       719.6285294985 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
```

HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0075423268 Hartrees.
Nuclear repulsion after empirical dispersion term = 719.6209871716 Hartrees.
Leave Link 301 at Fri Aug 21 17:58:24 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14229 LenP2D= 33675.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 3.73D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 565 565 565 565 565 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 17:58:25 2026, MaxMem= 805306368 cpu: 2.4 elap: 0.4
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 17:58:25 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 -0.000000 0.000000
Rot= 0.999999 -0.001243 -0.000003 0.000078 Ang= -0.14 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Supporting Information file

Petite list used in FoFCou.
Harris En= -582.859453822486
Leave Link 401 at Fri Aug 21 17:58:27 2026, MaxMem= 805306368 cpu: 14.7 elap: 2.5
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.969282774191
DIIS: error= 3.74D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.969282774191 IErMin= 1 ErrMin= 3.74D-03
ErrMax= 3.74D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-02 BMatP= 1.34D-02
IDIUse=3 WtCom= 9.63D-01 WtEn= 3.74D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.952 Goal= None Shift= 0.000
GapD= 0.952 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=4.02D-03 MaxDP=1.17D-01 OVMax= 2.45D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 3.95D-03 CP: 1.09D+00
E= -608.978425951833 Delta-E= -0.009143177642 Rises=F Damp=F
DIIS: error= 1.21D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.978425951833 IErMin= 2 ErrMin= 1.21D-03
ErrMax= 1.21D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.65D-04 BMatP= 1.34D-02
IDIUse=3 WtCom= 9.88D-01 WtEn= 1.21D-02
Coeff-Com: 0.588D-01 0.941D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.581D-01 0.942D+00
Gap= 0.237 Goal= None Shift= 0.000
RMSDP=1.30D-03 MaxDP=4.19D-02 DE=-9.14D-03 OVMax= 1.27D-02

Cycle 3 Pass 0 IDiag 1:
RMSU= 1.09D-03 CP: 1.07D+00 8.29D-01
E= -608.979317444236 Delta-E= -0.000891492404 Rises=F Damp=F
DIIS: error= 1.06D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.979317444236 IErMin= 3 ErrMin= 1.06D-03
ErrMax= 1.06D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.65D-04 BMatP= 6.65D-04
IDIUse=3 WtCom= 9.89D-01 WtEn= 1.06D-02
Coeff-Com: -0.118D-01 0.328D+00 0.684D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.117D-01 0.325D+00 0.687D+00
Gap= 0.238 Goal= None Shift= 0.000
RMSDP=4.22D+02 MaxDP=1.75D+04 DE=-8.91D-04 OVMax= 9.91D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -608.979136013339 Delta-E= 0.000181430898 Rises=F Damp=F
DIIS: error= 6.73D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.979136013339 IErMin= 1 ErrMin= 6.73D-04
ErrMax= 6.73D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.65D-04 BMatP= 2.65D-04
IDIUse=3 WtCom= 9.93D-01 WtEn= 6.73D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=2.86D-03 MaxDP=6.55D-02 DE= 1.81D-04 OVMax= 8.39D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 2.51D-03 CP: 8.57D-01
E= -608.979327433085 Delta-E= -0.000191419747 Rises=F Damp=F
DIIS: error= 9.67D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.979327433085 IErMin= 1 ErrMin= 6.73D-04
ErrMax= 9.67D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-04 BMatP= 2.65D-04
IDIUse=3 WtCom= 9.90D-01 WtEn= 9.67D-03
Coeff-Com: 0.442D+00 0.558D+00
Coeff-En: 0.993D-01 0.901D+00
Coeff: 0.439D+00 0.561D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=1.15D-04 MaxDP=2.82D-03 DE=-1.91D-04 OVMax= 5.22D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 7.24D-05 CP: 8.52D-01 1.03D+00
E= -608.979497931207 Delta-E= -0.000170498121 Rises=F Damp=F
DIIS: error= 4.57D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.979497931207 IErMin= 3 ErrMin= 4.57D-04
ErrMax= 4.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-05 BMatP= 1.86D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.57D-03

Coeff-Com: 0.456D-01 0.307D+00 0.647D+00
Coeff-En: 0.000D+00 0.990D-01 0.901D+00
Coeff: 0.454D-01 0.306D+00 0.649D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=8.35D-05 MaxDP=1.77D-03 DE=-1.70D-04 OVMax= 2.92D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.61D-05 CP: 8.49D-01 1.05D+00 1.50D+00
E= -608.979556649518 Delta-E= -0.000058718311 Rises=F Damp=F
DIIS: error= 2.89D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.979556649518 IErMin= 4 ErrMin= 2.89D-04
ErrMax= 2.89D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.00D-06 BMatP= 4.17D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 2.89D-03
Coeff-Com: -0.453D-01 0.588D-01 0.302D+00 0.685D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.452D-01 0.587D-01 0.301D+00 0.685D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.01D-05 MaxDP=7.42D-04 DE=-5.87D-05 OVMax= 2.61D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.03D-05 CP: 8.48D-01 1.06D+00 1.73D+00 1.30D+00
E= -608.979572010534 Delta-E= -0.000015361016 Rises=F Damp=F
DIIS: error= 1.07D-04 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.979572010534 IErMin= 5 ErrMin= 1.07D-04
ErrMax= 1.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-06 BMatP= 6.00D-06
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.07D-03
Coeff-Com: -0.200D-01-0.751D-01-0.129D+00 0.148D+00 0.108D+01
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.200D-01-0.750D-01-0.129D+00 0.147D+00 0.108D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=1.23D-05 MaxDP=3.88D-04 DE=-1.54D-05 OVMax= 2.25D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 8.63D-06 CP: 8.48D-01 1.06D+00 1.80D+00 1.43D+00 1.48D+00
E= -608.979578936793 Delta-E= -0.000006926258 Rises=F Damp=F
DIIS: error= 7.85D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.979578936793 IErMin= 6 ErrMin= 7.85D-05
ErrMax= 7.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.62D-07 BMatP= 1.02D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.317D-02-0.440D-01-0.124D+00-0.108D+00 0.439D+00 0.834D+00
Coeff: 0.317D-02-0.440D-01-0.124D+00-0.108D+00 0.439D+00 0.834D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=7.17D-06 MaxDP=2.29D-04 DE=-6.93D-06 OVMax= 1.33D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 3.45D-06 CP: 8.48D-01 1.06D+00 1.79D+00 1.45D+00 1.80D+00
CP: 1.35D+00
E= -608.979580293514 Delta-E= -0.000001356721 Rises=F Damp=F

DIIS: error= 2.00D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.979580293514 IErMin= 7 ErrMin= 2.00D-05
ErrMax= 2.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.64D-08 BMatP= 2.62D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.409D-02-0.145D-01-0.520D-01-0.771D-01 0.104D+00 0.437D+00
Coeff-Com: 0.598D+00
Coeff: 0.409D-02-0.145D-01-0.520D-01-0.771D-01 0.104D+00 0.437D+00
Coeff: 0.598D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.14D-06 MaxDP=9.40D-05 DE=-1.36D-06 OVMax= 3.27D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.22D-06 CP: 8.48D-01 1.06D+00 1.78D+00 1.43D+00 1.84D+00
CP: 1.52D+00 1.20D+00
E= -608.979580500584 Delta-E= -0.000000207069 Rises=F Damp=F
DIIS: error= 1.61D-05 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.979580500584 IErMin= 8 ErrMin= 1.61D-05
ErrMax= 1.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-08 BMatP= 6.64D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.131D-04 0.121D-01 0.290D-01 0.162D-01-0.121D+00-0.184D+00
Coeff-Com: 0.131D+00 0.112D+01
Coeff: -0.131D-04 0.121D-01 0.290D-01 0.162D-01-0.121D+00-0.184D+00
Coeff: 0.131D+00 0.112D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.30D-06 MaxDP=1.17D-04 DE=-2.07D-07 OVMax= 3.23D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 8.29D-07 CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.84D+00
CP: 1.66D+00 1.40D+00 2.24D+00
E= -608.979580601792 Delta-E= -0.000000101208 Rises=F Damp=F
DIIS: error= 8.25D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.979580601792 IErMin= 9 ErrMin= 8.25D-06
ErrMax= 8.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.17D-09 BMatP= 1.22D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.138D-02 0.117D-01 0.337D-01 0.344D-01-0.946D-01-0.252D+00
Coeff-Com: -0.136D+00 0.618D+00 0.785D+00
Coeff: -0.138D-02 0.117D-01 0.337D-01 0.344D-01-0.946D-01-0.252D+00
Coeff: -0.136D+00 0.618D+00 0.785D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=1.12D-06 MaxDP=3.43D-05 DE=-1.01D-07 OVMax= 1.72D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 4.13D-07 CP: 8.49D-01 1.06D+00 1.75D+00 1.41D+00 1.84D+00
CP: 1.68D+00 1.52D+00 2.75D+00 1.49D+00
E= -608.979580627730 Delta-E= -0.000000025938 Rises=F Damp=F
DIIS: error= 2.45D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.979580627730 IErMin=10 ErrMin= 2.45D-06
ErrMax= 2.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.07D-10 BMatP= 5.17D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.319D-03 0.846D-03 0.291D-02 0.501D-02-0.126D-02-0.283D-01
Coeff-Com: -0.504D-01-0.368D-01 0.174D+00 0.934D+00
Coeff: -0.319D-03 0.846D-03 0.291D-02 0.501D-02-0.126D-02-0.283D-01
Coeff: -0.504D-01-0.368D-01 0.174D+00 0.934D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=5.59D-07 MaxDP=1.05D-05 DE=-2.59D-08 OVMax= 4.78D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 2.15D-07 CP: 8.49D-01 1.06D+00 1.75D+00 1.41D+00 1.83D+00
CP: 1.67D+00 1.51D+00 2.86D+00 1.66D+00 1.36D+00
E= -608.979580631407 Delta-E= -0.000000003677 Rises=F Damp=F
DIIS: error= 1.51D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.979580631407 IErMin=11 ErrMin= 1.51D-06
ErrMax= 1.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-10 BMatP= 5.07D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.253D-03-0.258D-02-0.755D-02-0.715D-02 0.222D-01 0.546D-01
Coeff-Com: 0.184D-01-0.161D+00-0.146D+00 0.229D+00 0.100D+01
Coeff: 0.253D-03-0.258D-02-0.755D-02-0.715D-02 0.222D-01 0.546D-01
Coeff: 0.184D-01-0.161D+00-0.146D+00 0.229D+00 0.100D+01
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=3.14D-07 MaxDP=8.55D-06 DE=-3.68D-09 OVMax= 3.02D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 5.86D-08 CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
CP: 1.67D+00 1.50D+00 2.88D+00 1.73D+00 1.60D+00
CP: 1.52D+00
E= -608.979580632563 Delta-E= -0.000000001156 Rises=F Damp=F
DIIS: error= 8.13D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.979580632563 IErMin=12 ErrMin= 8.13D-07
ErrMax= 8.13D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.18D-11 BMatP= 1.37D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.138D-03-0.998D-03-0.295D-02-0.324D-02 0.734D-02 0.231D-01
Coeff-Com: 0.153D-01-0.463D-01-0.797D-01-0.101D+00 0.358D+00 0.831D+00
Coeff: 0.138D-03-0.998D-03-0.295D-02-0.324D-02 0.734D-02 0.231D-01
Coeff: 0.153D-01-0.463D-01-0.797D-01-0.101D+00 0.358D+00 0.831D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=6.60D-08 MaxDP=1.69D-06 DE=-1.16D-09 OVMax= 1.36D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 3.48D-08 CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
CP: 1.67D+00 1.51D+00 2.89D+00 1.73D+00 1.64D+00
CP: 1.63D+00 1.47D+00
E= -608.979580632860 Delta-E= -0.000000000297 Rises=F Damp=F
DIIS: error= 4.75D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.979580632860 IErMin=13 ErrMin= 4.75D-07
ErrMax= 4.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.95D-11 BMatP= 4.18D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.288D-04 0.488D-03 0.148D-02 0.115D-02-0.507D-02-0.919D-02
Coeff-Com: 0.565D-03 0.382D-01 0.186D-01-0.143D+00-0.203D+00 0.443D+00
Coeff-Com: 0.857D+00
Coeff: -0.288D-04 0.488D-03 0.148D-02 0.115D-02-0.507D-02-0.919D-02
Coeff: 0.565D-03 0.382D-01 0.186D-01-0.143D+00-0.203D+00 0.443D+00
Coeff: 0.857D+00
Gap=   0.239 Goal=   None   Shift=   0.000
RMSDP=8.59D-08 MaxDP=1.71D-06 DE=-2.97D-10 OVMax= 9.53D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 2.25D-08   CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
               CP: 1.67D+00 1.51D+00 2.89D+00 1.73D+00 1.62D+00
               CP: 1.65D+00 1.87D+00 1.64D+00
E= -608.979580632984   Delta-E=   -0.000000000124 Rises=F Damp=F
DIIS: error= 2.57D-07 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.979580632984   IErMin=14 ErrMin= 2.57D-07
ErrMax= 2.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.99D-12 BMatP= 1.95D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.790D-04 0.740D-03 0.224D-02 0.221D-02-0.651D-02-0.158D-01
Coeff-Com: -0.664D-02 0.447D-01 0.484D-01-0.541D-01-0.279D+00-0.827D-01
Coeff-Com: 0.533D+00 0.814D+00
Coeff: -0.790D-04 0.740D-03 0.224D-02 0.221D-02-0.651D-02-0.158D-01
Coeff: -0.664D-02 0.447D-01 0.484D-01-0.541D-01-0.279D+00-0.827D-01
Coeff: 0.533D+00 0.814D+00
Gap=   0.239 Goal=   None   Shift=   0.000
RMSDP=4.71D-08 MaxDP=1.10D-06 DE=-1.24D-10 OVMax= 6.40D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.24D-08   CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
               CP: 1.67D+00 1.51D+00 2.90D+00 1.73D+00 1.61D+00
               CP: 1.64D+00 2.07D+00 2.10D+00 1.42D+00
E= -608.979580633028   Delta-E=   -0.000000000044 Rises=F Damp=F
DIIS: error= 5.98D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -608.979580633028   IErMin=15 ErrMin= 5.98D-08
ErrMax= 5.98D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.76D-13 BMatP= 6.99D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.197D-05-0.270D-04-0.530D-04 0.144D-04 0.267D-03 0.234D-03
Coeff-Com: -0.102D-02-0.301D-02 0.330D-02 0.181D-01 0.109D-01-0.866D-01
Coeff-Com: -0.926D-01 0.737D-01 0.108D+01
Coeff: -0.197D-05-0.270D-04-0.530D-04 0.144D-04 0.267D-03 0.234D-03
Coeff: -0.102D-02-0.301D-02 0.330D-02 0.181D-01 0.109D-01-0.866D-01
Coeff: -0.926D-01 0.737D-01 0.108D+01
Gap=   0.239 Goal=   None   Shift=   0.000
RMSDP=2.52D-08 MaxDP=7.35D-07 DE=-4.39D-11 OVMax= 1.87D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 7.70D-09   CP: 8.49D-01 1.06D+00 1.76D+00 1.41D+00 1.83D+00
               CP: 1.67D+00 1.51D+00 2.90D+00 1.73D+00 1.60D+00

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CP: 1.63D+00 2.05D+00 2.10D+00 1.58D+00 1.76D+00
E= -608.979580633025 Delta-E= 0.000000000003 Rises=F Damp=F
DIIS: error= 1.84D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -608.979580633028 IErMin=16 ErrMin= 1.84D-08
ErrMax= 1.84D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-13 BMatP= 4.76D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.112D-04-0.125D-03-0.357D-03-0.328D-03 0.110D-02 0.247D-02
Coeff-Com: 0.548D-03-0.796D-02-0.573D-02 0.148D-01 0.453D-01-0.172D-01
Coeff-Com: -0.119D+00-0.860D-01 0.387D+00 0.785D+00
Coeff: 0.112D-04-0.125D-03-0.357D-03-0.328D-03 0.110D-02 0.247D-02
Coeff: 0.548D-03-0.796D-02-0.573D-02 0.148D-01 0.453D-01-0.172D-01
Coeff: -0.119D+00-0.860D-01 0.387D+00 0.785D+00
Gap= 0.239 Goal= None Shift= 0.000
RMSDP=9.94D-09 MaxDP=2.85D-07 DE= 2.73D-12 OVMax= 5.24D-07

SCF Done: E(RwB97XD) = -608.979580633 A.U. after 19 cycles
NFock= 19 Conv=0.99D-08 -V/T= 2.0044
KE= 6.063388954549D+02 PE=-2.850316487064D+03 EE= 9.153770238045D+02
Leave Link 502 at Fri Aug 21 18:05:44 2026, MaxMem= 805306368 cpu: 2618.5 elap: 436.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14229 LenP2D= 33675.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 18:05:44 2026, MaxMem= 805306368 cpu: 1.6 elap: 0.3
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 18:05:44 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 18:12:01 2026, MaxMem= 805306368 cpu: 2261.8 elap: 377.0
(Enter /home/user/gauss16/g16/l716.exe)

Supporting Information file

Dipole = 1.54326253D+00-5.66485486D-03-2.47702163D-04
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.002462975 -0.016721085 -0.000524258
2 6 0.013014191 0.010590509 0.000786127
3 6 -0.002404723 0.016738796 0.000566928
4 6 -0.015130804 -0.007220260 -0.001264458
5 6 0.012955217 -0.010618834 -0.000856015
6 6 0.015872091 -0.001797620 0.001637859
7 6 -0.015083237 0.007287560 0.001307176
8 6 -0.014916770 0.004093483 -0.001993098
9 6 0.015820067 0.001736194 -0.001647810
10 6 0.010578336 -0.008182589 0.003265646
11 6 -0.014908145 -0.004075424 0.001962257
12 6 -0.011348485 0.013227849 -0.004350077
13 6 0.010611786 0.008194740 -0.003212285
14 6 -0.011546297 -0.013272040 0.004388538
15 6 0.004367130 -0.000441283 0.003803457
16 6 0.004582618 0.000460005 -0.003869988

Cartesian Forces: Max 0.016738796 RMS 0.008899233
Leave Link 716 at Fri Aug 21 18:12:01 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.012519492 RMS 0.004300779
Search for a local minimum.
Step number 2 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .43008D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2
DE= -1.59D-02 DEPred=-1.53D-02 R= 1.04D+00
TightC=F SS= 1.41D+00 RLast= 2.59D-01 DXNew= 5.0454D-01 7.7596D-01
Trust test= 1.04D+00 RLast= 2.59D-01 DXMaxT set to 5.05D-01
ITU= 1 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.01283 0.01334 0.01662 0.01726 0.02624
Eigenvalues --- 0.02870 0.03118 0.03421 0.03430 0.03926
Eigenvalues --- 0.03968 0.04046 0.04660 0.08421 0.09211
Eigenvalues --- 0.24390 0.24598 0.24995 0.24996 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25001
Eigenvalues --- 0.26478 0.28117 0.31408 0.33940 0.51191
Eigenvalues --- 0.51323 0.57377 0.57674 0.58063 0.58170
Eigenvalues --- 0.58236 0.78665 0.79080 0.79694 0.80909
Eigenvalues --- 0.82168 0.84474
RFO step: Lambda=-2.28359973D-03 EMin= 1.28298139D-02
Quartic linear search produced a step of 0.06826.
Iteration 1 RMS(Cart)= 0.00835754 RMS(Int)= 0.00008185
Iteration 2 RMS(Cart)= 0.00006329 RMS(Int)= 0.00005289
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005289
ITry= 1 IFail=0 DXMaxC= 2.04D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.32138	-0.00485	-0.00432	-0.00715	-0.01147	2.30991
R2	2.51156	0.01252	-0.00092	0.02286	0.02194	2.53350
R3	2.51170	0.01234	-0.00078	0.02245	0.02167	2.53338
R4	2.32131	-0.00484	-0.00432	-0.00713	-0.01144	2.30987
R5	2.31655	-0.00465	-0.00417	-0.00676	-0.01093	2.30563
R6	2.51187	0.01234	-0.00079	0.02246	0.02168	2.53355
R7	2.51729	0.01161	-0.00058	0.02126	0.02069	2.53798
R8	2.31644	-0.00461	-0.00417	-0.00671	-0.01088	2.30556
R9	2.30718	-0.00394	-0.00400	-0.00566	-0.00966	2.29752
R10	2.51748	0.01160	-0.00058	0.02125	0.02067	2.53814
R11	2.58156	0.00981	-0.00016	0.02025	0.02009	2.60165
R12	2.30718	-0.00393	-0.00400	-0.00565	-0.00965	2.29752
R13	2.65342	-0.00486	-0.00576	-0.01301	-0.01875	2.63467
R14	2.78000	-0.00474	-0.00498	-0.01653	-0.02152	2.75848
R15	2.58151	0.00984	-0.00014	0.02032	0.02017	2.60168
R16	2.78096	-0.00489	-0.00505	-0.01714	-0.02221	2.75876
R17	2.71064	-0.00262	-0.00436	-0.00731	-0.01167	2.69897
A1	2.61114	-0.00015	0.00002	-0.00071	-0.00069	2.61045
A2	2.64342	-0.00019	0.00005	-0.00087	-0.00082	2.64260
A3	2.61666	-0.00022	0.00002	-0.00098	-0.00096	2.61570
A4	2.72154	-0.00016	-0.00003	-0.00073	-0.00077	2.72077
A5	2.63877	-0.00016	0.00003	-0.00070	-0.00067	2.63810
A6	2.77512	0.00032	0.00011	0.00134	0.00143	2.77655
A7	2.72590	-0.00024	-0.00005	-0.00104	-0.00110	2.72480
A8	2.77198	0.00036	0.00010	0.00155	0.00163	2.77362
A9	2.82435	0.00064	-0.00030	0.00285	0.00250	2.82685
A10	2.32211	-0.00062	0.00022	-0.00588	-0.00567	2.31644
A11	2.51368	-0.00002	0.00108	-0.00324	-0.00216	2.51152
A12	1.44740	0.00064	-0.00128	0.00913	0.00771	1.45511
A13	2.82264	0.00066	-0.00030	0.00296	0.00262	2.82526
A14	2.32252	-0.00063	0.00022	-0.00589	-0.00568	2.31684
A15	1.44721	0.00065	-0.00127	0.00915	0.00775	1.45496
A16	2.51345	-0.00002	0.00107	-0.00327	-0.00219	2.51126
A17	1.42960	-0.00014	-0.00173	0.00690	0.00500	1.43461

A18	1.42916	-0.00005	-0.00169	0.00728	0.00541	1.43458
A19	2.88997	0.00002	-0.00016	0.00051	0.00033	2.89031
A20	2.89168	0.00002	-0.00012	0.00045	0.00032	2.89200
A21	3.12819	0.00013	0.00045	0.00595	0.00633	3.13452
A22	3.12813	0.00013	0.00046	0.00591	0.00631	3.13443
D1	0.05267	0.00016	0.00052	0.00399	0.00450	0.05718
D2	-0.04216	-0.00017	0.00004	-0.00511	-0.00507	-0.04722
D3	-0.03407	-0.00011	-0.00020	-0.00117	-0.00139	-0.03546
D4	0.04957	0.00018	0.00054	0.00443	0.00497	0.05454
D5	0.04534	0.00022	0.00011	0.00781	0.00788	0.05322
D6	-0.02994	-0.00013	-0.00022	-0.00161	-0.00185	-0.03179
D7	0.06529	-0.00026	-0.00134	0.00386	0.00244	0.06773
D8	0.04334	0.00021	0.00011	0.00784	0.00791	0.05124
D9	0.06850	-0.00027	-0.00134	0.00347	0.00206	0.07056
D10	-0.51939	-0.00079	0.00057	-0.02513	-0.02459	-0.54398
D11	2.62135	-0.00008	-0.00201	0.00176	-0.00029	2.62106
D12	0.68885	0.00058	0.00073	0.01360	0.01433	0.70317
D13	-2.45318	0.00018	0.00229	-0.00157	0.00067	-2.45251
D14	-2.45224	0.00016	0.00228	-0.00231	-0.00008	-2.45232
D15	0.68892	-0.00024	0.00385	-0.01748	-0.01374	0.67518
D16	2.42972	0.00033	-0.00204	0.00140	-0.00066	2.42906
D17	-0.71250	0.00085	-0.00393	0.02120	0.01730	-0.69519
D18	-0.52464	-0.00076	0.00058	-0.02429	-0.02374	-0.54838
D19	2.61768	-0.00009	-0.00201	0.00133	-0.00073	2.61696
D20	-0.71227	0.00081	-0.00395	0.02105	0.01714	-0.69513
D21	2.42878	0.00032	-0.00204	0.00219	0.00013	2.42891
D22	0.67547	-0.00077	0.00346	-0.01857	-0.01522	0.66025

Item	Value	Threshold	Converged?
Maximum Force	0.012519	0.000450	NO
RMS Force	0.004301	0.000300	NO
Maximum Displacement	0.020446	0.001800	NO
RMS Displacement	0.008336	0.001200	NO

Predicted change in Energy=-1.228655D-03
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 18:12:01 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.619798	-0.669410	0.016948
2	6	0	3.002568	-1.723696	0.057595
3	6	0	3.617587	0.670849	-0.016107
4	6	0	1.854674	-2.416159	0.065177

5	6	0	3.002424	1.726322	-0.056609
6	6	0	0.643685	-2.564756	0.059669
7	6	0	1.852651	2.415819	-0.065424
8	6	0	-0.659563	-2.243063	0.017052
9	6	0	0.641906	2.566146	-0.060425
10	6	0	-1.729388	-1.667920	-0.036242
11	6	0	-0.660956	2.242474	-0.018247
12	6	0	-2.679412	-0.679225	-0.160061
13	6	0	-1.730912	1.667539	0.034748
14	6	0	-2.679645	0.677754	0.159961
15	6	0	-4.047958	-0.405478	-0.587773
16	6	0	-4.047459	0.402802	0.589738

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.222353	0.000000			
3	C	1.340668	2.473364	0.000000		
4	C	2.483772	1.340606	3.555853	0.000000	
5	C	2.475094	3.451908	1.222329	4.300269	0.000000
6	C	3.528656	2.504340	4.395336	1.220085	4.898012
7	C	3.556435	4.298026	2.482408	4.833743	1.340694
8	C	4.559530	3.698998	5.175519	2.520648	5.401073
9	C	4.398028	4.897898	3.528285	5.129323	2.505467
10	C	5.441842	4.733215	5.836128	3.662738	5.823344
11	C	5.177370	5.399784	4.558064	5.295113	3.699762
12	C	6.301705	5.781280	6.441710	4.860618	6.170950
13	C	5.838814	5.822958	5.440811	5.434515	4.734582
14	C	6.443468	6.169683	6.299696	5.490112	5.782067
15	C	7.696093	7.201675	7.761821	6.269789	7.384754
16	C	7.763025	7.382957	7.693623	6.561775	7.202105

		6	7	8	9	10
6	C	0.000000				
7	C	5.126731	0.000000			
8	C	1.343040	5.293694	0.000000		
9	C	5.132308	1.220052	4.982802	0.000000	
10	C	2.538699	5.432198	1.215795	4.852930	0.000000
11	C	4.981729	2.520019	4.485676	1.343128	4.053769
12	C	3.827072	5.488884	2.560615	4.644730	1.376733
13	C	4.853005	3.662223	4.054740	2.539058	3.336215
14	C	4.644185	4.859359	3.554199	3.827178	2.538438
15	C	5.205111	6.561231	3.901763	5.577049	2.696982
16	C	5.576218	6.268395	4.336636	5.205085	3.170677

		11	12	13	14	15
11	C	0.000000				
12	C	3.553955	0.000000			
13	C	1.215797	2.538682	0.000000		
14	C	2.560314	1.394205	1.376752	0.000000	

```
   15  C    4.336795   1.459724   3.170747   1.898626   0.000000
   16  C    3.901594   1.898561   2.697029   1.459871   1.428233
              16
   16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 2.65D-04
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.619654   -0.670227    0.015356
     2          6           0        3.002197   -1.724472    0.053571
     3          6           0        3.617731    0.670105   -0.014600
     4          6           0        1.854154   -2.416703    0.059564
     5          6           0        3.002795    1.725801   -0.052652
     6          6           0        0.643133   -2.565026    0.053728
     7          6           0        1.853171    2.415564   -0.059858
     8          6           0       -0.660046   -2.242954    0.011871
     9          6           0        0.642458    2.566141   -0.054496
    10          6           0       -1.729748   -1.667458   -0.040079
    11          6           0       -0.660473    2.242653   -0.013052
    12          6           0       -2.679560   -0.678275   -0.161599
    13          6           0       -1.730552    1.667828    0.038627
    14          6           0       -2.679497    0.677960    0.161561
    15          6           0       -4.048052   -0.403244   -0.588660
    16          6           0       -4.047365    0.402310    0.590718
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8537904           0.3947969           0.2726563
 Leave Link  202 at Fri Aug 21 18:12:01 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       719.0512270591 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
```

HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0075260663 Hartrees.
Nuclear repulsion after empirical dispersion term = 719.0437009928 Hartrees.
Leave Link 301 at Fri Aug 21 18:12:01 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14219 LenP2D= 33635.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 3.85D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 565 565 565 565 565 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 18:12:02 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 18:12:02 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 0.000000 -0.000000
Rot= 1.000000 0.000089 -0.000003 0.000029 Ang= 0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Supporting Information file

Petite list used in FoFCou.
Harris En= -582.860177073713
Leave Link 401 at Fri Aug 21 18:12:06 2026, MaxMem= 805306368 cpu: 24.7 elap: 4.1
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.979722802012
DIIS: error= 3.10D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.979722802012 IErMin= 1 ErrMin= 3.10D-03
ErrMax= 3.10D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-03 BMatP= 2.22D-03
IDIUse=3 WtCom= 9.69D-01 WtEn= 3.10D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.952 Goal= None Shift= 0.000
GapD= 0.952 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=4.78D-03 MaxDP=1.64D-01 OVMax= 1.06D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 4.64D-03 CP: 1.14D+00
E= -608.981036803820 Delta-E= -0.001314001808 Rises=F Damp=F
DIIS: error= 6.32D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981036803820 IErMin= 2 ErrMin= 6.32D-04
ErrMax= 6.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-04 BMatP= 2.22D-03
IDIUse=3 WtCom= 9.94D-01 WtEn= 6.32D-03
Coeff-Com: 0.526D-01 0.947D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.522D-01 0.948D+00
Gap= 0.241 Goal= None Shift= 0.000
RMSDP=1.25D-03 MaxDP=2.97D-02 DE=-1.31D-03 OVMax= 6.77D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 1.14D-03 CP: 1.13D+00 8.90D-01
E= -608.981151855228 Delta-E= -0.000115051408 Rises=F Damp=F
DIIS: error= 2.33D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981151855228 IErMin= 2 ErrMin= 6.32D-04
ErrMax= 2.33D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-04 BMatP= 1.23D-04
IDIUse=3 WtCom= 1.72D-01 WtEn= 8.28D-01
Coeff-Com: 0.306D-01 0.730D+00 0.240D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.525D-02 0.125D+00 0.869D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=4.31D+02 MaxDP=1.70D+04 DE=-1.15D-04 OVMax= 9.94D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -608.980960456240 Delta-E= 0.000191398988 Rises=F Damp=F
DIIS: error= 5.94D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.980960456240 IErMin= 1 ErrMin= 5.94D-04
ErrMax= 5.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-04 BMatP= 1.38D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 5.94D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=4.17D-03 MaxDP=1.29D-01 DE= 1.91D-04 OVMax= 5.64D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.29D-03 CP: 7.56D-01
E= -608.981059486248 Delta-E= -0.000099030008 Rises=F Damp=F
DIIS: error= 3.53D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981059486248 IErMin= 2 ErrMin= 3.53D-04
ErrMax= 3.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.81D-05 BMatP= 1.38D-04
IDIUse=3 WtCom= 9.96D-01 WtEn= 3.53D-03
Coeff-Com: 0.225D+00 0.775D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.224D+00 0.776D+00
Gap= 0.242 Goal= None Shift= 0.000
RMSDP=2.37D-04 MaxDP=6.29D-03 DE=-9.90D-05 OVMax= 3.34D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.13D-04 CP: 7.44D-01 1.05D+00
E= -608.981080497832 Delta-E= -0.000021011583 Rises=F Damp=F
DIIS: error= 3.02D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981080497832 IErMin= 3 ErrMin= 3.02D-04
ErrMax= 3.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-05 BMatP= 2.81D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.02D-03

Coeff-Com: -0.950D-02 0.429D+00 0.581D+00
Coeff-En: 0.000D+00 0.278D+00 0.722D+00
Coeff: -0.947D-02 0.428D+00 0.581D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=8.34D-05 MaxDP=2.19D-03 DE=-2.10D-05 OVMax= 1.95D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.54D-05 CP: 7.39D-01 1.07D+00 1.28D+00
E= -608.981100782059 Delta-E= -0.000020284228 Rises=F Damp=F
DIIS: error= 1.02D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981100782059 IErMin= 4 ErrMin= 1.02D-04
ErrMax= 1.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-06 BMatP= 1.65D-05
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.02D-03
Coeff-Com: -0.194D-01 0.186D+00 0.319D+00 0.515D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.193D-01 0.185D+00 0.319D+00 0.515D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=1.48D-05 MaxDP=3.83D-04 DE=-2.03D-05 OVMax= 6.26D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.64D-06 CP: 7.39D-01 1.07D+00 1.34D+00 1.15D+00
E= -608.981103732968 Delta-E= -0.000002950909 Rises=F Damp=F
DIIS: error= 7.14D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981103732968 IErMin= 5 ErrMin= 7.14D-05
ErrMax= 7.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.30D-07 BMatP= 1.75D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.563D-02-0.195D+00-0.255D+00-0.426D-02 0.145D+01
Coeff: 0.563D-02-0.195D+00-0.255D+00-0.426D-02 0.145D+01
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=1.57D-05 MaxDP=3.42D-04 DE=-2.95D-06 OVMax= 1.51D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.15D-06 CP: 7.38D-01 1.07D+00 1.42D+00 1.28D+00 1.99D+00
E= -608.981105814259 Delta-E= -0.000002081291 Rises=F Damp=F
DIIS: error= 2.45D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981105814259 IErMin= 6 ErrMin= 2.45D-05
ErrMax= 2.45D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.07D-08 BMatP= 2.30D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.596D-02-0.134D+00-0.186D+00-0.807D-01 0.779D+00 0.615D+00
Coeff: 0.596D-02-0.134D+00-0.186D+00-0.807D-01 0.779D+00 0.615D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=3.62D-06 MaxDP=9.99D-05 DE=-2.08D-06 OVMax= 3.77D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.47D-06 CP: 7.38D-01 1.07D+00 1.41D+00 1.28D+00 2.23D+00
CP: 1.23D+00
E= -608.981106025962 Delta-E= -0.000000211703 Rises=F Damp=F
DIIS: error= 8.00D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -608.981106025962 IErMin= 7 ErrMin= 8.00D-06
ErrMax= 8.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.90D-09 BMatP= 7.07D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.123D-02-0.180D-01-0.287D-01-0.302D-01 0.474D-01 0.223D+00
Coeff-Com: 0.805D+00
Coeff: 0.123D-02-0.180D-01-0.287D-01-0.302D-01 0.474D-01 0.223D+00
Coeff: 0.805D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=5.71D-06 MaxDP=1.54D-04 DE=-2.12D-07 OVMax= 1.57D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 7.72D-07 CP: 7.39D-01 1.07D+00 1.39D+00 1.24D+00 2.25D+00
CP: 1.36D+00 1.85D+00
E= -608.981106062581 Delta-E= -0.000000036619 Rises=F Damp=F
DIIS: error= 5.03D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981106062581 IErMin= 8 ErrMin= 5.03D-06
ErrMax= 5.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-09 BMatP= 7.90D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.119D-02 0.320D-01 0.419D-01 0.801D-02-0.219D+00-0.561D-01
Coeff-Com: 0.442D+00 0.753D+00
Coeff: -0.119D-02 0.320D-01 0.419D-01 0.801D-02-0.219D+00-0.561D-01
Coeff: 0.442D+00 0.753D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=3.40D-06 MaxDP=9.30D-05 DE=-3.66D-08 OVMax= 9.35D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.16D-07 CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.24D+00
CP: 1.42D+00 2.38D+00 1.59D+00
E= -608.981106076013 Delta-E= -0.000000013432 Rises=F Damp=F
DIIS: error= 2.30D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981106076013 IErMin= 9 ErrMin= 2.30D-06
ErrMax= 2.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.67D-10 BMatP= 3.14D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.842D-03 0.176D-01 0.247D-01 0.136D-01-0.893D-01-0.867D-01
Coeff-Com: -0.107D+00 0.236D+00 0.993D+00
Coeff: -0.842D-03 0.176D-01 0.247D-01 0.136D-01-0.893D-01-0.867D-01
Coeff: -0.107D+00 0.236D+00 0.993D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=7.21D-07 MaxDP=2.24D-05 DE=-1.34D-08 OVMax= 4.73D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.86D-07 CP: 7.39D-01 1.07D+00 1.37D+00 1.21D+00 2.24D+00
CP: 1.43D+00 2.55D+00 1.80D+00 1.62D+00
E= -608.981106080172 Delta-E= -0.000000004160 Rises=F Damp=F
DIIS: error= 1.10D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981106080172 IErMin=10 ErrMin= 1.10D-06
ErrMax= 1.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-10 BMatP= 5.67D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.533D-04-0.283D-02-0.343D-02 0.135D-02 0.283D-01-0.113D-01
Coeff-Com: -0.137D+00-0.121D+00 0.290D+00 0.955D+00
Coeff: 0.533D-04-0.283D-02-0.343D-02 0.135D-02 0.283D-01-0.113D-01
Coeff: -0.137D+00-0.121D+00 0.290D+00 0.955D+00
Gap=   0.243 Goal=   None   Shift=   0.000
RMSDP=7.41D-07 MaxDP=1.88D-05 DE=-4.16D-09 OVMax= 2.37D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 8.08D-08   CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.24D+00
               CP: 1.43D+00 2.51D+00 1.76D+00 1.96D+00 1.54D+00
E= -608.981106080997   Delta-E=   -0.000000000825 Rises=F Damp=F
DIIS: error= 5.77D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981106080997   IErMin=11 ErrMin= 5.77D-07
ErrMax= 5.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-11 BMatP= 1.09D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.153D-03-0.373D-02-0.518D-02-0.194D-02 0.231D-01 0.889D-02
Coeff-Com: -0.256D-01-0.683D-01-0.682D-01 0.312D+00 0.829D+00
Coeff: 0.153D-03-0.373D-02-0.518D-02-0.194D-02 0.231D-01 0.889D-02
Coeff: -0.256D-01-0.683D-01-0.682D-01 0.312D+00 0.829D+00
Gap=   0.243 Goal=   None   Shift=   0.000
RMSDP=3.66D-07 MaxDP=1.03D-05 DE=-8.25D-10 OVMax= 9.58D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 3.06D-08   CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.25D+00
               CP: 1.43D+00 2.46D+00 1.69D+00 1.99D+00 1.73D+00
               CP: 1.29D+00
E= -608.981106081146   Delta-E=   -0.000000000148 Rises=F Damp=F
DIIS: error= 3.42D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981106081146   IErMin=12 ErrMin= 3.42D-07
ErrMax= 3.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.61D-12 BMatP= 2.34D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.250D-04-0.248D-03-0.476D-03-0.834D-03-0.458D-03 0.380D-02
Coeff-Com: 0.250D-01 0.122D-01-0.819D-01-0.140D+00 0.147D+00 0.104D+01
Coeff: 0.250D-04-0.248D-03-0.476D-03-0.834D-03-0.458D-03 0.380D-02
Coeff: 0.250D-01 0.122D-01-0.819D-01-0.140D+00 0.147D+00 0.104D+01
Gap=   0.243 Goal=   None   Shift=   0.000
RMSDP=8.58D-08 MaxDP=2.73D-06 DE=-1.48D-10 OVMax= 6.56D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.51D-08   CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.26D+00
               CP: 1.42D+00 2.45D+00 1.66D+00 1.98D+00 1.77D+00
               CP: 1.47D+00 1.66D+00
E= -608.981106081205   Delta-E=   -0.000000000059 Rises=F Damp=F
DIIS: error= 2.07D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981106081205   IErMin=13 ErrMin= 2.07D-07
ErrMax= 2.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.45D-12 BMatP= 6.61D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.531D-04 0.155D-02 0.206D-02 0.374D-03-0.107D-01-0.201D-02

Coeff-Com: 0.281D-01 0.399D-01-0.241D-01-0.244D+00-0.274D+00 0.727D+00
Coeff-Com: 0.756D+00
Coeff: -0.531D-04 0.155D-02 0.206D-02 0.374D-03-0.107D-01-0.201D-02
Coeff: 0.281D-01 0.399D-01-0.241D-01-0.244D+00-0.274D+00 0.727D+00
Coeff: 0.756D+00
Gap=   0.243 Goal=   None   Shift=   0.000
RMSDP=2.97D-08 MaxDP=7.17D-07 DE=-5.91D-11 OVMax= 4.68D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 8.44D-09   CP: 7.39D-01 1.07D+00 1.37D+00 1.23D+00 2.26D+00
               CP: 1.42D+00 2.44D+00 1.66D+00 1.97D+00 1.77D+00
               CP: 1.52D+00 2.10D+00 1.58D+00
E= -608.981106081225   Delta-E=   -0.000000000020 Rises=F Damp=F
DIIS: error= 5.99D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.981106081225   IErMin=14 ErrMin= 5.99D-08
ErrMax= 5.99D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.06D-13 BMatP= 4.45D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.231D-04 0.569D-03 0.784D-03 0.330D-03-0.340D-02-0.148D-02
Coeff-Com: 0.427D-02 0.104D-01 0.856D-02-0.488D-01-0.127D+00 0.157D-01
Coeff-Com: 0.270D+00 0.870D+00
Coeff: -0.231D-04 0.569D-03 0.784D-03 0.330D-03-0.340D-02-0.148D-02
Coeff: 0.427D-02 0.104D-01 0.856D-02-0.488D-01-0.127D+00 0.157D-01
Coeff: 0.270D+00 0.870D+00
Gap=   0.243 Goal=   None   Shift=   0.000
RMSDP=4.48D-08 MaxDP=1.17D-06 DE=-2.00D-11 OVMax= 1.67D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 5.63D-09   CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.25D+00
               CP: 1.42D+00 2.45D+00 1.66D+00 1.97D+00 1.76D+00
               CP: 1.50D+00 2.12D+00 1.87D+00 1.42D+00
E= -608.981106081237   Delta-E=   -0.000000000012 Rises=F Damp=F
DIIS: error= 2.43D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -608.981106081237   IErMin=15 ErrMin= 2.43D-08
ErrMax= 2.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.27D-14 BMatP= 5.06D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.535D-05-0.187D-03-0.244D-03 0.389D-05 0.141D-02-0.148D-04
Coeff-Com: -0.513D-02-0.599D-02 0.781D-02 0.425D-01 0.240D-01-0.159D+00
Coeff-Com: -0.106D+00 0.294D+00 0.907D+00
Coeff: 0.535D-05-0.187D-03-0.244D-03 0.389D-05 0.141D-02-0.148D-04
Coeff: -0.513D-02-0.599D-02 0.781D-02 0.425D-01 0.240D-01-0.159D+00
Coeff: -0.106D+00 0.294D+00 0.907D+00
Gap=   0.243 Goal=   None   Shift=   0.000
RMSDP=2.16D-08 MaxDP=6.13D-07 DE=-1.18D-11 OVMax= 5.87D-07

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.51D-09   CP: 7.39D-01 1.07D+00 1.37D+00 1.22D+00 2.25D+00
               CP: 1.42D+00 2.46D+00 1.67D+00 1.97D+00 1.76D+00
               CP: 1.47D+00 2.08D+00 1.92D+00 1.74D+00 1.54D+00

Supporting Information file

E= -608.981106081232 Delta-E= 0.000000000004 Rises=F Damp=F
DIIS: error= 7.18D-09 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -608.981106081237 IErMin=16 ErrMin= 7.18D-09
ErrMax= 7.18D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-15 BMatP= 8.27D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.253D-05-0.679D-04-0.924D-04-0.301D-04 0.416D-03 0.135D-03
Coeff-Com: -0.887D-03-0.152D-02 0.292D-03 0.832D-02 0.131D-01-0.187D-01
Coeff-Com: -0.316D-01-0.414D-01 0.977D-01 0.974D+00
Coeff: 0.253D-05-0.679D-04-0.924D-04-0.301D-04 0.416D-03 0.135D-03
Coeff: -0.887D-03-0.152D-02 0.292D-03 0.832D-02 0.131D-01-0.187D-01
Coeff: -0.316D-01-0.414D-01 0.977D-01 0.974D+00
Gap= 0.243 Goal= None Shift= 0.000
RMSDP=2.64D-09 MaxDP=6.32D-08 DE= 4.09D-12 OVMax= 9.82D-08

SCF Done: E(RwB97XD) = -608.981106081 A.U. after 19 cycles
NFock= 19 Conv=0.26D-08 -V/T= 2.0043
KE= 6.063506560153D+02 PE=-2.849183397747D+03 EE= 9.148079346575D+02
Leave Link 502 at Fri Aug 21 18:24:15 2026, MaxMem= 805306368 cpu: 4371.6 elap: 728.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14219 LenP2D= 33635.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 18:24:15 2026, MaxMem= 805306368 cpu: 2.3 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 18:24:16 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 18:32:51 2026, MaxMem= 805306368 cpu: 3094.5 elap: 515.8
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.53457090D+00-5.28608494D-03-3.87975051D-04

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000154283	-0.005241617	-0.000500907
2	6	0.004345088	0.002474836	0.000754583
3	6	0.000239313	0.005272667	0.000535298
4	6	-0.004070830	-0.002930740	-0.001067360
5	6	0.004277109	-0.002535123	-0.000818853
6	6	0.004075288	-0.000736859	0.000996782
7	6	-0.004045571	0.003013648	0.001114809
8	6	-0.003974278	0.000050000	-0.000965724
9	6	0.004067988	0.000662888	-0.001012631
10	6	0.002538325	-0.002251863	0.002136582
11	6	-0.003979765	-0.000017155	0.000942031
12	6	-0.003189845	0.001811514	-0.001847456
13	6	0.002557635	0.002231574	-0.002084464
14	6	-0.003252023	-0.001798597	0.001837039
15	6	0.000087545	-0.001712116	-0.004206451
16	6	0.000169740	0.001706944	0.004186724

Cartesian Forces: Max 0.005272667 RMS 0.002647994
Leave Link 716 at Fri Aug 21 18:32:51 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.005565741 RMS 0.001771487
Search for a local minimum.
Step number 3 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .17715D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2 3
DE= -1.53D-03 DEPred=-1.23D-03 R= 1.24D+00
TightC=F SS= 1.41D+00 RLast= 9.04D-02 DXNew= 8.4853D-01 2.7111D-01
Trust test= 1.24D+00 RLast= 9.04D-02 DXMaxT set to 5.05D-01
ITU= 1 1 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.01281 0.01325 0.01632 0.01725 0.02624
Eigenvalues --- 0.02859 0.03105 0.03410 0.03422 0.03926
Eigenvalues --- 0.03966 0.04047 0.04725 0.08413 0.09213
Eigenvalues --- 0.23684 0.24564 0.24884 0.24996 0.24997
Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25000

```
    Eigenvalues ---    0.25266   0.28151   0.32543   0.35661   0.42307
    Eigenvalues ---    0.51320   0.53483   0.57377   0.57873   0.58159
    Eigenvalues ---    0.58183   0.78664   0.79200   0.79694   0.81167
    Eigenvalues ---    0.82167   0.88990
 RFO step:  Lambda=-4.24577900D-04 EMin= 1.28124421D-02
 Quartic linear search produced a step of  0.31972.
 Iteration  1 RMS(Cart)=  0.01191570 RMS(Int)=  0.00015219
 Iteration  2 RMS(Cart)=  0.00015562 RMS(Int)=  0.00003672
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00003672
  ITry=  1 IFail=0 DXMaxC= 3.14D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)   (Quad)   (Total)
    R1        2.30991   0.00038  -0.00367   0.00064  -0.00302   2.30689
    R2        2.53350   0.00557   0.00701   0.00772   0.01474   2.54824
    R3        2.53338   0.00532   0.00693   0.00721   0.01414   2.54752
    R4        2.30987   0.00038  -0.00366   0.00063  -0.00302   2.30685
    R5        2.30563   0.00043  -0.00349   0.00063  -0.00286   2.30276
    R6        2.53355   0.00531   0.00693   0.00720   0.01414   2.54768
    R7        2.53798   0.00461   0.00661   0.00594   0.01256   2.55053
    R8        2.30556   0.00042  -0.00348   0.00062  -0.00286   2.30270
    R9        2.29752   0.00084  -0.00309   0.00107  -0.00202   2.29549
   R10        2.53814   0.00460   0.00661   0.00593   0.01254   2.55068
   R11        2.60165   0.00447   0.00642   0.00713   0.01355   2.61520
   R12        2.29752   0.00084  -0.00309   0.00106  -0.00203   2.29550
   R13        2.63467   0.00136  -0.00600   0.00443  -0.00159   2.63307
   R14        2.75848   0.00032  -0.00688   0.00208  -0.00479   2.75369
   R15        2.60168   0.00447   0.00645   0.00712   0.01356   2.61525
   R16        2.75876   0.00027  -0.00710   0.00196  -0.00513   2.75363
   R17        2.69897   0.00352  -0.00373   0.01478   0.01104   2.71001
    A1        2.61045   0.00004  -0.00022   0.00174   0.00153   2.61199
    A2        2.64260  -0.00001  -0.00026   0.00131   0.00105   2.64365
    A3        2.61570  -0.00003  -0.00031   0.00143   0.00113   2.61683
    A4        2.72077  -0.00014  -0.00025   0.00020  -0.00006   2.72071
    A5        2.63810   0.00004  -0.00021   0.00156   0.00136   2.63945
    A6        2.77655   0.00020   0.00046   0.00118   0.00161   2.77816
    A7        2.72480  -0.00021  -0.00035  -0.00007  -0.00043   2.72437
    A8        2.77362   0.00025   0.00052   0.00143   0.00193   2.77554
    A9        2.82685   0.00037   0.00080   0.00103   0.00177   2.82862
   A10        2.31644  -0.00019  -0.00181   0.00245   0.00062   2.31705
   A11        2.51152   0.00002  -0.00069   0.00405   0.00341   2.51493
   A12        1.45511   0.00018   0.00247  -0.00657  -0.00421   1.45091
   A13        2.82526   0.00040   0.00084   0.00117   0.00195   2.82720
   A14        2.31684  -0.00019  -0.00182   0.00247   0.00064   2.31748
   A15        1.45496   0.00017   0.00248  -0.00661  -0.00424   1.45071
   A16        2.51126   0.00002  -0.00070   0.00409   0.00344   2.51470
   A17        1.43461  -0.00053   0.00160  -0.00976  -0.00827   1.42634
   A18        1.43458  -0.00049   0.00173  -0.00963  -0.00801   1.42656
```

A19	2.89031	-0.00037	0.00011	-0.01224	-0.01218	2.87813
A20	2.89200	-0.00038	0.00010	-0.01241	-0.01236	2.87964
A21	3.13452	-0.00029	0.00202	-0.00613	-0.00409	3.13043
A22	3.13443	-0.00029	0.00202	-0.00606	-0.00403	3.13041
D1	0.05718	0.00004	0.00144	0.00128	0.00271	0.05989
D2	-0.04722	-0.00016	-0.00162	-0.00456	-0.00619	-0.05342
D3	-0.03546	-0.00015	-0.00045	-0.00371	-0.00416	-0.03962
D4	0.05454	0.00005	0.00159	0.00164	0.00323	0.05777
D5	0.05322	0.00016	0.00252	0.00614	0.00866	0.06188
D6	-0.03179	-0.00017	-0.00059	-0.00412	-0.00471	-0.03651
D7	0.06773	-0.00017	0.00078	-0.00285	-0.00206	0.06567
D8	0.05124	0.00016	0.00253	0.00618	0.00871	0.05995
D9	0.07056	-0.00018	0.00066	-0.00309	-0.00242	0.06814
D10	-0.54398	-0.00021	-0.00786	-0.01211	-0.01998	-0.56396
D11	2.62106	-0.00048	-0.00009	-0.00623	-0.00630	2.61476
D12	0.70317	0.00064	0.00458	0.02872	0.03329	0.73646
D13	-2.45251	0.00081	0.00022	0.02563	0.02584	-2.42666
D14	-2.45232	0.00080	-0.00003	0.02529	0.02527	-2.42705
D15	0.67518	0.00097	-0.00439	0.02220	0.01782	0.69301
D16	2.42906	0.00012	-0.00021	-0.02396	-0.02414	2.40492
D17	-0.69519	-0.00008	0.00553	-0.01963	-0.01403	-0.70922
D18	-0.54838	-0.00019	-0.00759	-0.01162	-0.01921	-0.56759
D19	2.61696	-0.00049	-0.00023	-0.00629	-0.00651	2.61045
D20	-0.69513	-0.00009	0.00548	-0.01965	-0.01410	-0.70923
D21	2.42891	0.00012	0.00004	-0.02356	-0.02349	2.40542
D22	0.66025	0.00047	-0.00486	0.01946	0.01456	0.67481

Item	Value	Threshold	Converged?
Maximum Force	0.005566	0.000450	NO
RMS Force	0.001771	0.000300	NO
Maximum Displacement	0.031438	0.001800	NO
RMS Displacement	0.011962	0.001200	NO

Predicted change in Energy=-3.144828D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 18:32:51 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.620486	-0.673288	0.016168
2	6	0	3.005594	-1.727069	0.057295
3	6	0	3.618433	0.674810	-0.015388
4	6	0	1.853025	-2.426249	0.065899
5	6	0	3.005453	1.729680	-0.056432

6	6	0	0.643887	-2.577540	0.063433
7	6	0	1.851107	2.426075	-0.066090
8	6	0	-0.667164	-2.259670	0.021566
9	6	0	0.642184	2.578836	-0.064030
10	6	0	-1.731249	-1.676635	-0.036300
11	6	0	-0.668510	2.259110	-0.022595
12	6	0	-2.679668	-0.677271	-0.166519
13	6	0	-1.732684	1.676199	0.034905
14	6	0	-2.679898	0.675792	0.166167
15	6	0	-4.040901	-0.391237	-0.600840
16	6	0	-4.040093	0.388456	0.602762

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220753	0.000000			
3	C	1.348468	2.479894	0.000000		
4	C	2.489832	1.348088	3.569291	0.000000	
5	C	2.481490	3.458619	1.220730	4.314488	0.000000
6	C	3.533915	2.510179	4.408165	1.218569	4.913605
7	C	3.569807	4.312386	2.488563	4.854120	1.348175
8	C	4.571715	3.711346	5.194120	2.526078	5.423017
9	C	4.410559	4.913374	3.533517	5.151106	2.511208
10	C	5.445229	4.738035	5.843700	3.663247	5.834358
11	C	5.195763	5.421720	4.570333	5.321519	3.712068
12	C	6.302803	5.785704	6.443372	4.863974	6.174636
13	C	5.846099	5.833868	5.444242	5.448702	4.739319
14	C	6.444948	6.173363	6.300947	5.493642	5.786488
15	C	7.691366	7.202130	7.755296	6.270900	7.378738
16	C	7.756021	7.376631	7.688767	6.552834	7.202301

		6	7	8	9	10
6	C	0.000000				
7	C	5.148818	0.000000			
8	C	1.349685	5.320299	0.000000		
9	C	5.157952	1.218538	5.013268	0.000000	
10	C	2.542212	5.446686	1.214723	4.872677	0.000000
11	C	5.012282	2.525517	4.518996	1.349763	4.076726
12	C	3.835351	5.492610	2.567008	4.652681	1.383902
13	C	4.872700	3.662795	4.077570	2.542546	3.353591
14	C	4.652125	4.862863	3.562154	3.835465	2.544571
15	C	5.212334	6.552783	3.906473	5.571425	2.702860
16	C	5.570250	6.269409	4.327471	5.212110	3.162873

		11	12	13	14	15
11	C	0.000000				
12	C	3.561995	0.000000			
13	C	1.214725	2.544833	0.000000		
14	C	2.566750	1.393363	1.383929	0.000000	
15	C	4.328016	1.457191	3.163278	1.891872	0.000000

```
   16  C    3.906148   1.891646   2.702754   1.457158   1.434078
             16
   16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 1.21D-03
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.620318   -0.674242    0.013975
     2          6           0        3.005162   -1.727994    0.051770
     3          6           0        3.618602    0.673949   -0.013307
     4          6           0        1.852419   -2.426910    0.058176
     5          6           0        3.005885    1.729098   -0.050996
     6          6           0        0.643243   -2.577890    0.055250
     7          6           0        1.851713    2.425810   -0.058428
     8          6           0       -0.667730   -2.259560    0.014412
     9          6           0        0.642828    2.578865   -0.055864
    10          6           0       -1.731669   -1.676078   -0.041588
    11          6           0       -0.667945    2.259338   -0.015422
    12          6           0       -2.679840   -0.676069   -0.168622
    13          6           0       -1.732264    1.676514    0.040248
    14          6           0       -2.679726    0.675932    0.168352
    15          6           0       -4.041008   -0.388318   -0.602012
    16          6           0       -4.039987    0.387554    0.604056
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8455681           0.3948289           0.2719550
 Leave Link  202 at Fri Aug 21 18:32:51 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.8042181906 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
```

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074879094 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.7967302812 Hartrees.
Leave Link 301 at Fri Aug 21 18:32:52 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14217 LenP2D= 33589.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 3.90D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 18:32:53 2026, MaxMem= 805306368 cpu: 6.4 elap: 1.1
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 18:32:53 2026, MaxMem= 805306368 cpu: 0.9 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 -0.000000 -0.000000
Rot= 1.000000 -0.000429 -0.000002 0.000017 Ang= -0.05 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.863687939798

Supporting Information file

```
 Leave Link  401 at Fri Aug 21 18:33:01 2026, MaxMem=    805306368 cpu:                46.7 elap:
7.8
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804634234 LenY=   804301882
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
       NFxFlg=          0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=          0 NGrid=          0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -608.980360925497
 DIIS: error= 1.85D-03 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -608.980360925497     IErMin= 1 ErrMin= 1.85D-03
 ErrMax= 1.85D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-03 BMatP= 1.83D-03
 IDIUse=3 WtCom= 9.82D-01 WtEn= 1.85D-02
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=     0.960 Goal=   None    Shift=    0.000
 GapD=    0.960 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
 RMSDP=3.94D-03 MaxDP=1.27D-01             OVMax= 7.46D-03

 Cycle   2  Pass 0  IDiag  1:
 RMSU=  3.84D-03    CP:  1.10D+00
 E= -608.981429218990     Delta-E=       -0.001068293492 Rises=F Damp=F
 DIIS: error= 5.42D-04 at cycle   2 NSaved=   2.
 NSaved= 2 IEnMin= 2 EnMin= -608.981429218990     IErMin= 2 ErrMin= 5.42D-04
 ErrMax= 5.42D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 6.34D-05 BMatP= 1.83D-03
 IDIUse=3 WtCom= 9.95D-01 WtEn= 5.42D-03
 Coeff-Com:  0.481D-02 0.995D+00
 Coeff-En:   0.000D+00 0.100D+01
 Coeff:      0.478D-02 0.995D+00
 Gap=     0.245 Goal=   None    Shift=    0.000
 RMSDP=1.07D-03 MaxDP=2.92D-02 DE=-1.07D-03 OVMax= 4.01D-03

 Cycle   3  Pass 0  IDiag  1:
```

RMSU= 1.05D-03 CP: 1.12D+00 1.06D+00
E= -608.981484156543 Delta-E= -0.000054937554 Rises=F Damp=F
DIIS: error= 2.15D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981484156543 IErMin= 2 ErrMin= 5.42D-04
ErrMax= 2.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-04 BMatP= 6.34D-05
IDIUse=3 WtCom= 1.78D-01 WtEn= 8.22D-01
Coeff-Com: 0.190D-02 0.882D+00 0.116D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.337D-03 0.157D+00 0.843D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=4.20D+02 MaxDP=1.66D+04 DE=-5.49D-05 OVMax= 9.92D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -608.981286893094 Delta-E= 0.000197263449 Rises=F Damp=F
DIIS: error= 5.88D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981286893094 IErMin= 1 ErrMin= 5.88D-04
ErrMax= 5.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-04 BMatP= 1.24D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 5.88D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=4.04D-03 MaxDP=1.25D-01 DE= 1.97D-04 OVMax= 2.69D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.24D-03 CP: 7.67D-01
E= -608.981365391536 Delta-E= -0.000078498442 Rises=F Damp=F
DIIS: error= 3.39D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981365391536 IErMin= 2 ErrMin= 3.39D-04
ErrMax= 3.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-05 BMatP= 1.24D-04
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.39D-03
Coeff-Com: 0.138D+00 0.862D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.138D+00 0.862D+00
Gap= 0.245 Goal= None Shift= 0.000
RMSDP=2.50D-04 MaxDP=6.22D-03 DE=-7.85D-05 OVMax= 1.94D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.19D-04 CP: 7.53D-01 1.05D+00
E= -608.981362120546 Delta-E= 0.000003270990 Rises=F Damp=F
DIIS: error= 3.38D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -608.981365391536 IErMin= 3 ErrMin= 3.38D-04
ErrMax= 3.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-05 BMatP= 1.54D-05
IDIUse=3 WtCom= 3.52D-01 WtEn= 6.48D-01
Coeff-Com: -0.172D-01 0.553D+00 0.464D+00
Coeff-En: 0.000D+00 0.536D+00 0.464D+00

Coeff: -0.605D-02 0.542D+00 0.464D+00
Gap= 0.245 Goal= None Shift= 0.000
RMSDP=5.61D-05 MaxDP=1.51D-03 DE= 3.27D-06 OVMax= 1.13D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.51D-05 CP: 7.50D-01 1.06D+00 1.21D+00
E= -608.981386295772 Delta-E= -0.000024175226 Rises=F Damp=F
DIIS: error= 5.20D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981386295772 IErMin= 4 ErrMin= 5.20D-05
ErrMax= 5.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.62D-07 BMatP= 1.54D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.136D-01 0.210D+00 0.215D+00 0.589D+00
Coeff: -0.136D-01 0.210D+00 0.215D+00 0.589D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.75D-05 MaxDP=4.88D-04 DE=-2.42D-05 OVMax= 3.88D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.32D-06 CP: 7.49D-01 1.07D+00 1.29D+00 1.19D+00
E= -608.981387332955 Delta-E= -0.000001037183 Rises=F Damp=F
DIIS: error= 3.29D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981387332955 IErMin= 5 ErrMin= 3.29D-05
ErrMax= 3.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.20D-08 BMatP= 5.62D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.671D-02-0.211D+00-0.178D+00 0.256D-02 0.138D+01
Coeff: 0.671D-02-0.211D+00-0.178D+00 0.256D-02 0.138D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.78D-05 MaxDP=4.73D-04 DE=-1.04D-06 OVMax= 7.76D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.28D-06 CP: 7.49D-01 1.07D+00 1.38D+00 1.37D+00 2.12D+00
E= -608.981387981709 Delta-E= -0.000000648754 Rises=F Damp=F
DIIS: error= 1.56D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981387981709 IErMin= 6 ErrMin= 1.56D-05
ErrMax= 1.56D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-08 BMatP= 8.20D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.541D-02-0.146D+00-0.127D+00-0.653D-01 0.802D+00 0.532D+00
Coeff: 0.541D-02-0.146D+00-0.127D+00-0.653D-01 0.802D+00 0.532D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.56D-06 MaxDP=4.70D-05 DE=-6.49D-07 OVMax= 1.75D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 7.71D-07 CP: 7.49D-01 1.07D+00 1.37D+00 1.37D+00 2.23D+00
CP: 1.08D+00
E= -608.981388049537 Delta-E= -0.000000067829 Rises=F Damp=F
DIIS: error= 4.74D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981388049537 IErMin= 7 ErrMin= 4.74D-06
ErrMax= 4.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-09 BMatP= 3.25D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.403D-04 0.958D-02 0.631D-02-0.261D-01-0.120D+00 0.184D+00
Coeff-Com: 0.947D+00
Coeff: -0.403D-04 0.958D-02 0.631D-02-0.261D-01-0.120D+00 0.184D+00
Coeff: 0.947D+00
Gap=   0.246 Goal=   None   Shift=   0.000
RMSDP=5.19D-06 MaxDP=1.35D-04 DE=-6.78D-08 OVMax= 1.14D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 6.11D-07   CP: 7.49D-01 1.07D+00 1.35D+00 1.34D+00 2.15D+00
               CP: 1.08D+00 2.27D+00
E= -608.981388067291   Delta-E=   -0.000000017753 Rises=F Damp=F
DIIS: error= 3.79D-06 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -608.981388067291   IErMin= 8 ErrMin= 3.79D-06
ErrMax= 3.79D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.04D-10 BMatP= 3.39D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.948D-03 0.293D-01 0.245D-01 0.473D-03-0.187D+00-0.725D-02
Coeff-Com: 0.399D+00 0.742D+00
Coeff: -0.948D-03 0.293D-01 0.245D-01 0.473D-03-0.187D+00-0.725D-02
Coeff: 0.399D+00 0.742D+00
Gap=   0.246 Goal=   None   Shift=   0.000
RMSDP=1.64D-06 MaxDP=4.66D-05 DE=-1.78D-08 OVMax= 4.85D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.53D-07   CP: 7.49D-01 1.07D+00 1.34D+00 1.32D+00 2.09D+00
               CP: 1.08D+00 2.73D+00 1.34D+00
E= -608.981388070704   Delta-E=   -0.000000003413 Rises=F Damp=F
DIIS: error= 1.04D-06 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -608.981388070704   IErMin= 9 ErrMin= 1.04D-06
ErrMax= 1.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-10 BMatP= 8.04D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.229D-03 0.442D-02 0.430D-02 0.823D-02-0.870D-02-0.545D-01
Coeff-Com: -0.196D+00 0.160D+00 0.108D+01
Coeff: -0.229D-03 0.442D-02 0.430D-02 0.823D-02-0.870D-02-0.545D-01
Coeff: -0.196D+00 0.160D+00 0.108D+01
Gap=   0.246 Goal=   None   Shift=   0.000
RMSDP=3.37D-07 MaxDP=1.17D-05 DE=-3.41D-09 OVMax= 2.87D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.47D-07   CP: 7.49D-01 1.07D+00 1.34D+00 1.32D+00 2.06D+00
               CP: 1.06D+00 2.90D+00 1.50D+00 1.64D+00
E= -608.981388071955   Delta-E=   -0.000000001251 Rises=F Damp=F
DIIS: error= 7.93D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981388071955   IErMin=10 ErrMin= 7.93D-07
ErrMax= 7.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.55D-11 BMatP= 1.58D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.111D-03-0.450D-02-0.351D-02 0.297D-02 0.368D-01-0.201D-01
Coeff-Com: -0.168D+00-0.974D-01 0.455D+00 0.799D+00
Coeff: 0.111D-03-0.450D-02-0.351D-02 0.297D-02 0.368D-01-0.201D-01

Coeff: -0.168D+00-0.974D-01 0.455D+00 0.799D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.61D-07 MaxDP=6.16D-06 DE=-1.25D-09 OVMax= 1.30D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 3.04D-08 CP: 7.49D-01 1.07D+00 1.34D+00 1.32D+00 2.07D+00
CP: 1.05D+00 2.89D+00 1.50D+00 1.94D+00 1.40D+00
E= -608.981388072164 Delta-E= -0.000000000209 Rises=F Damp=F
DIIS: error= 3.05D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981388072164 IErMin=11 ErrMin= 3.05D-07
ErrMax= 3.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-11 BMatP= 4.55D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.999D-04-0.315D-02-0.264D-02-0.109D-03 0.205D-01-0.918D-05
Coeff-Com: -0.521D-01-0.799D-01 0.398D-01 0.417D+00 0.660D+00
Coeff: 0.999D-04-0.315D-02-0.264D-02-0.109D-03 0.205D-01-0.918D-05
Coeff: -0.521D-01-0.799D-01 0.398D-01 0.417D+00 0.660D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.41D-07 MaxDP=3.74D-06 DE=-2.09D-10 OVMax= 4.46D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.43D-08 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.07D+00
CP: 1.05D+00 2.87D+00 1.49D+00 1.96D+00 1.55D+00
CP: 1.37D+00
E= -608.981388072213 Delta-E= -0.000000000049 Rises=F Damp=F
DIIS: error= 1.99D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981388072213 IErMin=12 ErrMin= 1.99D-07
ErrMax= 1.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.05D-12 BMatP= 1.35D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.436D-05 0.143D-03 0.265D-04-0.897D-03-0.293D-02 0.550D-02
Coeff-Com: 0.281D-01 0.936D-03-0.116D+00-0.655D-01 0.266D+00 0.885D+00
Coeff: 0.436D-05 0.143D-03 0.265D-04-0.897D-03-0.293D-02 0.550D-02
Coeff: 0.281D-01 0.936D-03-0.116D+00-0.655D-01 0.266D+00 0.885D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=6.22D-08 MaxDP=1.86D-06 DE=-4.87D-11 OVMax= 3.12D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 9.75D-09 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.08D+00
CP: 1.05D+00 2.86D+00 1.47D+00 1.94D+00 1.60D+00
CP: 1.69D+00 1.51D+00
E= -608.981388072231 Delta-E= -0.000000000018 Rises=F Damp=F
DIIS: error= 1.19D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981388072231 IErMin=13 ErrMin= 1.19D-07
ErrMax= 1.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.81D-13 BMatP= 3.05D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.326D-04 0.115D-02 0.920D-03-0.361D-03-0.810D-02 0.216D-02
Coeff-Com: 0.302D-01 0.286D-01-0.679D-01-0.171D+00-0.120D+00 0.340D+00
Coeff-Com: 0.964D+00
Coeff: -0.326D-04 0.115D-02 0.920D-03-0.361D-03-0.810D-02 0.216D-02

Coeff: 0.302D-01 0.286D-01-0.679D-01-0.171D+00-0.120D+00 0.340D+00
Coeff: 0.964D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.19D-08 MaxDP=2.40D-07 DE=-1.82D-11 OVMax= 2.47D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 5.13D-09 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.08D+00
CP: 1.06D+00 2.85D+00 1.47D+00 1.93D+00 1.61D+00
CP: 1.84D+00 1.85D+00 1.52D+00
E= -608.981388072233 Delta-E= -0.000000000002 Rises=F Damp=F
DIIS: error= 5.17D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -608.981388072233 IErMin=14 ErrMin= 5.17D-08
ErrMax= 5.17D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-13 BMatP= 8.81D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.397D-05 0.510D-04 0.626D-04 0.237D-03 0.273D-03-0.160D-02
Coeff-Com: -0.566D-02 0.326D-02 0.258D-01 0.864D-02-0.847D-01-0.251D+00
Coeff-Com: 0.121D+00 0.118D+01
Coeff: -0.397D-05 0.510D-04 0.626D-04 0.237D-03 0.273D-03-0.160D-02
Coeff: -0.566D-02 0.326D-02 0.258D-01 0.864D-02-0.847D-01-0.251D+00
Coeff: 0.121D+00 0.118D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.59D-08 MaxDP=6.51D-07 DE=-1.82D-12 OVMax= 1.42D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 3.27D-09 CP: 7.49D-01 1.07D+00 1.34D+00 1.33D+00 2.08D+00
CP: 1.05D+00 2.86D+00 1.47D+00 1.93D+00 1.60D+00
CP: 1.84D+00 1.90D+00 1.82D+00 1.75D+00
E= -608.981388072236 Delta-E= -0.000000000003 Rises=F Damp=F
DIIS: error= 1.25D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -608.981388072236 IErMin=15 ErrMin= 1.25D-08
ErrMax= 1.25D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-14 BMatP= 1.63D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.523D-05-0.193D-03-0.153D-03 0.724D-04 0.141D-02-0.660D-03
Coeff-Com: -0.580D-02-0.428D-02 0.145D-01 0.307D-01 0.117D-01-0.964D-01
Coeff-Com: -0.130D+00 0.130D+00 0.105D+01
Coeff: 0.523D-05-0.193D-03-0.153D-03 0.724D-04 0.141D-02-0.660D-03
Coeff: -0.580D-02-0.428D-02 0.145D-01 0.307D-01 0.117D-01-0.964D-01
Coeff: -0.130D+00 0.130D+00 0.105D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.00D-09 MaxDP=1.51D-07 DE=-3.41D-12 OVMax= 4.06D-07

SCF Done: E(RwB97XD) = -608.981388072 A.U. after 18 cycles
NFock= 18 Conv=0.50D-08 -V/T= 2.0045
KE= 6.062575326491D+02 PE=-2.846607848744D+03 EE= 9.135721977414D+02
Leave Link 502 at Fri Aug 21 18:44:12 2026, MaxMem= 805306368 cpu: 4025.5 elap: 671.2
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.

Supporting Information file

Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14217 LenP2D= 33589.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 18:44:12 2026, MaxMem= 805306368 cpu: 2.2 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 18:44:12 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 2611.4 elap: 435.3
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.51345453D+00-4.72278216D-03-4.77546478D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000134277	0.000292559	-0.000412978
2	6	-0.000256779	-0.000172245	0.000613995
3	6	0.000238411	-0.000264418	0.000440196
4	6	0.000501151	-0.000232070	-0.000863098
5	6	-0.000332742	0.000104360	-0.000670177
6	6	-0.000479261	0.000025035	0.000862827
7	6	0.000532306	0.000320156	0.000909665
8	6	0.000526655	-0.000253227	-0.001090145
9	6	-0.000484767	-0.000095891	-0.000880248
10	6	-0.000286670	0.000839198	0.001169892
11	6	0.000518843	0.000284454	0.001069359
12	6	-0.000215107	-0.001473423	-0.002548339
13	6	-0.000271391	-0.000865391	-0.001126214
14	6	-0.000214759	0.001499044	0.002523731
15	6	0.000043768	-0.003273910	-0.002172394
16	6	0.000046065	0.003265772	0.002173929

Supporting Information file

Cartesian Forces: Max 0.003273910 RMS 0.001130740
Leave Link 716 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003236618 RMS 0.000624034
Search for a local minimum.
Step number 4 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .62403D-03 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 1 2 3 4
DE= -2.82D-04 DEPred=-3.14D-04 R= 8.97D-01
TightC=F SS= 1.41D+00 RLast= 8.74D-02 DXNew= 8.4853D-01 2.6229D-01
Trust test= 8.97D-01 RLast= 8.74D-02 DXMaxT set to 5.05D-01
ITU= 1 1 1 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.01293 0.01365 0.01670 0.01734 0.02624
Eigenvalues --- 0.02815 0.03059 0.03365 0.03423 0.03926
Eigenvalues --- 0.03965 0.04047 0.06031 0.08438 0.09287
Eigenvalues --- 0.19449 0.24521 0.24683 0.24993 0.24994
Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25001
Eigenvalues --- 0.25072 0.28102 0.32093 0.38069 0.43397
Eigenvalues --- 0.51325 0.53457 0.57383 0.57862 0.58159
Eigenvalues --- 0.58183 0.78671 0.79015 0.79698 0.80820
Eigenvalues --- 0.82173 0.83868
RFO step: Lambda=-1.49434008D-04 EMin= 1.29347083D-02
Quartic linear search produced a step of -0.08283.
Iteration 1 RMS(Cart)= 0.00633165 RMS(Int)= 0.00005952
Iteration 2 RMS(Cart)= 0.00004072 RMS(Int)= 0.00002866
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002866
ITry= 1 IFail=0 DXMaxC= 2.16D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.30689	0.00034	0.00025	-0.00128	-0.00103	2.30586
R2	2.54824	-0.00001	-0.00122	0.00380	0.00258	2.55081
R3	2.54752	-0.00002	-0.00117	0.00365	0.00248	2.55000
R4	2.30685	0.00034	0.00025	-0.00128	-0.00103	2.30581
R5	2.30276	0.00039	0.00024	-0.00114	-0.00091	2.30185
R6	2.54768	-0.00003	-0.00117	0.00364	0.00247	2.55015
R7	2.55053	-0.00004	-0.00104	0.00325	0.00221	2.55274
R8	2.30270	0.00038	0.00024	-0.00115	-0.00091	2.30179

R9	2.29549	0.00053	0.00017	-0.00072	-0.00055	2.29494
R10	2.55068	-0.00005	-0.00104	0.00323	0.00219	2.55288
R11	2.61520	-0.00020	-0.00112	0.00335	0.00222	2.61742
R12	2.29550	0.00053	0.00017	-0.00073	-0.00056	2.29494
R13	2.63307	0.00175	0.00013	0.00360	0.00375	2.63682
R14	2.75369	-0.00000	0.00040	-0.00328	-0.00292	2.75077
R15	2.61525	-0.00021	-0.00112	0.00333	0.00221	2.61746
R16	2.75363	0.00000	0.00042	-0.00338	-0.00299	2.75064
R17	2.71001	0.00324	-0.00091	0.01120	0.01033	2.72034
A1	2.61199	0.00006	-0.00013	-0.00006	-0.00018	2.61180
A2	2.64365	0.00004	-0.00009	-0.00019	-0.00028	2.64337
A3	2.61683	-0.00001	-0.00009	-0.00043	-0.00052	2.61631
A4	2.72071	-0.00030	0.00000	-0.00163	-0.00163	2.71908
A5	2.63945	0.00009	-0.00011	0.00010	-0.00002	2.63943
A6	2.77816	0.00002	-0.00013	0.00022	0.00008	2.77823
A7	2.72437	-0.00037	0.00004	-0.00196	-0.00193	2.72244
A8	2.77554	0.00007	-0.00016	0.00049	0.00032	2.77586
A9	2.82862	0.00030	-0.00015	0.00155	0.00138	2.83000
A10	2.31705	-0.00062	-0.00005	-0.00502	-0.00506	2.31199
A11	2.51493	-0.00001	-0.00028	-0.00191	-0.00218	2.51275
A12	1.45091	0.00063	0.00035	0.00674	0.00703	1.45794
A13	2.82720	0.00032	-0.00016	0.00169	0.00151	2.82872
A14	2.31748	-0.00062	-0.00005	-0.00501	-0.00505	2.31243
A15	1.45071	0.00062	0.00035	0.00670	0.00700	1.45772
A16	2.51470	-0.00001	-0.00028	-0.00187	-0.00214	2.51256
A17	1.42634	0.00014	0.00068	0.00408	0.00469	1.43103
A18	1.42656	0.00014	0.00066	0.00418	0.00477	1.43133
A19	2.87813	0.00037	0.00101	0.00317	0.00417	2.88230
A20	2.87964	0.00036	0.00102	0.00303	0.00404	2.88369
A21	3.13043	0.00022	0.00034	0.00720	0.00753	3.13795
A22	3.13041	0.00021	0.00033	0.00711	0.00743	3.13784
D1	0.05989	0.00016	-0.00022	0.00371	0.00349	0.06338
D2	-0.05342	0.00007	0.00051	-0.00140	-0.00088	-0.05430
D3	-0.03962	-0.00005	0.00034	-0.00278	-0.00244	-0.04205
D4	0.05777	0.00018	-0.00027	0.00417	0.00390	0.06167
D5	0.06188	0.00017	-0.00072	0.00749	0.00677	0.06865
D6	-0.03651	-0.00006	0.00039	-0.00324	-0.00285	-0.03936
D7	0.06567	-0.00011	0.00017	0.00307	0.00323	0.06891
D8	0.05995	0.00017	-0.00072	0.00760	0.00687	0.06683
D9	0.06814	-0.00012	0.00020	0.00272	0.00291	0.07105
D10	-0.56396	-0.00058	0.00165	-0.01787	-0.01623	-0.58019
D11	2.61476	0.00002	0.00052	-0.00572	-0.00519	2.60956
D12	0.73646	0.00035	-0.00276	0.00360	0.00080	0.73727
D13	-2.42666	-0.00000	-0.00214	-0.00315	-0.00535	-2.43201
D14	-2.42705	-0.00000	-0.00209	-0.00362	-0.00577	-2.43283
D15	0.69301	-0.00035	-0.00148	-0.01036	-0.01192	0.68108
D16	2.40492	0.00089	0.00200	0.00603	0.00797	2.41289
D17	-0.70922	0.00134	0.00116	0.01513	0.01627	-0.69295

```
  D18       -0.56759  -0.00057   0.00159  -0.01721  -0.01563  -0.58322
  D19        2.61045   0.00002   0.00054  -0.00586  -0.00532   2.60513
  D20       -0.70923   0.00134   0.00117   0.01510   0.01626  -0.69298
  D21        2.40542   0.00089   0.00195   0.00661   0.00850   2.41392
  D22        0.67481  -0.00067  -0.00121  -0.01186  -0.01312   0.66169
         Item               Value     Threshold  Converged?
 Maximum Force            0.003237     0.000450     NO
 RMS     Force            0.000624     0.000300     NO
 Maximum Displacement     0.021642     0.001800     NO
 RMS     Displacement     0.006324     0.001200     NO
 Predicted change in Energy=-7.735845D-05
 Lowest energy point so far.  Saving SCF results.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link  103 at Fri Aug 21 18:51:28 2026, MaxMem=  805306368 cpu:                  0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l202.exe)
                      Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.623692   -0.673916    0.017066
     2          6           0        3.008781   -1.726993    0.059683
     3          6           0        3.621775    0.675505   -0.016183
     4          6           0        1.854749   -2.426303    0.067283
     5          6           0        3.008632    1.729586   -0.058843
     6          6           0        0.645777   -2.575001    0.063189
     7          6           0        1.852919    2.426261   -0.067458
     8          6           0       -0.665657   -2.254519    0.015860
     9          6           0        0.644135    2.576223   -0.063808
    10          6           0       -1.730943   -1.673869   -0.037545
    11          6           0       -0.666956    2.253978   -0.016972
    12          6           0       -2.684409   -0.677794   -0.168605
    13          6           0       -1.732292    1.673393    0.036135
    14          6           0       -2.684622    0.676321    0.168094
    15          6           0       -4.048276   -0.402689   -0.596499
    16          6           0       -4.047307    0.399817    0.598604
 ---------------------------------------------------------------------
               Distance matrix (angstroms):
                    1          2          3          4          5
    1  C    0.000000
    2  C    1.220206   0.000000
    3  C    1.349832   2.480628   0.000000
    4  C    2.490490   1.349400   3.570792   0.000000
    5  C    2.482112   3.458610   1.220184   4.314946   0.000000
    6  C    3.533303   2.510561   4.407794   1.218089   4.911969
    7  C    3.571257   4.312968   2.489302   4.854434   1.349482
```

```
   8  C    4.571304   3.712371   5.193086   2.526776   5.420247
   9  C    4.409956   4.911667   3.532894   5.148595   2.511507
  10  C    5.447477   4.741018   5.845648   3.665287   5.835026
  11  C    5.194554   5.418953   4.569988   5.317060   3.713043
  12  C    6.310835   5.793561   6.451558   4.869998   6.182091
  13  C    5.847802   5.834462   5.446517   5.447507   4.742208
  14  C    6.452966   6.180817   6.309088   5.499302   5.794308
  15  C    7.701242   7.210160   7.767171   6.275454   7.391592
  16  C    7.767581   7.389325   7.698622   6.565327   7.210187
                6          7          8          9         10
   6  C    0.000000
   7  C    5.146540   0.000000
   8  C    1.350854   5.316001   0.000000
   9  C    5.152790   1.218057   5.005794   0.000000
  10  C    2.543813   5.445735   1.214430   4.868775   0.000000
  11  C    5.004871   2.526263   4.508617   1.350924   4.069457
  12  C    3.839696   5.498430   2.568161   4.656051   1.385078
  13  C    4.868757   3.664871   4.070211   2.544110   3.348074
  14  C    4.655497   4.868989   3.562193   3.839795   2.544639
  15  C    5.214237   6.565588   3.904660   5.583583   2.701548
  16  C    5.582226   6.273977   4.338277   5.213939   3.173390
               11         12         13         14         15
  11  C    0.000000
  12  C    3.562077   0.000000
  13  C    1.214430   2.544902   0.000000
  14  C    2.567922   1.395347   1.385098   0.000000
  15  C    4.339016   1.455647   3.173976   1.899584   0.000000
  16  C    3.904308   1.899300   2.701418   1.455577   1.439544
               16
  16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 8.27D-04
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.623506   -0.674963    0.015259
    2          6           0        3.008302   -1.727976    0.055163
    3          6           0        3.621962    0.674540   -0.014500
    4          6           0        1.854077   -2.426983    0.060974
    5          6           0        3.009111    1.728897   -0.054423
    6          6           0        0.645064   -2.575335    0.056517
```

```
     7        6        0        1.853592    2.425913   -0.061215
     8        6        0       -0.666282   -2.254368    0.010040
     9        6        0        0.644849    2.576201   -0.057156
    10        6        0       -1.731408   -1.673286   -0.041844
    11        6        0       -0.666331    2.254199   -0.011131
    12        6        0       -2.684600   -0.676610   -0.170310
    13        6        0       -1.731827    1.673775    0.040494
    14        6        0       -2.684431    0.676629    0.169890
    15        6        0       -4.048398   -0.400022   -0.597467
    16        6        0       -4.047185    0.399390    0.599707
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8468943           0.3938762           0.2716111
 Leave Link  202 at Fri Aug 21 18:51:28 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.4701327343 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0074897369 Hartrees.
 Nuclear repulsion after empirical dispersion term =      717.4626429974 Hartrees.
 Leave Link  301 at Fri Aug 21 18:51:28 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33574.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  4.01D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
```

Supporting Information file

IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 563 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 18:51:28 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000292 -0.000001 0.000014 Ang= 0.03 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.36D+04 ExpMxC= 4.63D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -582.864964196537
Leave Link 401 at Fri Aug 21 18:51:34 2026, MaxMem= 805306368 cpu: 31.1 elap: 5.2
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Supporting Information file

Symmetry not used in FoFCou.
E= -608.981207400464
DIIS: error= 6.29D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981207400464 IErMin= 1 ErrMin= 6.29D-04
ErrMax= 6.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.37D-04 BMatP= 5.37D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 6.29D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.959 Goal= None Shift= 0.000
RMSDP=3.35D-03 MaxDP=9.85D-02 OVMax= 3.59D-03

Cycle 2 Pass 0 IDiag 1:
RMSU= 3.28D-03 CP: 1.08D+00
E= -608.981587035798 Delta-E= -0.000379635334 Rises=F Damp=F
DIIS: error= 4.51D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981587035798 IErMin= 2 ErrMin= 4.51D-04
ErrMax= 4.51D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-05 BMatP= 5.37D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.51D-03
Coeff-Com: 0.332D-01 0.967D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.330D-01 0.967D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=9.95D-04 MaxDP=3.17D-02 DE=-3.80D-04 OVMax= 2.13D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 9.85D-04 CP: 1.09D+00 1.04D+00
E= -608.981565874565 Delta-E= 0.000021161233 Rises=F Damp=F
DIIS: error= 1.39D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -608.981587035798 IErMin= 2 ErrMin= 4.51D-04
ErrMax= 1.39D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-04 BMatP= 3.13D-05
IDIUse=3 WtCom= 2.12D-01 WtEn= 7.88D-01
Rare condition: small coef for last iteration: 0.000D+00
Coeff-Com: 0.270D-01 0.877D+00 0.964D-01
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.270D-01 0.877D+00 0.964D-01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.88D-03 MaxDP=1.13D-01 DE= 2.12D-05 OVMax= 7.47D-04

Cycle 4 Pass 0 IDiag 1:
RMSU= 1.71D-03 CP: 1.17D+00 1.71D+00 6.19D-01
E= -608.981594686058 Delta-E= -0.000028811493 Rises=F Damp=F
DIIS: error= 1.82D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981594686058 IErMin= 2 ErrMin= 4.51D-04
ErrMax= 1.82D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.79D-04 BMatP= 3.13D-05
IDIUse=3 WtCom= 1.90D-01 WtEn= 8.10D-01
Coeff-Com: -0.290D-01 0.827D+00 0.738D+00-0.536D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.551D-02 0.157D+00 0.140D+00 0.708D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.75D+02 MaxDP=1.46D+04 DE=-2.88D-05 OVMax= 9.84D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 5 Pass 1 IDiag 1:
E= -608.981372450888 Delta-E= 0.000222235170 Rises=F Damp=F
DIIS: error= 6.32D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981372450888 IErMin= 1 ErrMin= 6.32D-04
ErrMax= 6.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-04 BMatP= 1.27D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 6.32D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.72D-03 MaxDP=2.03D-01 DE= 2.22D-04 OVMax= 1.73D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 4.11D-03 CP: 6.55D-01
E= -608.981454486177 Delta-E= -0.000082035289 Rises=F Damp=F
DIIS: error= 1.02D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981454486177 IErMin= 2 ErrMin= 1.02D-04
ErrMax= 1.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-06 BMatP= 1.27D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.02D-03
Coeff-Com: -0.633D-02 0.101D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.632D-02 0.101D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.88D-04 MaxDP=9.95D-03 DE=-8.20D-05 OVMax= 1.17D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.70D-04 CP: 6.33D-01 1.06D+00
E= -608.981451868728 Delta-E= 0.000002617449 Rises=F Damp=F
DIIS: error= 1.72D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -608.981454486177 IErMin= 2 ErrMin= 1.02D-04
ErrMax= 1.72D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.94D-06 BMatP= 2.37D-06
IDIUse=3 WtCom= 4.33D-01 WtEn= 5.67D-01
Coeff-Com: -0.219D-01 0.634D+00 0.388D+00
Coeff-En: 0.000D+00 0.646D+00 0.354D+00
Coeff: -0.947D-02 0.641D+00 0.368D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.99D-05 MaxDP=5.11D-04 DE= 2.62D-06 OVMax= 4.31D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 5.26D-06 CP: 6.32D-01 1.06D+00 1.06D+00
E= -608.981457847689 Delta-E= -0.000005978960 Rises=F Damp=F
DIIS: error= 1.21D-05 at cycle 4 NSaved= 4.

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NSaved= 4 IEnMin= 4 EnMin= -608.981457847689 IErMin= 4 ErrMin= 1.21D-05
ErrMax= 1.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.25D-08 BMatP= 2.37D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.289D-02 0.339D-01 0.162D-01 0.953D+00
Coeff: -0.289D-02 0.339D-01 0.162D-01 0.953D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.05D-05 MaxDP=7.79D-04 DE=-5.98D-06 OVMax= 2.38D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.63D-06 CP: 6.30D-01 1.06D+00 1.16D+00 1.50D+00
E= -608.981458013438 Delta-E= -0.000000165750 Rises=F Damp=F
DIIS: error= 1.26D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981458013438 IErMin= 4 ErrMin= 1.21D-05
ErrMax= 1.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-08 BMatP= 4.25D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.484D-02-0.165D+00-0.102D+00 0.468D+00 0.794D+00
Coeff: 0.484D-02-0.165D+00-0.102D+00 0.468D+00 0.794D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.14D-05 MaxDP=3.00D-04 DE=-1.66D-07 OVMax= 2.58D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.08D-06 CP: 6.30D-01 1.07D+00 1.20D+00 1.65D+00 1.55D+00
E= -608.981458095696 Delta-E= -0.000000082257 Rises=F Damp=F
DIIS: error= 4.10D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981458095696 IErMin= 6 ErrMin= 4.10D-06
ErrMax= 4.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.14D-09 BMatP= 2.42D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.248D-02-0.728D-01-0.441D-01 0.902D-02 0.335D+00 0.770D+00
Coeff: 0.248D-02-0.728D-01-0.441D-01 0.902D-02 0.335D+00 0.770D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.51D-06 MaxDP=4.48D-05 DE=-8.23D-08 OVMax= 1.17D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 5.99D-07 CP: 6.30D-01 1.07D+00 1.19D+00 1.64D+00 1.57D+00
CP: 1.18D+00
E= -608.981458113165 Delta-E= -0.000000017470 Rises=F Damp=F
DIIS: error= 2.35D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981458113165 IErMin= 7 ErrMin= 2.35D-06
ErrMax= 2.35D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.77D-09 BMatP= 5.14D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.372D-03 0.202D-01 0.132D-01-0.187D+00-0.994D-01 0.452D+00
Coeff-Com: 0.801D+00
Coeff: -0.372D-03 0.202D-01 0.132D-01-0.187D+00-0.994D-01 0.452D+00
Coeff: 0.801D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.23D-06 MaxDP=9.63D-05 DE=-1.75D-08 OVMax= 8.11D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.28D-07 CP: 6.30D-01 1.06D+00 1.18D+00 1.60D+00 1.48D+00
CP: 1.24D+00 2.01D+00
E= -608.981458119197 Delta-E= -0.000000006032 Rises=F Damp=F
DIIS: error= 8.57D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981458119197 IErMin= 8 ErrMin= 8.57D-07
ErrMax= 8.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-10 BMatP= 1.77D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.423D-03 0.158D-01 0.100D-01-0.693D-01-0.676D-01 0.801D-01
Coeff-Com: 0.299D+00 0.732D+00
Coeff: -0.423D-03 0.158D-01 0.100D-01-0.693D-01-0.676D-01 0.801D-01
Coeff: 0.299D+00 0.732D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.09D-06 MaxDP=3.23D-05 DE=-6.03D-09 OVMax= 2.07D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 8.12D-08 CP: 6.30D-01 1.06D+00 1.18D+00 1.58D+00 1.43D+00
CP: 1.25D+00 2.28D+00 1.27D+00
E= -608.981458119731 Delta-E= -0.000000000534 Rises=F Damp=F
DIIS: error= 4.59D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981458119731 IErMin= 9 ErrMin= 4.59D-07
ErrMax= 4.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.27D-11 BMatP= 1.58D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.828D-05-0.108D-02-0.538D-03 0.258D-01 0.686D-02-0.907D-01
Coeff-Com: -0.113D+00 0.174D+00 0.998D+00
Coeff: -0.828D-05-0.108D-02-0.538D-03 0.258D-01 0.686D-02-0.907D-01
Coeff: -0.113D+00 0.174D+00 0.998D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=3.85D-07 MaxDP=1.23D-05 DE=-5.34D-10 OVMax= 1.18D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 4.57D-08 CP: 6.30D-01 1.06D+00 1.18D+00 1.57D+00 1.40D+00
CP: 1.22D+00 2.45D+00 1.46D+00 1.63D+00
E= -608.981458119909 Delta-E= -0.000000000178 Rises=F Damp=F
DIIS: error= 1.88D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981458119909 IErMin=10 ErrMin= 1.88D-07
ErrMax= 1.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.83D-12 BMatP= 3.27D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.106D-03-0.451D-02-0.277D-02 0.283D-01 0.201D-01-0.576D-01
Coeff-Com: -0.120D+00-0.107D+00 0.413D+00 0.830D+00
Coeff: 0.106D-03-0.451D-02-0.277D-02 0.283D-01 0.201D-01-0.576D-01
Coeff: -0.120D+00-0.107D+00 0.413D+00 0.830D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.02D-08 MaxDP=1.28D-06 DE=-1.78D-10 OVMax= 5.45D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.66D-08 CP: 6.30D-01 1.06D+00 1.18D+00 1.57D+00 1.40D+00
CP: 1.23D+00 2.48D+00 1.49D+00 1.84D+00 1.40D+00
E= -608.981458119942 Delta-E= -0.000000000033 Rises=F Damp=F

DIIS: error= 1.01D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981458119942 IErMin=11 ErrMin= 1.01D-07
ErrMax= 1.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.59D-13 BMatP= 7.83D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.315D-04-0.116D-02-0.735D-03 0.497D-02 0.431D-02-0.561D-02
Coeff-Com: -0.204D-01-0.533D-01-0.268D-02 0.217D+00 0.857D+00
Coeff: 0.315D-04-0.116D-02-0.735D-03 0.497D-02 0.431D-02-0.561D-02
Coeff: -0.204D-01-0.533D-01-0.268D-02 0.217D+00 0.857D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=8.49D-08 MaxDP=2.49D-06 DE=-3.27D-11 OVMax= 1.42D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 8.13D-09 CP: 6.30D-01 1.06D+00 1.18D+00 1.58D+00 1.40D+00
CP: 1.23D+00 2.46D+00 1.47D+00 1.80D+00 1.50D+00
CP: 1.44D+00
E= -608.981458119947 Delta-E= -0.000000000006 Rises=F Damp=F
DIIS: error= 5.66D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981458119947 IErMin=12 ErrMin= 5.66D-08
ErrMax= 5.66D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.10D-13 BMatP= 8.59D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.907D-05 0.476D-03 0.280D-03-0.398D-02-0.272D-02 0.108D-01
Coeff-Com: 0.183D-01-0.186D-02-0.958D-01-0.939D-01 0.475D+00 0.693D+00
Coeff: -0.907D-05 0.476D-03 0.280D-03-0.398D-02-0.272D-02 0.108D-01
Coeff: 0.183D-01-0.186D-02-0.958D-01-0.939D-01 0.475D+00 0.693D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=4.24D-08 MaxDP=1.32D-06 DE=-5.68D-12 OVMax= 6.35D-07

Cycle 17 Pass 1 IDiag 1:
RMSU= 2.91D-09 CP: 6.30D-01 1.06D+00 1.18D+00 1.58D+00 1.40D+00
CP: 1.23D+00 2.45D+00 1.46D+00 1.76D+00 1.50D+00
CP: 1.67D+00 1.52D+00
E= -608.981458119951 Delta-E= -0.000000000003 Rises=F Damp=F
DIIS: error= 3.07D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981458119951 IErMin=13 ErrMin= 3.07D-08
ErrMax= 3.07D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.26D-14 BMatP= 4.10D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.843D-05 0.375D-03 0.228D-03-0.246D-02-0.187D-02 0.581D-02
Coeff-Com: 0.112D-01 0.571D-02-0.412D-01-0.790D-01 0.901D-01 0.346D+00
Coeff-Com: 0.665D+00
Coeff: -0.843D-05 0.375D-03 0.228D-03-0.246D-02-0.187D-02 0.581D-02
Coeff: 0.112D-01 0.571D-02-0.412D-01-0.790D-01 0.901D-01 0.346D+00
Coeff: 0.665D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=6.24D-09 MaxDP=2.41D-07 DE=-3.41D-12 OVMax= 1.83D-07

SCF Done: E(RwB97XD) = -608.981458120 A.U. after 17 cycles
NFock= 17 Conv=0.62D-08 -V/T= 2.0045
KE= 6.062394251116D+02 PE=-2.845931996889D+03 EE= 9.132484706602D+02

Supporting Information file

Leave Link 502 at Fri Aug 21 19:01:46 2026, MaxMem= 805306368 cpu: 3669.8 elap: 611.9
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33574.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 19:01:46 2026, MaxMem= 805306368 cpu: 2.1 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 19:01:46 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 19:07:50 2026, MaxMem= 805306368 cpu: 2184.6 elap: 364.2
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.52170194D+00-4.32614017D-03-6.02178276D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000366109	0.001501681	-0.000429897
2	6	-0.001136658	-0.000996602	0.000615564
3	6	0.000466820	-0.001476295	0.000451283
4	6	0.001568849	0.000319341	-0.000848618
5	6	-0.001208745	0.000932572	-0.000661704
6	6	-0.001623330	0.000289293	0.000495399
7	6	0.001603371	-0.000239380	0.000889992
8	6	0.001262388	-0.000730216	-0.000437065
9	6	-0.001630788	-0.000351065	-0.000515084
10	6	-0.000769507	0.001119645	0.000907088
11	6	0.001256279	0.000760538	0.000424827
12	6	-0.000549147	-0.001561225	-0.000523419

```
    13        6        -0.000763250   -0.001143648   -0.000878908
    14        6        -0.000539752    0.001580204    0.000514140
    15        6         0.000850168   -0.000620293   -0.001862224
    16        6         0.000847192    0.000615450    0.001858625
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.001862224 RMS     0.001005218
 Leave Link  716 at Fri Aug 21 19:07:50 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.001473907 RMS     0.000466734
 Search for a local minimum.
 Step number   5 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .46673D-03 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
 DE= -7.00D-05 DEPred=-7.74D-05 R= 9.05D-01
 TightC=F SS=  1.41D+00  RLast= 4.80D-02 DXNew= 8.4853D-01 1.4389D-01
 Trust test= 9.05D-01 RLast= 4.80D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  0
    Eigenvalues ---    0.01289   0.01312   0.01576   0.01731   0.02623
    Eigenvalues ---    0.02656   0.02994   0.03291   0.03423   0.03926
    Eigenvalues ---    0.03940   0.04047   0.08431   0.08693   0.09336
    Eigenvalues ---    0.16413   0.24486   0.24573   0.24987   0.24990
    Eigenvalues ---    0.24997   0.24999   0.25000   0.25000   0.25002
    Eigenvalues ---    0.25076   0.28167   0.32373   0.35757   0.49754
    Eigenvalues ---    0.51323   0.56192   0.57382   0.57878   0.58161
    Eigenvalues ---    0.58184   0.78669   0.79213   0.79697   0.81247
    Eigenvalues ---    0.82170   0.87164
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:     5    4
 RFO step:  Lambda=-4.49650053D-05.
 NNeg= 0 NGDIIS= 2 SimSw=  2.50D-01 Rises=F DC= -7.00D-05 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.3553990294D-02 NUsed= 2 OKEnD=T EnDIS=F
 InvSVX:  RCond= 5.73D-04 Info=           0 Equed=N FErr=  1.89D-15 BErr=  4.78D-17
 DidBck=F Rises=F RFO-DIIS coefs:    1.16138   -0.16138
 Iteration  1 RMS(Cart)=  0.00317740 RMS(Int)=  0.00001082
 Iteration  2 RMS(Cart)=  0.00000975 RMS(Int)=  0.00000574
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000574
  ITry=  1  IFail=0  DXMaxC=  8.45D-03  DCOld=  1.00D+10  DXMaxT=  5.05D-01  DXLimC=
3.00D+00 Rises=F
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
```

Supporting Information file

		(Linear)	(Quad)	(Total)		
R1	2.30586	0.00077	-0.00017	0.00096	0.00079	2.30665
R2	2.55081	-0.00085	0.00042	-0.00064	-0.00023	2.55059
R3	2.55000	-0.00082	0.00040	-0.00061	-0.00021	2.54979
R4	2.30581	0.00077	-0.00017	0.00096	0.00080	2.30661
R5	2.30185	0.00082	-0.00015	0.00099	0.00084	2.30270
R6	2.55015	-0.00082	0.00040	-0.00062	-0.00022	2.54993
R7	2.55274	-0.00084	0.00036	-0.00070	-0.00035	2.55240
R8	2.30179	0.00082	-0.00015	0.00099	0.00085	2.30264
R9	2.29494	0.00061	-0.00009	0.00077	0.00068	2.29562
R10	2.55288	-0.00084	0.00035	-0.00071	-0.00036	2.55252
R11	2.61742	-0.00063	0.00036	-0.00063	-0.00027	2.61715
R12	2.29494	0.00061	-0.00009	0.00077	0.00068	2.29562
R13	2.63682	0.00082	0.00061	0.00204	0.00265	2.63947
R14	2.75077	-0.00056	-0.00047	-0.00230	-0.00277	2.74800
R15	2.61746	-0.00064	0.00036	-0.00064	-0.00029	2.61717
R16	2.75064	-0.00055	-0.00048	-0.00230	-0.00278	2.74786
R17	2.72034	0.00147	0.00167	0.00530	0.00697	2.72731
A1	2.61180	0.00004	-0.00003	0.00042	0.00039	2.61219
A2	2.64337	0.00005	-0.00005	0.00039	0.00034	2.64370
A3	2.61631	-0.00003	-0.00008	0.00015	0.00007	2.61638
A4	2.71908	-0.00015	-0.00026	-0.00056	-0.00083	2.71825
A5	2.63943	0.00010	-0.00000	0.00061	0.00060	2.64004
A6	2.77823	0.00009	0.00001	0.00029	0.00030	2.77853
A7	2.72244	-0.00021	-0.00031	-0.00078	-0.00109	2.72135
A8	2.77586	0.00013	0.00005	0.00046	0.00051	2.77637
A9	2.83000	0.00016	0.00022	0.00043	0.00064	2.83065
A10	2.31199	-0.00017	-0.00082	-0.00021	-0.00103	2.31096
A11	2.51275	0.00021	-0.00035	0.00166	0.00131	2.51406
A12	1.45794	-0.00003	0.00114	-0.00141	-0.00029	1.45765
A13	2.82872	0.00018	0.00024	0.00053	0.00076	2.82948
A14	2.31243	-0.00017	-0.00082	-0.00021	-0.00103	2.31140
A15	1.45772	-0.00004	0.00113	-0.00143	-0.00031	1.45741
A16	2.51256	0.00021	-0.00035	0.00168	0.00134	2.51390
A17	1.43103	-0.00025	0.00076	-0.00244	-0.00170	1.42933
A18	1.43133	-0.00025	0.00077	-0.00243	-0.00167	1.42966
A19	2.88230	-0.00005	0.00067	-0.00148	-0.00081	2.88148
A20	2.88369	-0.00006	0.00065	-0.00159	-0.00095	2.88274
A21	3.13795	-0.00028	0.00121	-0.00468	-0.00348	3.13448
A22	3.13784	-0.00028	0.00120	-0.00466	-0.00347	3.13437
D1	0.06338	-0.00001	0.00056	0.00011	0.00068	0.06405
D2	-0.05430	-0.00012	-0.00014	-0.00403	-0.00417	-0.05847
D3	-0.04205	-0.00013	-0.00039	-0.00425	-0.00465	-0.04670
D4	0.06167	0.00000	0.00063	0.00037	0.00100	0.06267
D5	0.06865	0.00017	0.00109	0.00436	0.00544	0.07409
D6	-0.03936	-0.00014	-0.00046	-0.00452	-0.00498	-0.04435
D7	0.06891	0.00002	0.00052	0.00664	0.00715	0.07605
D8	0.06683	0.00017	0.00111	0.00446	0.00556	0.07238

D9	0.07105	0.00001	0.00047	0.00654	0.00700	0.07805
D10	-0.58019	-0.00001	-0.00262	-0.00685	-0.00947	-0.58966
D11	2.60956	-0.00038	-0.00084	-0.00857	-0.00942	2.60015
D12	0.73727	0.00022	0.00013	0.00381	0.00394	0.74120
D13	-2.43201	0.00045	-0.00086	0.00492	0.00405	-2.42796
D14	-2.43283	0.00045	-0.00093	0.00489	0.00395	-2.42887
D15	0.68108	0.00068	-0.00192	0.00600	0.00407	0.68515
D16	2.41289	0.00017	0.00129	-0.00272	-0.00144	2.41146
D17	-0.69295	-0.00010	0.00263	-0.00399	-0.00136	-0.69431
D18	-0.58322	-0.00001	-0.00252	-0.00665	-0.00918	-0.59240
D19	2.60513	-0.00038	-0.00086	-0.00843	-0.00929	2.59584
D20	-0.69298	-0.00010	0.00262	-0.00399	-0.00136	-0.69434
D21	2.41392	0.00017	0.00137	-0.00268	-0.00131	2.41261
D22	0.66169	0.00052	-0.00212	0.00514	0.00301	0.66470

Item	Value	Threshold	Converged?
Maximum Force	0.001474	0.000450	NO
RMS Force	0.000467	0.000300	NO
Maximum Displacement	0.008451	0.001800	NO
RMS Displacement	0.003181	0.001200	NO

Predicted change in Energy=-2.250658D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 19:07:50 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.623129	-0.673877	0.015098
2	6	0	3.008357	-1.727593	0.055919
3	6	0	3.621328	0.675516	-0.014229
4	6	0	1.854860	-2.427570	0.063431
5	6	0	3.008171	1.730145	-0.055146
6	6	0	0.645400	-2.576017	0.063048
7	6	0	1.853081	2.427633	-0.063601
8	6	0	-0.666017	-2.255591	0.020331
9	6	0	0.643787	2.577171	-0.063619
10	6	0	-1.731218	-1.674031	-0.033082
11	6	0	-0.667302	2.255070	-0.021380
12	6	0	-2.684730	-0.678697	-0.167900
13	6	0	-1.732514	1.673504	0.031742
14	6	0	-2.684933	0.677220	0.167354
15	6	0	-4.046190	-0.403359	-0.598308
16	6	0	-4.045210	0.400475	0.600342

Supporting Information file

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220627	0.000000			
3	C	1.349712	2.481045	0.000000		
4	C	2.490894	1.349289	3.571496	0.000000	
5	C	2.482424	3.459522	1.220606	4.316339	0.000000
6	C	3.533738	2.510665	4.408467	1.218535	4.913215
7	C	3.571921	4.314493	2.489789	4.856864	1.349367
8	C	4.571502	3.712287	5.193641	2.527104	5.421388
9	C	4.410441	4.912889	3.533339	5.150755	2.511541
10	C	5.447170	4.740713	5.845551	3.665663	5.835298
11	C	5.194984	5.420152	4.570272	5.319362	3.712922
12	C	6.310515	5.793230	6.451656	4.870312	6.182584
13	C	5.847511	5.834715	5.446257	5.448767	4.741819
14	C	6.452929	6.181350	6.308874	5.500930	5.793927
15	C	7.698565	7.207513	7.765047	6.273572	7.389917
16	C	7.765318	7.387684	7.696048	6.564825	7.207487

		6	7	8	9	10
6	C	0.000000				
7	C	5.148887	0.000000			
8	C	1.350672	5.318410	0.000000		
9	C	5.154745	1.218505	5.007817	0.000000	
10	C	2.543842	5.447180	1.214791	4.869733	0.000000
11	C	5.006967	2.526637	4.510854	1.350736	4.070613
12	C	3.839651	5.500172	2.568506	4.657315	1.384936
13	C	4.869690	3.665282	4.071282	2.544113	3.348163
14	C	4.656774	4.869379	3.563568	3.839731	2.545216
15	C	5.212375	6.565198	3.903722	5.582592	2.700589
16	C	5.581220	6.272163	4.337054	5.212058	3.171649

		11	12	13	14	15
11	C	0.000000				
12	C	3.563492	0.000000			
13	C	1.214791	2.545471	0.000000		
14	C	2.568281	1.396749	1.384946	0.000000	
15	C	4.337854	1.454179	3.172290	1.899187	0.000000
16	C	3.903374	1.898872	2.700458	1.454105	1.443230

		16
16	C	0.000000

Stoichiometry C16
Framework group C1[X(C16)]
Deg. of freedom 42
Full point group C1 NOp 1
RotChk: IX=0 Diff= 4.76D-05
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Supporting Information file

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.622934	-0.674962	0.013312
2	6	0	3.007857	-1.728602	0.051451
3	6	0	3.621523	0.674501	-0.012568
4	6	0	1.854157	-2.428261	0.057195
5	6	0	3.008671	1.729409	-0.050779
6	6	0	0.644655	-2.576356	0.056455
7	6	0	1.853783	2.427250	-0.057431
8	6	0	-0.666670	-2.255443	0.014580
9	6	0	0.644532	2.577139	-0.057045
10	6	0	-1.731703	-1.673439	-0.037328
11	6	0	-0.666649	2.255311	-0.015606
12	6	0	-2.684929	-0.677488	-0.169586
13	6	0	-1.732028	1.673919	0.036049
14	6	0	-2.684733	0.677568	0.169131
15	6	0	-4.046317	-0.400657	-0.599265
16	6	0	-4.045084	0.400111	0.601435

Rotational constants (GHZ): 0.8461707 0.3940196 0.2716098
Leave Link 202 at Fri Aug 21 19:07:50 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 717.4044189663 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074872213 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.3969317449 Hartrees.
Leave Link 301 at Fri Aug 21 19:07:50 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

```
      NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33574.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  4.03D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=          32
 NSgBfM=   562   562   562   562   562 MxSgAt=    16 MxSgA2=    16.
 Leave Link  302 at Fri Aug 21 19:07:51 2026, MaxMem=    805306368 cpu:                3.4 elap:
0.6
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Aug 21 19:07:51 2026, MaxMem=    805306368 cpu:                0.5 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca.chk"
 B after Tr=     0.000000    0.000000    0.000000
      Rot=    1.000000    0.000016   -0.000000    0.000006 Ang=   0.00 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Leave Link  401 at Fri Aug 21 19:07:51 2026, MaxMem=    805306368 cpu:                1.5 elap:
0.3
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804634234 LenY=   804301882
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
      NFxFlg=          0 DoJE=T BraDBF=F KetDBF=F FulRan=T
      wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=          0 NGrid=          0
      NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -608.981418093463
 DIIS: error= 5.62D-04 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -608.981418093463     IErMin= 1 ErrMin= 5.62D-04
```

ErrMax= 5.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-04 BMatP= 1.59D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 5.62D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.960 Goal=   None   Shift=   0.000
RMSDP=3.18D-05 MaxDP=8.52D-04   OVMax= 1.56D-03

Cycle   2 Pass 1 IDiag 1:
RMSU= 3.17D-05   CP: 1.00D+00
E= -608.981488559122   Delta-E=   -0.000070465659 Rises=F Damp=F
DIIS: error= 5.27D-05 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -608.981488559122   IErMin= 2 ErrMin= 5.27D-05
ErrMax= 5.27D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-06 BMatP= 1.59D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.276D-01 0.103D+01
Coeff: -0.276D-01 0.103D+01
Gap=   0.246 Goal=   None   Shift=   0.000
RMSDP=1.10D-05 MaxDP=4.06D-04 DE=-7.05D-05 OVMax= 8.97D-04

Cycle   3 Pass 1 IDiag 1:
RMSU= 1.02D-05   CP: 1.00D+00 1.11D+00
E= -608.981491935081   Delta-E=   -0.000003375959 Rises=F Damp=F
DIIS: error= 3.02D-05 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -608.981491935081   IErMin= 3 ErrMin= 3.02D-05
ErrMax= 3.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-07 BMatP= 1.49D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.120D-01 0.228D+00 0.784D+00
Coeff: -0.120D-01 0.228D+00 0.784D+00
Gap=   0.246 Goal=   None   Shift=   0.000
RMSDP=4.70D-06 MaxDP=1.51D-04 DE=-3.38D-06 OVMax= 3.72D-04

Cycle   4 Pass 1 IDiag 1:
RMSU= 4.56D-06   CP: 1.00D+00 1.13D+00 1.07D+00
E= -608.981492491209   Delta-E=   -0.000000556128 Rises=F Damp=F
DIIS: error= 2.54D-05 at cycle   4 NSaved=   4.
NSaved= 4 IEnMin= 4 EnMin= -608.981492491209   IErMin= 4 ErrMin= 2.54D-05
ErrMax= 2.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-07 BMatP= 3.50D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.674D-04-0.993D-01 0.418D+00 0.682D+00
Coeff: -0.674D-04-0.993D-01 0.418D+00 0.682D+00
Gap=   0.246 Goal=   None   Shift=   0.000
RMSDP=2.71D-06 MaxDP=1.07D-04 DE=-5.56D-07 OVMax= 3.29D-04

Cycle   5 Pass 1 IDiag 1:
RMSU= 1.39D-06   CP: 1.00D+00 1.15D+00 1.29D+00 1.01D+00
E= -608.981492831449   Delta-E=   -0.000000340240 Rises=F Damp=F
DIIS: error= 1.31D-05 at cycle   5 NSaved=   5.

NSaved= 5 IEnMin= 5 EnMin= -608.981492831449 IErMin= 5 ErrMin= 1.31D-05
ErrMax= 1.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-08 BMatP= 2.02D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.243D-02-0.975D-01 0.671D-01 0.327D+00 0.701D+00
Coeff: 0.243D-02-0.975D-01 0.671D-01 0.327D+00 0.701D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.43D-06 MaxDP=3.96D-05 DE=-3.40D-07 OVMax= 1.84D-04

Cycle 6 Pass 1 IDiag 1:
RMSU= 6.41D-07 CP: 1.00D+00 1.16D+00 1.40D+00 1.09D+00 1.21D+00
E= -608.981492909410 Delta-E= -0.000000077961 Rises=F Damp=F
DIIS: error= 5.93D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981492909410 IErMin= 6 ErrMin= 5.93D-06
ErrMax= 5.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.94D-09 BMatP= 3.13D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.138D-02-0.324D-01-0.522D-01 0.291D-01 0.359D+00 0.695D+00
Coeff: 0.138D-02-0.324D-01-0.522D-01 0.291D-01 0.359D+00 0.695D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=7.47D-07 MaxDP=3.05D-05 DE=-7.80D-08 OVMax= 7.98D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.91D-07 CP: 1.00D+00 1.16D+00 1.43D+00 1.20D+00 1.33D+00
CP: 1.26D+00
E= -608.981492935472 Delta-E= -0.000000026062 Rises=F Damp=F
DIIS: error= 3.13D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981492935472 IErMin= 7 ErrMin= 3.13D-06
ErrMax= 3.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-09 BMatP= 7.94D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.497D-03 0.270D-01-0.365D-01-0.108D+00-0.186D+00 0.165D+00
Coeff-Com: 0.114D+01
Coeff: -0.497D-03 0.270D-01-0.365D-01-0.108D+00-0.186D+00 0.165D+00
Coeff: 0.114D+01
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.96D-07 MaxDP=2.20D-05 DE=-2.61D-08 OVMax= 1.10D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.98D-07 CP: 1.00D+00 1.16D+00 1.45D+00 1.23D+00 1.53D+00
CP: 1.78D+00 1.62D+00
E= -608.981492944810 Delta-E= -0.000000009338 Rises=F Damp=F
DIIS: error= 8.22D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981492944810 IErMin= 8 ErrMin= 8.22D-07
ErrMax= 8.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-10 BMatP= 1.26D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.294D-03 0.114D-01-0.541D-02-0.332D-01-0.933D-01-0.278D-01
Coeff-Com: 0.346D+00 0.803D+00
Coeff: -0.294D-03 0.114D-01-0.541D-02-0.332D-01-0.933D-01-0.278D-01
Coeff: 0.346D+00 0.803D+00
Gap= 0.246 Goal= None Shift= 0.000

RMSDP=1.79D-07 MaxDP=5.03D-06 DE=-9.34D-09 OVMax= 2.49D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.65D-08 CP: 1.00D+00 1.16D+00 1.45D+00 1.22D+00 1.57D+00
CP: 1.92D+00 1.85D+00 1.40D+00
E= -608.981492945459 Delta-E= -0.000000000649 Rises=F Damp=F
DIIS: error= 7.10D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981492945459 IErMin= 9 ErrMin= 7.10D-07
ErrMax= 7.10D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.20D-11 BMatP= 1.53D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.134D-04-0.915D-03 0.394D-02 0.953D-02 0.210D-02-0.493D-01
Coeff-Com: -0.822D-01 0.291D+00 0.825D+00
Coeff: -0.134D-04-0.915D-03 0.394D-02 0.953D-02 0.210D-02-0.493D-01
Coeff: -0.822D-01 0.291D+00 0.825D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=1.14D-07 MaxDP=3.10D-06 DE=-6.49D-10 OVMax= 1.19D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.64D-08 CP: 1.00D+00 1.16D+00 1.44D+00 1.22D+00 1.57D+00
CP: 1.98D+00 2.00D+00 1.67D+00 1.31D+00
E= -608.981492945609 Delta-E= -0.000000000151 Rises=F Damp=F
DIIS: error= 5.30D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981492945609 IErMin=10 ErrMin= 5.30D-07
ErrMax= 5.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-11 BMatP= 4.20D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.668D-04-0.334D-02 0.318D-02 0.141D-01 0.250D-01-0.224D-01
Coeff-Com: -0.128D+00-0.532D-01 0.474D+00 0.691D+00
Coeff: 0.668D-04-0.334D-02 0.318D-02 0.141D-01 0.250D-01-0.224D-01
Coeff: -0.128D+00-0.532D-01 0.474D+00 0.691D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=5.76D-08 MaxDP=1.55D-06 DE=-1.51D-10 OVMax= 4.81D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.28D-08 CP: 1.00D+00 1.16D+00 1.44D+00 1.22D+00 1.57D+00
CP: 2.00D+00 2.07D+00 1.82D+00 1.55D+00 1.07D+00
E= -608.981492945658 Delta-E= -0.000000000048 Rises=F Damp=F
DIIS: error= 2.06D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981492945658 IErMin=11 ErrMin= 2.06D-07
ErrMax= 2.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.30D-12 BMatP= 1.63D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.279D-04-0.108D-02 0.214D-03 0.368D-02 0.916D-02 0.592D-03
Coeff-Com: -0.308D-01-0.768D-01 0.180D-02 0.274D+00 0.819D+00
Coeff: 0.279D-04-0.108D-02 0.214D-03 0.368D-02 0.916D-02 0.592D-03
Coeff: -0.308D-01-0.768D-01 0.180D-02 0.274D+00 0.819D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=2.26D-08 MaxDP=6.34D-07 DE=-4.84D-11 OVMax= 2.60D-06

Cycle 12 Pass 1 IDiag 1:

Supporting Information file

RMSU= 5.91D-09 CP: 1.00D+00 1.16D+00 1.44D+00 1.22D+00 1.57D+00
CP: 2.01D+00 2.09D+00 1.87D+00 1.66D+00 1.31D+00
CP: 1.33D+00
E= -608.981492945667 Delta-E= -0.000000000009 Rises=F Damp=F
DIIS: error= 4.95D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981492945667 IErMin=12 ErrMin= 4.95D-08
ErrMax= 4.95D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.19D-13 BMatP= 2.30D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.100D-04 0.590D-03-0.848D-03-0.257D-02-0.392D-02 0.564D-02
Coeff-Com: 0.257D-01-0.924D-02-0.125D+00-0.853D-01 0.197D+00 0.997D+00
Coeff: -0.100D-04 0.590D-03-0.848D-03-0.257D-02-0.392D-02 0.564D-02
Coeff: 0.257D-01-0.924D-02-0.125D+00-0.853D-01 0.197D+00 0.997D+00
Gap= 0.246 Goal= None Shift= 0.000
RMSDP=9.06D-09 MaxDP=3.03D-07 DE=-8.87D-12 OVMax= 1.22D-06

SCF Done: E(RwB97XD) = -608.981492946 A.U. after 12 cycles
NFock= 12 Conv=0.91D-08 -V/T= 2.0045
KE= 6.062281313365D+02 PE=-2.845787776720D+03 EE= 9.131812206933D+02
Leave Link 502 at Fri Aug 21 19:16:15 2026, MaxMem= 805306368 cpu: 3020.1 elap: 503.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33574.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 19:16:15 2026, MaxMem= 805306368 cpu: 2.4 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 19:16:15 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 2804.1 elap: 467.4
(Enter /home/user/gauss16/g16/l716.exe)

Supporting Information file

Dipole = 1.52052001D+00-3.98676189D-03-6.17266069D-04
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 0.000021466 0.000902890 -0.000355004
2 6 -0.000774787 -0.000403534 0.000545450
3 6 0.000115466 -0.000878709 0.000372289
4 6 0.000807076 0.000262011 -0.000733817
5 6 -0.000843303 0.000344761 -0.000584743
6 6 -0.000792127 0.000337263 0.000595476
7 6 0.000838677 -0.000190302 0.000772042
8 6 0.000626878 -0.000329529 -0.000673302
9 6 -0.000798538 -0.000391532 -0.000615185
10 6 -0.000145826 0.000649434 0.000831218
11 6 0.000622351 0.000354605 0.000662792
12 6 -0.000515214 -0.001110012 -0.000528565
13 6 -0.000138688 -0.000666860 -0.000808893
14 6 -0.000511674 0.001120127 0.000523333
15 6 0.000748131 -0.000316335 -0.000845076
16 6 0.000740113 0.000315722 0.000841985

Cartesian Forces: Max 0.001120127 RMS 0.000635984
Leave Link 716 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000864453 RMS 0.000315437
Search for a local minimum.
Step number 6 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .31544D-03 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 1 2 3 4 5
6
DE= -3.48D-05 DEPred=-2.25D-05 R= 1.55D+00
TightC=F SS= 1.41D+00 RLast= 2.78D-02 DXNew= 8.4853D-01 8.3335D-02
Trust test= 1.55D+00 RLast= 2.78D-02 DXMaxT set to 5.05D-01
ITU= 1 1 1 1 1 0
Eigenvalues --- 0.00976 0.01290 0.01453 0.01732 0.02205
Eigenvalues --- 0.02625 0.02941 0.03354 0.03422 0.03926
Eigenvalues --- 0.04047 0.04309 0.08292 0.08430 0.09348

```
    Eigenvalues ---    0.14864   0.24488   0.24582   0.24990   0.24995
    Eigenvalues ---    0.24997   0.24999   0.25000   0.25000   0.25041
    Eigenvalues ---    0.25097   0.28163   0.32013   0.34279   0.42598
    Eigenvalues ---    0.51322   0.53498   0.57382   0.57897   0.58160
    Eigenvalues ---    0.58184   0.78669   0.79249   0.79697   0.81363
    Eigenvalues ---    0.82171   0.99189
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:     6    5    4
 RFO step:  Lambda=-6.98031378D-05.
 NNeg= 0 NGDIIS= 3 SimSw=  2.50D-01 Rises=F DC= -3.48D-05 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.8686524034D-02 NUsed= 3 OKEnD=T EnDIS=F
 InvSVX:  RCond= 6.75D-05 Info=           0 Equed=N FErr=  3.60D-14 BErr=  3.80D-17
 DidBck=F Rises=F RFO-DIIS coefs:    2.92281   -1.56131   -0.36151
 Iteration  1 RMS(Cart)=  0.00353550 RMS(Int)=  0.00003533
 Iteration  2 RMS(Cart)=  0.00003195 RMS(Int)=  0.00002444
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00002444
  ITry=  1  IFail=0  DXMaxC=  1.07D-02  DCOld=  1.00D+10  DXMaxT=  5.05D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)    (Quad)   (Total)
   R1        2.30665   0.00007   0.00115  -0.00046   0.00070   2.30735
   R2        2.55059  -0.00086   0.00050  -0.00150  -0.00100   2.54958
   R3        2.54979  -0.00081   0.00049  -0.00138  -0.00088   2.54890
   R4        2.30661   0.00007   0.00116  -0.00046   0.00071   2.30732
   R5        2.30270   0.00007   0.00129  -0.00053   0.00076   2.30346
   R6        2.54993  -0.00082   0.00048  -0.00139  -0.00091   2.54903
   R7        2.55240  -0.00074   0.00014  -0.00112  -0.00098   2.55142
   R8        2.30264   0.00007   0.00130  -0.00053   0.00077   2.30341
   R9        2.29562  -0.00005   0.00111  -0.00063   0.00048   2.29610
  R10        2.55252  -0.00075   0.00011  -0.00112  -0.00101   2.55151
  R11        2.61715  -0.00053   0.00029  -0.00076  -0.00047   2.61668
  R12        2.29562  -0.00005   0.00111  -0.00063   0.00048   2.29610
  R13        2.63947   0.00051   0.00645   0.00014   0.00658   2.64605
  R14        2.74800  -0.00057  -0.00639  -0.00178  -0.00817   2.73983
  R15        2.61717  -0.00053   0.00024  -0.00076  -0.00052   2.61665
  R16        2.74786  -0.00056  -0.00643  -0.00177  -0.00819   2.73967
  R17        2.72731   0.00068   0.01713  -0.00149   0.01563   2.74294
   A1        2.61219   0.00002   0.00068  -0.00005   0.00062   2.61281
   A2        2.64370   0.00005   0.00054   0.00016   0.00069   2.64440
   A3        2.61638  -0.00005  -0.00006  -0.00026  -0.00033   2.61605
   A4        2.71825  -0.00010  -0.00218  -0.00001  -0.00221   2.71605
   A5        2.64004   0.00010   0.00115   0.00034   0.00148   2.64151
   A6        2.77853   0.00010   0.00061   0.00051   0.00109   2.77962
   A7        2.72135  -0.00015  -0.00280  -0.00017  -0.00299   2.71836
   A8        2.77637   0.00014   0.00110   0.00061   0.00168   2.77805
   A9        2.83065   0.00007   0.00174  -0.00016   0.00152   2.83216
  A10        2.31096  -0.00016  -0.00381   0.00045  -0.00338   2.30759
  A11        2.51406   0.00021   0.00174   0.00171   0.00347   2.51753
```

A12	1.45765	-0.00004	0.00199	-0.00210	-0.00011	1.45754
A13	2.82948	0.00008	0.00201	-0.00009	0.00185	2.83133
A14	2.31140	-0.00016	-0.00380	0.00042	-0.00340	2.30800
A15	1.45741	-0.00004	0.00193	-0.00207	-0.00015	1.45725
A16	2.51390	0.00021	0.00181	0.00171	0.00353	2.51744
A17	1.42933	-0.00010	-0.00158	-0.00151	-0.00312	1.42621
A18	1.42966	-0.00010	-0.00149	-0.00155	-0.00307	1.42659
A19	2.88148	-0.00000	-0.00006	-0.00145	-0.00155	2.87994
A20	2.88274	-0.00001	-0.00036	-0.00150	-0.00190	2.88084
A21	3.13448	0.00005	-0.00397	0.01199	0.00797	3.14244
A22	3.13437	0.00005	-0.00399	0.01204	0.00799	3.14236
D1	0.06405	0.00010	0.00256	0.00470	0.00729	0.07134
D2	-0.05847	0.00003	-0.00834	0.00522	-0.00309	-0.06156
D3	-0.04670	-0.00009	-0.00981	-0.00047	-0.01028	-0.05697
D4	0.06267	0.00010	0.00333	0.00480	0.00816	0.07082
D5	0.07409	0.00010	0.01291	0.00285	0.01575	0.08984
D6	-0.04435	-0.00010	-0.01062	-0.00067	-0.01129	-0.05563
D7	0.07605	-0.00010	0.01491	-0.01079	0.00408	0.08014
D8	0.07238	0.00011	0.01317	0.00297	0.01612	0.08851
D9	0.07805	-0.00010	0.01451	-0.01078	0.00368	0.08173
D10	-0.58966	-0.00010	-0.02408	-0.00186	-0.02596	-0.61563
D11	2.60015	-0.00029	-0.01998	-0.00494	-0.02494	2.57521
D12	0.74120	0.00012	0.00786	0.00091	0.00875	0.74996
D13	-2.42796	0.00024	0.00585	0.00253	0.00837	-2.41959
D14	-2.42887	0.00024	0.00551	0.00279	0.00828	-2.42059
D15	0.68515	0.00036	0.00351	0.00441	0.00790	0.69305
D16	2.41146	0.00014	0.00012	-0.00210	-0.00198	2.40948
D17	-0.69431	0.00000	0.00327	-0.00439	-0.00110	-0.69541
D18	-0.59240	-0.00010	-0.02331	-0.00194	-0.02527	-0.61768
D19	2.59584	-0.00029	-0.01978	-0.00459	-0.02439	2.57145
D20	-0.69434	0.00000	0.00326	-0.00439	-0.00111	-0.69544
D21	2.41261	0.00014	0.00055	-0.00242	-0.00187	2.41074
D22	0.66470	0.00032	0.00104	0.00466	0.00570	0.67039

Item	Value	Threshold	Converged?
Maximum Force	0.000864	0.000450	NO
RMS Force	0.000315	0.000300	NO
Maximum Displacement	0.010717	0.001800	NO
RMS Displacement	0.003554	0.001200	NO

Predicted change in Energy=-3.505190D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Atomic Atomic Coordinates (Angstroms)

Supporting Information file

Number	Number	Type	X	Y	Z
1	6	0	3.621413	-0.673513	0.016004
2	6	0	3.006863	-1.727693	0.059215
3	6	0	3.619958	0.675306	-0.015233
4	6	0	1.854626	-2.428861	0.064763
5	6	0	3.006567	1.730131	-0.058679
6	6	0	0.644621	-2.576164	0.064452
7	6	0	1.853000	2.429231	-0.064873
8	6	0	-0.666262	-2.256528	0.016222
9	6	0	0.643092	2.577125	-0.064859
10	6	0	-1.731138	-1.673437	-0.032526
11	6	0	-0.667501	2.256040	-0.017052
12	6	0	-2.685711	-0.679890	-0.170407
13	6	0	-1.732278	1.672747	0.031426
14	6	0	-2.685895	0.678374	0.169840
15	6	0	-4.041135	-0.402545	-0.603979
16	6	0	-4.040220	0.399675	0.605688

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220997	0.000000			
3	C	1.349182	2.481095	0.000000		
4	C	2.491016	1.348821	3.571925	0.000000	
5	C	2.482161	3.459834	1.220980	4.317340	0.000000
6	C	3.533231	2.510004	4.408065	1.218938	4.913057
7	C	3.572234	4.315880	2.490152	4.859822	1.348887
8	C	4.570569	3.711249	5.193103	2.527238	5.421138
9	C	4.409488	4.912664	3.532861	5.152137	2.510667
10	C	5.445366	4.739200	5.843896	3.665765	5.833593
11	C	5.194051	5.420046	4.569576	5.321289	3.711750
12	C	6.309882	5.792756	6.451518	4.871228	6.182452
13	C	5.845271	5.832943	5.444584	5.448869	4.740049
14	C	6.452395	6.181334	6.308568	5.502934	5.793318
15	C	7.692363	7.202092	7.758913	6.270022	7.383479
16	C	7.758872	7.381444	7.690243	6.560673	7.201993

		6	7	8	9	10
6	C	0.000000				
7	C	5.150814	0.000000			
8	C	1.350151	5.320676	0.000000		
9	C	5.154912	1.218913	5.008511	0.000000	
10	C	2.543334	5.447842	1.215043	4.868809	0.000000
11	C	5.007845	2.526897	4.512691	1.350199	4.070916
12	C	3.839548	5.502515	2.568811	4.658349	1.384687
13	C	4.868674	3.665482	4.071341	2.543533	3.346795
14	C	4.657839	4.870539	3.565973	3.839596	2.546278
15	C	5.208429	6.561282	3.900214	5.577730	2.697743

```
  16  C    5.576405   6.268875   4.334337   5.208103   3.168118
             11         12         13         14         15
  11  C    0.000000
  12  C    3.566002   0.000000
  13  C    1.215044   2.546501   0.000000
  14  C    2.568632   1.400232   1.384673   0.000000
  15  C    4.335200   1.449855   3.168816   1.898383   0.000000
  16  C    3.899888   1.898020   2.697607   1.449770   1.451500
             16
  16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 6.92D-05
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.621195   -0.674726    0.014197
     2          6           0        3.006304   -1.728815    0.054688
     3          6           0        3.620176    0.674170   -0.013546
     4          6           0        1.853840   -2.429622    0.058440
     5          6           0        3.007126    1.729303   -0.054250
     6          6           0        0.643787   -2.576531    0.057768
     7          6           0        1.853786    2.428791   -0.058613
     8          6           0       -0.666993   -2.256346    0.010389
     9          6           0        0.643927    2.577076   -0.058196
    10          6           0       -1.731680   -1.672786   -0.036830
    11          6           0       -0.666770    2.256293   -0.011198
    12          6           0       -2.685934   -0.678576   -0.172121
    13          6           0       -1.731735    1.673221    0.035788
    14          6           0       -2.685672    0.678803    0.171643
    15          6           0       -4.041275   -0.399670   -0.604951
    16          6           0       -4.040080    0.399414    0.606791
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8455567           0.3943858           0.2717769
 Leave Link  202 at Fri Aug 21 19:24:03 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
```

48 alpha electrons 48 beta electrons
nuclear repulsion energy 717.4564325114 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074870116 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.4489454998 Hartrees.
Leave Link 301 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14214 LenP2D= 33578.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.18D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 564 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 19:24:03 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 19:24:04 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 0.000000 -0.000000
Rot= 1.000000 -0.000017 0.000000 0.000017 Ang= -0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 19:24:04 2026, MaxMem= 805306368 cpu: 1.9 elap: 0.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981346938310
DIIS: error= 5.51D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981346938310 IErMin= 1 ErrMin= 5.51D-04
ErrMax= 5.51D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-04 BMatP= 2.40D-04
IDIUse=3 WtCom= 9.94D-01 WtEn= 5.51D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=1.17D-04 MaxDP=2.84D-03 OVMax= 3.31D-03

Cycle 2 Pass 1 IDiag 1:
RMSU= 1.14D-04 CP: 9.97D-01
E= -608.981504442509 Delta-E= -0.000157504199 Rises=F Damp=F
DIIS: error= 1.00D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981504442509 IErMin= 2 ErrMin= 1.00D-04
ErrMax= 1.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.13D-06 BMatP= 2.40D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.00D-03
Coeff-Com: -0.309D-01 0.103D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.309D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.09D-05 MaxDP=9.02D-04 DE=-1.58D-04 OVMax= 2.24D-03

Cycle 3 Pass 1 IDiag 1:
RMSU= 1.78D-05 CP: 9.96D-01 1.09D+00
E= -608.981518282894 Delta-E= -0.000013840385 Rises=F Damp=F
DIIS: error= 8.16D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981518282894 IErMin= 3 ErrMin= 8.16D-05
ErrMax= 8.16D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-06 BMatP= 5.13D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.236D-01 0.345D+00 0.679D+00

Coeff: -0.236D-01 0.345D+00 0.679D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=8.83D-06 MaxDP=3.25D-04 DE=-1.38D-05 OVMax= 9.23D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 8.29D-06 CP: 9.97D-01 1.10D+00 9.09D-01
E= -608.981521772383 Delta-E= -0.000003489489 Rises=F Damp=F
DIIS: error= 5.60D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981521772383 IErMin= 4 ErrMin= 5.60D-05
ErrMax= 5.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.88D-07 BMatP= 2.16D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.289D-03-0.162D+00 0.334D+00 0.828D+00
Coeff: 0.289D-03-0.162D+00 0.334D+00 0.828D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=6.02D-06 MaxDP=2.81D-04 DE=-3.49D-06 OVMax= 8.85D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.21D-06 CP: 9.97D-01 1.10D+00 1.18D+00 1.18D+00
E= -608.981523731732 Delta-E= -0.000001959349 Rises=F Damp=F
DIIS: error= 2.76D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981523731732 IErMin= 5 ErrMin= 2.76D-05
ErrMax= 2.76D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-07 BMatP= 7.88D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.411D-02-0.141D+00 0.614D-01 0.409D+00 0.667D+00
Coeff: 0.411D-02-0.141D+00 0.614D-01 0.409D+00 0.667D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.74D-06 MaxDP=1.11D-04 DE=-1.96D-06 OVMax= 4.60D-04

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.47D-06 CP: 9.97D-01 1.10D+00 1.30D+00 1.30D+00 1.17D+00
E= -608.981524145941 Delta-E= -0.000000414209 Rises=F Damp=F
DIIS: error= 1.19D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981524145941 IErMin= 6 ErrMin= 1.19D-05
ErrMax= 1.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.88D-08 BMatP= 1.51D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.233D-02-0.285D-01-0.754D-01-0.369D-01 0.354D+00 0.784D+00
Coeff: 0.233D-02-0.285D-01-0.754D-01-0.369D-01 0.354D+00 0.784D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.04D-06 MaxDP=1.05D-04 DE=-4.14D-07 OVMax= 2.56D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 8.65D-07 CP: 9.97D-01 1.10D+00 1.33D+00 1.48D+00 1.40D+00
CP: 1.28D+00
E= -608.981524300102 Delta-E= -0.000000154161 Rises=F Damp=F
DIIS: error= 4.90D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981524300102 IErMin= 7 ErrMin= 4.90D-06
ErrMax= 4.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.88D-09 BMatP= 3.88D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.605D-03 0.314D-01-0.300D-01-0.101D+00-0.114D+00 0.114D+00
Coeff-Com: 0.110D+01
Coeff: -0.605D-03 0.314D-01-0.300D-01-0.101D+00-0.114D+00 0.114D+00
Coeff: 0.110D+01
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=1.13D-06 MaxDP=4.58D-05 DE=-1.54D-07 OVMax= 1.99D-04

Cycle   8 Pass 1 IDiag 1:
RMSU= 3.61D-07   CP: 9.97D-01 1.10D+00 1.35D+00 1.55D+00 1.58D+00
               CP: 1.58D+00 1.38D+00
E= -608.981524331009   Delta-E=   -0.000000030907 Rises=F Damp=F
DIIS: error= 3.27D-06 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -608.981524331009   IErMin= 8 ErrMin= 3.27D-06
ErrMax= 3.27D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.42D-10 BMatP= 3.88D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.451D-03 0.149D-01-0.601D-02-0.330D-01-0.779D-01-0.300D-01
Coeff-Com: 0.433D+00 0.700D+00
Coeff: -0.451D-03 0.149D-01-0.601D-02-0.330D-01-0.779D-01-0.300D-01
Coeff: 0.433D+00 0.700D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=2.54D-07 MaxDP=8.84D-06 DE=-3.09D-08 OVMax= 4.69D-05

Cycle   9 Pass 1 IDiag 1:
RMSU= 1.28D-07   CP: 9.97D-01 1.10D+00 1.35D+00 1.56D+00 1.59D+00
               CP: 1.67D+00 1.50D+00 1.27D+00
E= -608.981524333915   Delta-E=   -0.000000002907 Rises=F Damp=F
DIIS: error= 1.92D-06 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -608.981524333915   IErMin= 9 ErrMin= 1.92D-06
ErrMax= 1.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-10 BMatP= 9.42D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.818D-04-0.928D-03 0.526D-02 0.144D-01-0.115D-01-0.603D-01
Coeff-Com: -0.825D-01 0.421D+00 0.715D+00
Coeff: -0.818D-04-0.928D-03 0.526D-02 0.144D-01-0.115D-01-0.603D-01
Coeff: -0.825D-01 0.421D+00 0.715D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=1.73D-07 MaxDP=5.17D-06 DE=-2.91D-09 OVMax= 2.63D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 6.71D-08   CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.60D+00
               CP: 1.70D+00 1.59D+00 1.54D+00 1.28D+00
E= -608.981524335260   Delta-E=   -0.000000001344 Rises=F Damp=F
DIIS: error= 7.67D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981524335260   IErMin=10 ErrMin= 7.67D-07
ErrMax= 7.67D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.22D-11 BMatP= 4.17D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.111D-03-0.489D-02 0.262D-02 0.158D-01 0.210D-01-0.157D-01
Coeff-Com: -0.155D+00-0.650D-01 0.230D+00 0.972D+00
Coeff: 0.111D-03-0.489D-02 0.262D-02 0.158D-01 0.210D-01-0.157D-01

Coeff: -0.155D+00-0.650D-01 0.230D+00 0.972D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.26D-07 MaxDP=4.13D-06 DE=-1.34D-09 OVMax= 1.70D-05

Cycle 11 Pass 1 IDiag 1:
RMSU= 3.52D-08 CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.60D+00
CP: 1.72D+00 1.64D+00 1.72D+00 1.66D+00 1.57D+00
E= -608.981524335633 Delta-E= -0.000000000373 Rises=F Damp=F
DIIS: error= 3.59D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981524335633 IErMin=11 ErrMin= 3.59D-07
ErrMax= 3.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.54D-12 BMatP= 6.22D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.418D-04-0.112D-02-0.324D-03 0.215D-02 0.726D-02 0.557D-02
Coeff-Com: -0.268D-01-0.902D-01-0.487D-01 0.250D+00 0.902D+00
Coeff: 0.418D-04-0.112D-02-0.324D-03 0.215D-02 0.726D-02 0.557D-02
Coeff: -0.268D-01-0.902D-01-0.487D-01 0.250D+00 0.902D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.16D-08 MaxDP=1.13D-06 DE=-3.73D-10 OVMax= 5.96D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.44D-08 CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.61D+00
CP: 1.73D+00 1.65D+00 1.76D+00 1.80D+00 1.84D+00
CP: 1.38D+00
E= -608.981524335692 Delta-E= -0.000000000059 Rises=F Damp=F
DIIS: error= 1.84D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981524335692 IErMin=12 ErrMin= 1.84D-07
ErrMax= 1.84D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.91D-12 BMatP= 9.54D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.132D-04 0.800D-03-0.772D-03-0.300D-02-0.253D-02 0.574D-02
Coeff-Com: 0.275D-01-0.163D-01-0.710D-01-0.146D+00 0.334D+00 0.871D+00
Coeff: -0.132D-04 0.800D-03-0.772D-03-0.300D-02-0.253D-02 0.574D-02
Coeff: 0.275D-01-0.163D-01-0.710D-01-0.146D+00 0.334D+00 0.871D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.73D-08 MaxDP=5.63D-07 DE=-5.91D-11 OVMax= 3.33D-06

Cycle 13 Pass 1 IDiag 1:
RMSU= 8.83D-09 CP: 9.97D-01 1.10D+00 1.34D+00 1.56D+00 1.60D+00
CP: 1.73D+00 1.65D+00 1.76D+00 1.84D+00 1.97D+00
CP: 1.62D+00 1.30D+00
E= -608.981524335716 Delta-E= -0.000000000025 Rises=F Damp=F
DIIS: error= 9.44D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -608.981524335716 IErMin=13 ErrMin= 9.44D-08
ErrMax= 9.44D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-12 BMatP= 2.91D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.172D-04 0.693D-03-0.324D-03-0.215D-02-0.298D-02 0.175D-02
Coeff-Com: 0.208D-01 0.131D-01-0.269D-01-0.131D+00-0.355D-01 0.447D+00
Coeff-Com: 0.716D+00
Coeff: -0.172D-04 0.693D-03-0.324D-03-0.215D-02-0.298D-02 0.175D-02

```
 Coeff:      0.208D-01 0.131D-01-0.269D-01-0.131D+00-0.355D-01 0.447D+00
 Coeff:      0.716D+00
 Gap=     0.247 Goal=   None    Shift=    0.000
 RMSDP=7.39D-09 MaxDP=2.22D-07 DE=-2.46D-11 OVMax= 1.69D-06

 SCF Done:  E(RwB97XD) =  -608.981524336     A.U. after   13 cycles
            NFock= 13  Conv=0.74D-08     -V/T= 2.0045
 KE= 6.062244414788D+02 PE=-2.845882832050D+03 EE= 9.132279207355D+02
 Leave Link  502 at Fri Aug 21 19:33:40 2026, MaxMem=    805306368 cpu:             3454.3 elap:
576.0
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14214 LenP2D=   33578.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 Leave Link  701 at Fri Aug 21 19:33:40 2026, MaxMem=    805306368 cpu:                2.2 elap:
0.4
 (Enter /home/user/gauss16/g16/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link  702 at Fri Aug 21 19:33:40 2026, MaxMem=    805306368 cpu:                0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l703.exe)
 Integral derivatives from FoFJK, PRISM(SPDF).
 Compute integral first derivatives, UseDBF=F ICtDFT=          0.
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=         800
        NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
        wScrn=  0.000000 ICntrl=      2527 IOpCl=  0 I1Cent=          0 NGrid=          0
        NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 Leave Link  703 at Fri Aug 21 19:40:31 2026, MaxMem=    805306368 cpu:             2465.1 elap:
411.0
 (Enter /home/user/gauss16/g16/l716.exe)
 Dipole        = 1.51961950D+00-3.02113427D-03-5.87945115D-04
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
     1        6        -0.000265558   -0.000020332   -0.000334886
     2        6        -0.000103310    0.000235385    0.000434918
     3        6        -0.000191714    0.000038929    0.000340126
     4        6        -0.000172783    0.000123021   -0.000591187
```

```
     5        6       -0.000159097   -0.000278344   -0.000451126
     6        6        0.000250443    0.000194974    0.000236237
     7        6       -0.000146623   -0.000074358    0.000615618
     8        6       -0.000185489    0.000120610   -0.000036054
     9        6        0.000243032   -0.000229011   -0.000254287
    10        6        0.000384268    0.000033002    0.000294546
    11        6       -0.000186095   -0.000107392    0.000029924
    12        6       -0.000051501   -0.000077549   -0.000361099
    13        6        0.000392697   -0.000036483   -0.000283553
    14        6       -0.000057920    0.000070676    0.000358308
    15        6        0.000136621    0.000393613    0.000827645
    16        6        0.000113029   -0.000386741   -0.000825130
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.000827645 RMS     0.000308833
 Leave Link  716 at Fri Aug 21 19:40:31 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000690566 RMS     0.000239370
 Search for a local minimum.
 Step number   7 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .23937D-03 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                                      6    7
 DE= -3.14D-05 DEPred=-3.51D-05 R= 8.96D-01
 TightC=F SS=  1.41D+00  RLast= 6.64D-02 DXNew= 8.4853D-01 1.9913D-01
 Trust test= 8.96D-01 RLast= 6.64D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  1  1  0
    Eigenvalues ---    0.00696   0.01290   0.01541   0.01732   0.02380
    Eigenvalues ---    0.02626   0.02939   0.03413   0.03422   0.03926
    Eigenvalues ---    0.04047   0.04753   0.08286   0.08440   0.09362
    Eigenvalues ---    0.15854   0.24430   0.24571   0.24988   0.24993
    Eigenvalues ---    0.24994   0.24998   0.25000   0.25000   0.25048
    Eigenvalues ---    0.25292   0.28162   0.31615   0.34593   0.40147
    Eigenvalues ---    0.51322   0.53330   0.57381   0.57901   0.58162
    Eigenvalues ---    0.58185   0.78669   0.79194   0.79696   0.81312
    Eigenvalues ---    0.82168   0.87719
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:     7    6    5    4
 RFO step:  Lambda=-1.55547474D-05.
 NNeg= 0 NGDIIS= 4 SimSw=  2.50D-01 Rises=F DC= -3.14D-05 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
```

Supporting Information file

RMS Error= 0.3559269524D-02 NUsed= 4 OKEnD=T EnDIS=F
InvSVX: RCond= 2.68D-05 Info= 0 Equed=N FErr= 1.19D-13 BErr= 6.21D-17
DidBck=T Rises=F RFO-DIIS coefs: 0.76669 1.02114 -0.65717 -0.13066
Iteration 1 RMS(Cart)= 0.00278217 RMS(Int)= 0.00001226
Iteration 2 RMS(Cart)= 0.00000605 RMS(Int)= 0.00001159
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001159
ITry= 1 IFail=0 DXMaxC= 7.00D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.30735	-0.00051	0.00033	-0.00086	-0.00053	2.30682
R2	2.54958	-0.00044	0.00039	-0.00111	-0.00071	2.54887
R3	2.54890	-0.00041	0.00036	-0.00102	-0.00066	2.54824
R4	2.30732	-0.00051	0.00033	-0.00086	-0.00053	2.30679
R5	2.30346	-0.00053	0.00037	-0.00090	-0.00054	2.30292
R6	2.54903	-0.00042	0.00036	-0.00103	-0.00067	2.54836
R7	2.55142	-0.00029	0.00025	-0.00074	-0.00050	2.55092
R8	2.30341	-0.00053	0.00037	-0.00090	-0.00053	2.30288
R9	2.29610	-0.00051	0.00035	-0.00088	-0.00053	2.29557
R10	2.55151	-0.00029	0.00024	-0.00075	-0.00050	2.55100
R11	2.61668	-0.00021	0.00019	-0.00056	-0.00037	2.61630
R12	2.29610	-0.00051	0.00035	-0.00088	-0.00053	2.29557
R13	2.64605	-0.00020	0.00104	-0.00109	-0.00005	2.64600
R14	2.73983	-0.00019	-0.00066	-0.00025	-0.00092	2.73891
R15	2.61665	-0.00021	0.00018	-0.00055	-0.00037	2.61628
R16	2.73967	-0.00018	-0.00067	-0.00022	-0.00090	2.73877
R17	2.74294	-0.00069	0.00319	-0.00418	-0.00099	2.74195
A1	2.61281	-0.00003	0.00014	-0.00026	-0.00012	2.61269
A2	2.64440	0.00001	0.00007	-0.00007	-0.00000	2.64439
A3	2.61605	-0.00008	0.00006	-0.00035	-0.00029	2.61576
A4	2.71605	0.00003	-0.00035	0.00031	-0.00004	2.71601
A5	2.64151	0.00005	0.00013	0.00002	0.00014	2.64166
A6	2.77962	0.00009	-0.00001	0.00031	0.00029	2.77991
A7	2.71836	-0.00000	-0.00042	0.00025	-0.00017	2.71819
A8	2.77805	0.00010	0.00005	0.00033	0.00037	2.77842
A9	2.83216	0.00001	0.00033	-0.00026	0.00005	2.83221
A10	2.30759	-0.00010	-0.00068	0.00021	-0.00049	2.30710
A11	2.51753	0.00015	-0.00006	0.00039	0.00033	2.51786
A12	1.45754	-0.00006	0.00072	-0.00056	0.00016	1.45770
A13	2.83133	0.00002	0.00036	-0.00024	0.00010	2.83143
A14	2.30800	-0.00010	-0.00068	0.00017	-0.00052	2.30749
A15	1.45725	-0.00005	0.00070	-0.00052	0.00018	1.45743
A16	2.51744	0.00015	-0.00005	0.00037	0.00033	2.51777
A17	1.42621	0.00011	-0.00000	0.00048	0.00047	1.42667
A18	1.42659	0.00009	0.00002	0.00042	0.00043	1.42702
A19	2.87994	-0.00000	0.00026	0.00008	0.00032	2.88026
A20	2.88084	-0.00000	0.00023	0.00008	0.00029	2.88113
A21	3.14244	-0.00024	-0.00362	0.00033	-0.00331	3.13913

A22	3.14236	-0.00024	-0.00363	0.00034	-0.00331	3.13905
D1	0.07134	-0.00005	-0.00071	0.00076	0.00006	0.07140
D2	-0.06156	-0.00019	-0.00268	-0.00016	-0.00282	-0.06438
D3	-0.05697	-0.00010	-0.00158	-0.00143	-0.00300	-0.05998
D4	0.07082	-0.00005	-0.00061	0.00073	0.00013	0.07096
D5	0.08984	0.00018	0.00150	0.00081	0.00230	0.09214
D6	-0.05563	-0.00010	-0.00167	-0.00146	-0.00313	-0.05876
D7	0.08014	0.00019	0.00510	0.00056	0.00564	0.08577
D8	0.08851	0.00019	0.00152	0.00089	0.00240	0.09090
D9	0.08173	0.00019	0.00503	0.00062	0.00562	0.08735
D10	-0.61563	-0.00006	-0.00353	0.00030	-0.00324	-0.61886
D11	2.57521	0.00004	-0.00228	-0.00103	-0.00331	2.57190
D12	0.74996	-0.00005	0.00116	-0.00194	-0.00079	0.74917
D13	-2.41959	-0.00011	0.00054	-0.00139	-0.00087	-2.42046
D14	-2.42059	-0.00010	0.00043	-0.00115	-0.00073	-2.42132
D15	0.69305	-0.00016	-0.00020	-0.00060	-0.00081	0.69224
D16	2.40948	-0.00005	0.00037	0.00050	0.00086	2.41035
D17	-0.69541	0.00002	0.00131	-0.00049	0.00082	-0.69459
D18	-0.61768	-0.00006	-0.00338	0.00015	-0.00325	-0.62092
D19	2.57145	0.00004	-0.00232	-0.00076	-0.00309	2.56836
D20	-0.69544	0.00003	0.00131	-0.00049	0.00083	-0.69461
D21	2.41074	-0.00005	0.00051	0.00019	0.00070	2.41143
D22	0.67039	-0.00005	-0.00067	0.00011	-0.00057	0.66982

Item	Value	Threshold	Converged?
Maximum Force	0.000691	0.000450	NO
RMS Force	0.000239	0.000300	YES
Maximum Displacement	0.007000	0.001800	NO
RMS Displacement	0.002783	0.001200	NO

Predicted change in Energy=-6.481618D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 19:40:31 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.621144	-0.673346	0.014334
2	6	0	3.006590	-1.727268	0.055827
3	6	0	3.619745	0.675169	-0.013595
4	6	0	1.854521	-2.428045	0.061249
5	6	0	3.006261	1.729686	-0.055321
6	6	0	0.644764	-2.575020	0.063740
7	6	0	1.852910	2.428465	-0.061358
8	6	0	-0.666001	-2.255378	0.019886

9	6	0	0.643240	2.575949	-0.064131
10	6	0	-1.730854	-1.672824	-0.028821
11	6	0	-0.667233	2.254873	-0.020680
12	6	0	-2.685862	-0.680270	-0.168840
13	6	0	-1.731972	1.672088	0.027772
14	6	0	-2.686047	0.678732	0.168338
15	6	0	-4.041019	-0.404323	-0.602516
16	6	0	-4.040189	0.401510	0.604119

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220717	0.000000			
3	C	1.348805	2.480420	0.000000		
4	C	2.490406	1.348473	3.570932	0.000000	
5	C	2.481431	3.458741	1.220701	4.315880	0.000000
6	C	3.532370	2.509375	4.406838	1.218655	4.911347
7	C	3.571220	4.314490	2.489585	4.858057	1.348534
8	C	4.569734	3.710541	5.191998	2.526768	5.419584
9	C	4.408173	4.910956	3.532011	5.150037	2.510001
10	C	5.444695	4.738513	5.843134	3.665159	5.832498
11	C	5.192868	5.418513	4.568775	5.319369	3.711008
12	C	6.309669	5.792295	6.451511	4.870599	6.182316
13	C	5.844407	5.831842	5.443936	5.447489	4.739311
14	C	6.452325	6.181231	6.308418	5.502753	5.792832
15	C	7.691659	7.200860	7.758830	6.268447	7.383601
16	C	7.758814	7.381695	7.689672	6.561151	7.200789

		6	7	8	9	10
6	C	0.000000				
7	C	5.148798	0.000000			
8	C	1.349889	5.318825	0.000000		
9	C	5.152556	1.218631	5.006285	0.000000	
10	C	2.542850	5.446558	1.214765	4.867201	0.000000
11	C	5.005630	2.526443	4.510434	1.349933	4.069172
12	C	3.838912	5.502384	2.568350	4.657987	1.384489
13	C	4.867041	3.664892	4.069563	2.543038	3.345391
14	C	4.657483	4.869955	3.565337	3.838963	2.545797
15	C	5.206956	6.561703	3.899300	5.578007	2.697236
16	C	5.576785	6.267378	4.334228	5.206655	3.168044

		11	12	13	14	15
11	C	0.000000				
12	C	3.565372	0.000000			
13	C	1.214765	2.546006	0.000000		
14	C	2.568182	1.400205	1.384477	0.000000	
15	C	4.335007	1.449370	3.168666	1.898202	0.000000
16	C	3.898995	1.897871	2.697112	1.449295	1.450977

		16
16	C	0.000000

Supporting Information file

Stoichiometry C16
Framework group C1[X(C16)]
Deg. of freedom 42
Full point group C1 NOp 1
RotChk: IX=0 Diff= 1.52D-04
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.620925	-0.674559	0.012603
2	6	0	3.006028	-1.728380	0.051489
3	6	0	3.619965	0.674022	-0.011977
4	6	0	1.853732	-2.428793	0.055190
5	6	0	3.006823	1.728839	-0.051075
6	6	0	0.643927	-2.575380	0.057336
7	6	0	1.853700	2.428007	-0.055358
8	6	0	-0.666735	-2.255203	0.014297
9	6	0	0.644078	2.575891	-0.057746
10	6	0	-1.731399	-1.672184	-0.032947
11	6	0	-0.666500	2.255135	-0.015070
12	6	0	-2.686086	-0.678974	-0.170485
13	6	0	-1.731427	1.672578	0.031952
14	6	0	-2.685824	0.679186	0.170066
15	6	0	-4.041160	-0.401510	-0.603453
16	6	0	-4.040049	0.401324	0.605179

Rotational constants (GHZ): 0.8462479 0.3944465 0.2718532
Leave Link 202 at Fri Aug 21 19:40:31 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 717.6062848131 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074903768 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.5987944362 Hartrees.
Leave Link 301 at Fri Aug 21 19:40:32 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14214 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.17D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 19:40:32 2026, MaxMem= 805306368 cpu: 3.4 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 19:40:32 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000054 0.000000 0.000001 Ang= 0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 19:40:33 2026, MaxMem= 805306368 cpu: 1.9 elap: 0.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F

Supporting Information file

IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981484875068
DIIS: error= 4.87D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981484875068 IErMin= 1 ErrMin= 4.87D-04
ErrMax= 4.87D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-04 BMatP= 1.10D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.87D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=1.99D-05 MaxDP=4.25D-04 OVMax= 9.48D-04

Cycle 2 Pass 1 IDiag 1:
RMSU= 1.97D-05 CP: 1.00D+00
E= -608.981529019781 Delta-E= -0.000044144714 Rises=F Damp=F
DIIS: error= 3.76D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981529019781 IErMin= 2 ErrMin= 3.76D-05
ErrMax= 3.76D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.82D-07 BMatP= 1.10D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.308D-01 0.103D+01
Coeff: -0.308D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.88D-06 MaxDP=1.50D-04 DE=-4.41D-05 OVMax= 3.36D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 5.84D-06 CP: 1.00D+00 1.03D+00
E= -608.981530579122 Delta-E= -0.000001559340 Rises=F Damp=F
DIIS: error= 1.98D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981530579122 IErMin= 3 ErrMin= 1.98D-05
ErrMax= 1.98D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-07 BMatP= 6.82D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.997D-02 0.187D+00 0.823D+00
Coeff: -0.997D-02 0.187D+00 0.823D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.30D-06 MaxDP=6.40D-05 DE=-1.56D-06 OVMax= 1.74D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 1.99D-06 CP: 1.00D+00 1.03D+00 1.19D+00
E= -608.981530704336 Delta-E= -0.000000125214 Rises=F Damp=F
DIIS: error= 2.66D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981530704336 IErMin= 3 ErrMin= 1.98D-05
ErrMax= 2.66D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-07 BMatP= 1.44D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.645D-03-0.112D+00 0.514D+00 0.597D+00
Coeff: 0.645D-03-0.112D+00 0.514D+00 0.597D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=1.45D-06 MaxDP=3.53D-05 DE=-1.25D-07 OVMax= 1.27D-04

Cycle   5 Pass 1 IDiag 1:
RMSU= 9.88D-07   CP: 1.00D+00 1.02D+00 1.37D+00 1.06D+00
E= -608.981530861839   Delta-E=   -0.000000157504 Rises=F Damp=F
DIIS: error= 5.53D-06 at cycle   5 NSaved=   5.
NSaved= 5 IEnMin= 5 EnMin= -608.981530861839   IErMin= 5 ErrMin= 5.53D-06
ErrMax= 5.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.62D-09 BMatP= 1.29D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.188D-02-0.781D-01 0.902D-01 0.255D+00 0.731D+00
Coeff: 0.188D-02-0.781D-01 0.902D-01 0.255D+00 0.731D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=6.73D-07 MaxDP=1.71D-05 DE=-1.58D-07 OVMax= 4.67D-05

Cycle   6 Pass 1 IDiag 1:
RMSU= 3.18D-07   CP: 1.00D+00 1.02D+00 1.45D+00 1.22D+00 1.07D+00
E= -608.981530879252   Delta-E=   -0.000000017413 Rises=F Damp=F
DIIS: error= 1.42D-06 at cycle   6 NSaved=   6.
NSaved= 6 IEnMin= 6 EnMin= -608.981530879252   IErMin= 6 ErrMin= 1.42D-06
ErrMax= 1.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-09 BMatP= 9.62D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.559D-03-0.110D-01-0.395D-01 0.195D-02 0.252D+00 0.796D+00
Coeff: 0.559D-03-0.110D-01-0.395D-01 0.195D-02 0.252D+00 0.796D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=3.27D-07 MaxDP=1.38D-05 DE=-1.74D-08 OVMax= 2.45D-05

Cycle   7 Pass 1 IDiag 1:
RMSU= 1.48D-07   CP: 1.00D+00 1.02D+00 1.47D+00 1.31D+00 1.24D+00
               CP: 1.34D+00
E= -608.981530882359   Delta-E=   -0.000000003107 Rises=F Damp=F
DIIS: error= 9.48D-07 at cycle   7 NSaved=   7.
NSaved= 7 IEnMin= 7 EnMin= -608.981530882359   IErMin= 7 ErrMin= 9.48D-07
ErrMax= 9.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-10 BMatP= 1.25D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.293D-03 0.158D-01-0.334D-01-0.641D-01-0.107D+00 0.241D+00
Coeff-Com: 0.948D+00
Coeff: -0.293D-03 0.158D-01-0.334D-01-0.641D-01-0.107D+00 0.241D+00
Coeff: 0.948D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=2.04D-07 MaxDP=9.33D-06 DE=-3.11D-09 OVMax= 1.62D-05

Cycle   8 Pass 1 IDiag 1:
RMSU= 8.32D-08   CP: 1.00D+00 1.02D+00 1.47D+00 1.35D+00 1.35D+00
               CP: 1.68D+00 1.44D+00
E= -608.981530883060   Delta-E=   -0.000000000700 Rises=F Damp=F

DIIS: error= 9.54D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981530883060 IErMin= 7 ErrMin= 9.48D-07
ErrMax= 9.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.58D-11 BMatP= 2.37D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.236D-03 0.105D-01-0.153D-01-0.380D-01-0.887D-01 0.481D-01
Coeff-Com: 0.560D+00 0.524D+00
Coeff: -0.236D-03 0.105D-01-0.153D-01-0.380D-01-0.887D-01 0.481D-01
Coeff: 0.560D+00 0.524D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.76D-08 MaxDP=2.11D-06 DE=-7.00D-10 OVMax= 3.99D-06

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.18D-08 CP: 1.00D+00 1.02D+00 1.47D+00 1.35D+00 1.37D+00
CP: 1.77D+00 1.59D+00 1.12D+00
E= -608.981530883213 Delta-E= -0.000000000153 Rises=F Damp=F
DIIS: error= 2.07D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981530883213 IErMin= 9 ErrMin= 2.07D-07
ErrMax= 2.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.44D-12 BMatP= 9.58D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.116D-04-0.931D-04 0.239D-02 0.155D-02-0.386D-02-0.373D-01
Coeff-Com: -0.300D-01 0.177D+00 0.890D+00
Coeff: -0.116D-04-0.931D-04 0.239D-02 0.155D-02-0.386D-02-0.373D-01
Coeff: -0.300D-01 0.177D+00 0.890D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.63D-08 MaxDP=1.36D-06 DE=-1.53D-10 OVMax= 2.83D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.12D-08 CP: 1.00D+00 1.02D+00 1.47D+00 1.35D+00 1.38D+00
CP: 1.83D+00 1.73D+00 1.37D+00 1.35D+00
E= -608.981530883226 Delta-E= -0.000000000013 Rises=F Damp=F
DIIS: error= 8.71D-08 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981530883226 IErMin=10 ErrMin= 8.71D-08
ErrMax= 8.71D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-12 BMatP= 7.44D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.364D-04-0.189D-02 0.381D-02 0.735D-02 0.140D-01-0.268D-01
Coeff-Com: -0.115D+00-0.582D-02 0.382D+00 0.742D+00
Coeff: 0.364D-04-0.189D-02 0.381D-02 0.735D-02 0.140D-01-0.268D-01
Coeff: -0.115D+00-0.582D-02 0.382D+00 0.742D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.99D-08 MaxDP=5.12D-07 DE=-1.34D-11 OVMax= 1.46D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 7.04D-09 CP: 1.00D+00 1.02D+00 1.46D+00 1.35D+00 1.37D+00
CP: 1.84D+00 1.78D+00 1.51D+00 1.45D+00 1.15D+00
E= -608.981530883229 Delta-E= -0.000000000003 Rises=F Damp=F
DIIS: error= 5.43D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981530883229 IErMin=11 ErrMin= 5.43D-08
ErrMax= 5.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.62D-13 BMatP= 1.69D-12

Supporting Information file

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.125D-04-0.505D-03 0.564D-03 0.167D-02 0.497D-02-0.407D-03
Coeff-Com: -0.250D-01-0.329D-01-0.702D-01 0.188D+00 0.934D+00
Coeff: 0.125D-04-0.505D-03 0.564D-03 0.167D-02 0.497D-02-0.407D-03
Coeff: -0.250D-01-0.329D-01-0.702D-01 0.188D+00 0.934D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=7.86D-09 MaxDP=1.86D-07 DE=-2.73D-12 OVMax= 7.87D-07

SCF Done: E(RwB97XD) = -608.981530883 A.U. after 11 cycles
NFock= 11 Conv=0.79D-08 -V/T= 2.0045
KE= 6.062400375314D+02 PE=-2.846196658125D+03 EE= 9.133762952744D+02
Leave Link 502 at Fri Aug 21 19:48:04 2026, MaxMem= 805306368 cpu: 2710.3 elap: 451.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14214 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 19:48:05 2026, MaxMem= 805306368 cpu: 2.2 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 19:48:05 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 19:56:25 2026, MaxMem= 805306368 cpu: 2999.7 elap: 500.1
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.51995985D+00-2.88711103D-03-5.41129412D-04
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 0.000026476 0.000082985 -0.000305987

```
     2        6       -0.000075764   -0.000079040    0.000413196
     3        6        0.000095902   -0.000065273    0.000310616
     4        6        0.000082831    0.000004516   -0.000503254
     5        6       -0.000127633    0.000038372   -0.000427881
     6        6       -0.000052520    0.000065103    0.000349726
     7        6        0.000107095    0.000041222    0.000526290
     8        6        0.000041604   -0.000087507   -0.000236160
     9        6       -0.000058946   -0.000097397   -0.000367517
    10        6       -0.000025773    0.000126774    0.000304796
    11        6        0.000039905    0.000100447    0.000230563
    12        6        0.000109040   -0.000110010   -0.000190401
    13        6       -0.000017488   -0.000130458   -0.000291650
    14        6        0.000101753    0.000104734    0.000184077
    15        6       -0.000112800    0.000348082    0.000424988
    16        6       -0.000133682   -0.000342550   -0.000421399
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000526290 RMS     0.000228542
 Leave Link  716 at Fri Aug 21 19:56:25 2026, MaxMem=    805306368 cpu:                  0.4 elap:
0.1
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000426578 RMS     0.000079605
 Search for a local minimum.
 Step number   8 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .79605D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                                      6    7    8
 DE= -6.55D-06 DEPred=-6.48D-06 R= 1.01D+00
 TightC=F SS=  1.41D+00  RLast= 1.34D-02 DXNew= 8.4853D-01 4.0069D-02
 Trust test= 1.01D+00 RLast= 1.34D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  1  1  1  0
    Eigenvalues ---    0.00716   0.01290   0.01554   0.01732   0.02369
    Eigenvalues ---    0.02625   0.02913   0.03422   0.03422   0.03926
    Eigenvalues ---    0.04047   0.06019   0.08167   0.08437   0.09356
    Eigenvalues ---    0.15990   0.23880   0.24444   0.24735   0.24989
    Eigenvalues ---    0.24994   0.24996   0.24998   0.25000   0.25000
    Eigenvalues ---    0.25060   0.28164   0.31343   0.32172   0.40829
    Eigenvalues ---    0.51321   0.53346   0.57380   0.57872   0.58159
    Eigenvalues ---    0.58183   0.78668   0.79313   0.79696   0.81411
    Eigenvalues ---    0.82169   0.92688
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:     8    7    6    5    4
```

Supporting Information file

RFO step: Lambda=-3.94495644D-06.
NNeg= 0 NGDIIS= 5 SimSw= 2.50D-01 Rises=F DC= -6.55D-06 SmlDif= 1.00D-05
NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj= 3.0
RMS Error= 0.2024303191D-02 NUsed= 5 OKEnD=F EnDIS=F
InvSVX: RCond= 2.47D-06 Info= 0 Equed=N FErr= 2.23D-13 BErr= 6.05D-17
DidBck=F Rises=F RFO-DIIS coefs: 1.86245 -0.66575 -0.40010 0.19083 0.01256
Iteration 1 RMS(Cart)= 0.00148293 RMS(Int)= 0.00000229
Iteration 2 RMS(Cart)= 0.00000213 RMS(Int)= 0.00000153
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000153
ITry= 1 IFail=0 DXMaxC= 4.56D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.30682	0.00007	-0.00047	0.00056	0.00009	2.30692
R2	2.54887	-0.00004	-0.00080	0.00043	-0.00036	2.54851
R3	2.54824	-0.00004	-0.00073	0.00037	-0.00036	2.54788
R4	2.30679	0.00007	-0.00046	0.00056	0.00010	2.30689
R5	2.30292	0.00005	-0.00047	0.00054	0.00006	2.30299
R6	2.54836	-0.00005	-0.00074	0.00037	-0.00037	2.54799
R7	2.55092	-0.00001	-0.00058	0.00032	-0.00026	2.55066
R8	2.30288	0.00005	-0.00047	0.00054	0.00007	2.30295
R9	2.29557	0.00005	-0.00049	0.00053	0.00004	2.29562
R10	2.55100	-0.00001	-0.00059	0.00032	-0.00027	2.55073
R11	2.61630	-0.00003	-0.00039	0.00012	-0.00027	2.61604
R12	2.29557	0.00005	-0.00049	0.00053	0.00004	2.29562
R13	2.64600	-0.00004	0.00066	-0.00024	0.00042	2.64643
R14	2.73891	0.00009	-0.00180	0.00154	-0.00025	2.73866
R15	2.61628	-0.00003	-0.00039	0.00013	-0.00026	2.61602
R16	2.73877	0.00010	-0.00178	0.00158	-0.00020	2.73857
R17	2.74195	-0.00043	0.00068	-0.00133	-0.00065	2.74130
A1	2.61269	-0.00004	-0.00006	-0.00011	-0.00017	2.61251
A2	2.64439	-0.00001	0.00007	-0.00010	-0.00003	2.64436
A3	2.61576	-0.00009	-0.00032	-0.00020	-0.00052	2.61523
A4	2.71601	0.00003	-0.00028	0.00021	-0.00008	2.71593
A5	2.64166	0.00003	0.00029	-0.00002	0.00027	2.64193
A6	2.77991	0.00008	0.00040	0.00011	0.00051	2.78042
A7	2.71819	-0.00001	-0.00049	0.00015	-0.00034	2.71785
A8	2.77842	0.00010	0.00054	0.00014	0.00068	2.77909
A9	2.83221	-0.00001	0.00019	-0.00020	-0.00001	2.83220
A10	2.30710	-0.00003	-0.00081	0.00014	-0.00067	2.30643
A11	2.51786	0.00009	0.00073	-0.00001	0.00072	2.51858
A12	1.45770	-0.00006	0.00008	-0.00015	-0.00006	1.45763
A13	2.83143	-0.00000	0.00027	-0.00018	0.00009	2.83152
A14	2.30749	-0.00004	-0.00084	0.00012	-0.00072	2.30677
A15	1.45743	-0.00005	0.00010	-0.00012	-0.00002	1.45742
A16	2.51777	0.00009	0.00073	-0.00002	0.00072	2.51849
A17	1.42667	0.00008	0.00008	0.00026	0.00034	1.42701
A18	1.42702	0.00006	0.00005	0.00021	0.00026	1.42728

A19	2.88026	0.00000	0.00009	-0.00011	-0.00002	2.88024
A20	2.88113	-0.00000	0.00002	-0.00013	-0.00012	2.88101
A21	3.13913	0.00000	-0.00068	0.00014	-0.00054	3.13859
A22	3.13905	0.00000	-0.00067	0.00018	-0.00050	3.13855
D1	0.07140	0.00004	0.00130	0.00075	0.00206	0.07345
D2	-0.06438	-0.00006	-0.00218	-0.00059	-0.00278	-0.06716
D3	-0.05998	-0.00007	-0.00364	-0.00090	-0.00453	-0.06451
D4	0.07096	0.00004	0.00147	0.00073	0.00220	0.07316
D5	0.09214	0.00011	0.00389	0.00089	0.00478	0.09692
D6	-0.05876	-0.00007	-0.00387	-0.00091	-0.00477	-0.06353
D7	0.08577	0.00004	0.00417	-0.00029	0.00388	0.08966
D8	0.09090	0.00011	0.00402	0.00096	0.00499	0.09589
D9	0.08735	0.00004	0.00412	-0.00034	0.00378	0.09113
D10	-0.61886	-0.00007	-0.00577	-0.00028	-0.00605	-0.62492
D11	2.57190	-0.00002	-0.00578	0.00048	-0.00530	2.56659
D12	0.74917	-0.00005	0.00023	0.00035	0.00058	0.74975
D13	-2.42046	-0.00008	0.00014	-0.00016	-0.00001	-2.42047
D14	-2.42132	-0.00008	0.00027	-0.00010	0.00017	-2.42115
D15	0.69224	-0.00011	0.00018	-0.00061	-0.00042	0.69182
D16	2.41035	-0.00008	0.00055	-0.00080	-0.00025	2.41010
D17	-0.69459	-0.00004	0.00057	-0.00023	0.00033	-0.69425
D18	-0.62092	-0.00007	-0.00571	-0.00026	-0.00597	-0.62689
D19	2.56836	-0.00001	-0.00551	0.00060	-0.00490	2.56346
D20	-0.69461	-0.00004	0.00057	-0.00023	0.00034	-0.69427
D21	2.41143	-0.00008	0.00039	-0.00086	-0.00047	2.41096
D22	0.66982	-0.00002	0.00018	-0.00034	-0.00017	0.66965

Item	Value	Threshold	Converged?
Maximum Force	0.000427	0.000450	YES
RMS Force	0.000080	0.000300	YES
Maximum Displacement	0.004565	0.001800	NO
RMS Displacement	0.001483	0.001200	NO

Predicted change in Energy=-1.950728D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 19:56:25 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.621585	-0.673243	0.013425
2	6	0	3.006759	-1.727084	0.054430
3	6	0	3.620302	0.675114	-0.012769
4	6	0	1.854674	-2.427473	0.059238
5	6	0	3.006358	1.729444	-0.054000

6	6	0	0.644839	-2.574046	0.063509
7	6	0	1.853089	2.427983	-0.059335
8	6	0	-0.665908	-2.254692	0.021351
9	6	0	0.643319	2.574913	-0.063851
10	6	0	-1.730931	-1.672323	-0.026406
11	6	0	-0.667143	2.254181	-0.022033
12	6	0	-2.686312	-0.680566	-0.168123
13	6	0	-1.732018	1.671521	0.025475
14	6	0	-2.686516	0.679000	0.167706
15	6	0	-4.041381	-0.405050	-0.601905
16	6	0	-4.040716	0.402319	0.603288

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220767	0.000000			
3	C	1.348613	2.480223	0.000000		
4	C	2.490259	1.348283	3.570528	0.000000	
5	C	2.481120	3.458228	1.220753	4.314991	0.000000
6	C	3.532219	2.509201	4.406386	1.218689	4.910254
7	C	3.570781	4.313755	2.489530	4.856904	1.348338
8	C	4.569862	3.710518	5.191967	2.526782	5.418907
9	C	4.407557	4.909889	3.531893	5.148436	2.509754
10	C	5.445106	4.738696	5.843488	3.665263	5.832211
11	C	5.192712	5.417921	4.568996	5.318275	3.710927
12	C	6.310513	5.792736	6.452549	4.870722	6.182852
13	C	5.844581	5.831583	5.444412	5.446765	4.739396
14	C	6.453255	6.181864	6.309400	5.503121	5.793219
15	C	7.692308	7.201029	7.759846	6.268235	7.384232
16	C	7.759873	7.382581	7.690588	6.561962	7.201009

		6	7	8	9	10
6	C	0.000000				
7	C	5.147354	0.000000			
8	C	1.349749	5.317829	0.000000		
9	C	5.150534	1.218668	5.004639	0.000000	
10	C	2.542730	5.445990	1.214787	4.865951	0.000000
11	C	5.004037	2.526493	4.509081	1.349788	4.068059
12	C	3.838683	5.502824	2.568230	4.657838	1.384348
13	C	4.865772	3.665027	4.068385	2.542896	3.344247
14	C	4.657369	4.870164	3.565224	3.838737	2.545495
15	C	5.206532	6.562411	3.899158	5.578180	2.697287
16	C	5.577144	6.267322	4.334476	5.206287	3.167927

		11	12	13	14	15
11	C	0.000000				
12	C	3.565267	0.000000			
13	C	1.214787	2.545677	0.000000		
14	C	2.568085	1.400429	1.384339	0.000000	
15	C	4.335117	1.449237	3.168424	1.898190	0.000000

16 C 3.898899 1.897926 2.697189 1.449187 1.450633
16
16 C 0.000000
Stoichiometry C16
Framework group C1[X(C16)]
Deg. of freedom 42
Full point group C1 NOp 1
RotChk: IX=0 Diff= 7.13D-05
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.621366	-0.674452	0.011736
2	6	0	3.006198	-1.728189	0.050186
3	6	0	3.620521	0.673966	-0.011178
4	6	0	1.853886	-2.428213	0.053307
5	6	0	3.006919	1.728592	-0.049836
6	6	0	0.644003	-2.574402	0.057238
7	6	0	1.853878	2.427518	-0.053455
8	6	0	-0.666641	-2.254520	0.015876
9	6	0	0.644156	2.574851	-0.057597
10	6	0	-1.731476	-1.671691	-0.030449
11	6	0	-0.666410	2.254445	-0.016541
12	6	0	-2.686536	-0.679281	-0.169739
13	6	0	-1.731474	1.672018	0.029565
14	6	0	-2.686292	0.679464	0.169396
15	6	0	-4.041520	-0.402271	-0.602831
16	6	0	-4.040577	0.402164	0.604323

Rotational constants (GHZ): 0.8467271 0.3943751 0.2718574
Leave Link 202 at Fri Aug 21 19:56:25 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 576 symmetry adapted cartesian basis functions of A symmetry.
There are 496 symmetry adapted basis functions of A symmetry.
496 basis functions, 816 primitive gaussians, 576 cartesian basis functions
48 alpha electrons 48 beta electrons
nuclear repulsion energy 717.6441226232 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 16 NActive= 16 NUniq= 16 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0074916892 Hartrees.
Nuclear repulsion after empirical dispersion term = 717.6366309340 Hartrees.
Leave Link 301 at Fri Aug 21 19:56:25 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33578.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 496 RedAO= T EigKep= 4.20D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 19:56:26 2026, MaxMem= 805306368 cpu: 6.9 elap: 1.2
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 19:56:27 2026, MaxMem= 805306368 cpu: 1.0 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 -0.000000 0.000000
Rot= 1.000000 0.000025 0.000001 -0.000000 Ang= 0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 19:56:27 2026, MaxMem= 805306368 cpu: 3.9 elap: 0.7
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Supporting Information file

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981520241532
DIIS: error= 2.60D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981520241532 IErMin= 1 ErrMin= 2.60D-04
ErrMax= 2.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.24D-05 BMatP= 3.24D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 2.60D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=2.35D-05 MaxDP=6.26D-04 OVMax= 5.20D-04

Cycle 2 Pass 1 IDiag 1:
RMSU= 2.28D-05 CP: 9.99D-01
E= -608.981533431867 Delta-E= -0.000013190335 Rises=F Damp=F
DIIS: error= 1.98D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981533431867 IErMin= 2 ErrMin= 1.98D-05
ErrMax= 1.98D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-07 BMatP= 3.24D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.301D-01 0.103D+01
Coeff: -0.301D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.73D-06 MaxDP=1.11D-04 DE=-1.32D-05 OVMax= 1.96D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 3.54D-06 CP: 9.99D-01 1.13D+00
E= -608.981533894336 Delta-E= -0.000000462469 Rises=F Damp=F
DIIS: error= 1.57D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981533894336 IErMin= 3 ErrMin= 1.57D-05
ErrMax= 1.57D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.62D-08 BMatP= 2.23D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.147D-01 0.344D+00 0.670D+00
Coeff: -0.147D-01 0.344D+00 0.670D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.53D-06 MaxDP=4.92D-05 DE=-4.62D-07 OVMax= 1.02D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 1.40D-06 CP: 9.99D-01 1.15D+00 1.07D+00
E= -608.981533976241 Delta-E= -0.000000081905 Rises=F Damp=F
DIIS: error= 1.51D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -608.981533976241 IErMin= 4 ErrMin= 1.51D-05
ErrMax= 1.51D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-08 BMatP= 8.62D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.828D-03-0.119D+00 0.394D+00 0.724D+00
Coeff: 0.828D-03-0.119D+00 0.394D+00 0.724D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.04D-06 MaxDP=2.74D-05 DE=-8.19D-08 OVMax= 9.87D-05

Cycle 5 Pass 1 IDiag 1:
RMSU= 5.54D-07 CP: 9.99D-01 1.17D+00 1.29D+00 1.10D+00
E= -608.981534031807 Delta-E= -0.000000055566 Rises=F Damp=F
DIIS: error= 4.24D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981534031807 IErMin= 5 ErrMin= 4.24D-06
ErrMax= 4.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.78D-09 BMatP= 3.96D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.214D-02-0.989D-01 0.120D+00 0.359D+00 0.619D+00
Coeff: 0.214D-02-0.989D-01 0.120D+00 0.359D+00 0.619D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.66D-07 MaxDP=1.06D-05 DE=-5.56D-08 OVMax= 3.87D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.27D-07 CP: 9.99D-01 1.17D+00 1.36D+00 1.17D+00 1.05D+00
E= -608.981534040992 Delta-E= -0.000000009185 Rises=F Damp=F
DIIS: error= 3.09D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981534040992 IErMin= 6 ErrMin= 3.09D-06
ErrMax= 3.09D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.14D-10 BMatP= 4.78D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.549D-03-0.615D-02-0.488D-01-0.510D-01 0.206D+00 0.899D+00
Coeff: 0.549D-03-0.615D-02-0.488D-01-0.510D-01 0.206D+00 0.899D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.65D-07 MaxDP=9.93D-06 DE=-9.19D-09 OVMax= 3.91D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.14D-07 CP: 9.99D-01 1.17D+00 1.39D+00 1.27D+00 1.27D+00
CP: 1.14D+00
E= -608.981534044533 Delta-E= -0.000000003541 Rises=F Damp=F
DIIS: error= 1.49D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981534044533 IErMin= 7 ErrMin= 1.49D-06
ErrMax= 1.49D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-10 BMatP= 7.14D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.412D-03 0.233D-01-0.396D-01-0.105D+00-0.112D+00 0.212D+00
Coeff-Com: 0.102D+01
Coeff: -0.412D-03 0.233D-01-0.396D-01-0.105D+00-0.112D+00 0.212D+00
Coeff: 0.102D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.41D-07 MaxDP=5.37D-06 DE=-3.54D-09 OVMax= 2.83D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.90D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.29D+00 1.40D+00
CP: 1.46D+00 1.41D+00
E= -608.981534045836 Delta-E= -0.000000001302 Rises=F Damp=F
DIIS: error= 7.98D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981534045836 IErMin= 8 ErrMin= 7.98D-07
ErrMax= 7.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.98D-11 BMatP= 1.71D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.350D-03 0.139D-01-0.104D-01-0.449D-01-0.103D+00-0.863D-01
Coeff-Com: 0.531D+00 0.700D+00
Coeff: -0.350D-03 0.139D-01-0.104D-01-0.449D-01-0.103D+00-0.863D-01
Coeff: 0.531D+00 0.700D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.43D-08 MaxDP=1.15D-06 DE=-1.30D-09 OVMax= 1.37D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.42D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.29D+00 1.43D+00
CP: 1.54D+00 1.67D+00 1.25D+00
E= -608.981534046165 Delta-E= -0.000000000330 Rises=F Damp=F
DIIS: error= 5.01D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981534046165 IErMin= 9 ErrMin= 5.01D-07
ErrMax= 5.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-11 BMatP= 6.98D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.408D-04-0.387D-03 0.649D-02 0.901D-02-0.147D-01-0.979D-01
Coeff-Com: -0.565D-01 0.318D+00 0.836D+00
Coeff: -0.408D-04-0.387D-03 0.649D-02 0.901D-02-0.147D-01-0.979D-01
Coeff: -0.565D-01 0.318D+00 0.836D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.77D-08 MaxDP=8.02D-07 DE=-3.30D-10 OVMax= 8.42D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.44D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.29D+00 1.43D+00
CP: 1.57D+00 1.80D+00 1.60D+00 1.41D+00
E= -608.981534046282 Delta-E= -0.000000000117 Rises=F Damp=F
DIIS: error= 2.51D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981534046282 IErMin=10 ErrMin= 2.51D-07
ErrMax= 2.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.79D-12 BMatP= 1.94D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.135D-03-0.643D-02 0.816D-02 0.254D-01 0.402D-01-0.150D-01
Coeff-Com: -0.286D+00-0.130D+00 0.456D+00 0.907D+00
Coeff: 0.135D-03-0.643D-02 0.816D-02 0.254D-01 0.402D-01-0.150D-01
Coeff: -0.286D+00-0.130D+00 0.456D+00 0.907D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.65D-08 MaxDP=1.06D-06 DE=-1.17D-10 OVMax= 7.09D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.19D-08 CP: 9.99D-01 1.17D+00 1.40D+00 1.27D+00 1.42D+00
CP: 1.60D+00 1.86D+00 1.91D+00 1.81D+00 1.49D+00
E= -608.981534046327 Delta-E= -0.000000000044 Rises=F Damp=F

Supporting Information file

DIIS: error= 8.03D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981534046327 IErMin=11 ErrMin= 8.03D-08
ErrMax= 8.03D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.72D-13 BMatP= 6.79D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.115D-04-0.158D-03-0.903D-03-0.792D-03 0.504D-02 0.175D-01
Coeff-Com: -0.305D-02-0.651D-01-0.129D+00 0.662D-01 0.111D+01
Coeff: 0.115D-04-0.158D-03-0.903D-03-0.792D-03 0.504D-02 0.175D-01
Coeff: -0.305D-02-0.651D-01-0.129D+00 0.662D-01 0.111D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.26D-08 MaxDP=5.19D-07 DE=-4.43D-11 OVMax= 2.15D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.30D-09 CP: 9.99D-01 1.17D+00 1.40D+00 1.27D+00 1.41D+00
CP: 1.61D+00 1.85D+00 1.97D+00 1.95D+00 1.94D+00
CP: 1.46D+00
E= -608.981534046337 Delta-E= -0.000000000010 Rises=F Damp=F
DIIS: error= 2.51D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981534046337 IErMin=12 ErrMin= 2.51D-08
ErrMax= 2.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.82D-13 BMatP= 5.72D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.186D-04 0.106D-02-0.185D-02-0.482D-02-0.487D-02 0.111D-01
Coeff-Com: 0.478D-01-0.828D-02-0.132D+00-0.131D+00 0.487D+00 0.736D+00
Coeff: -0.186D-04 0.106D-02-0.185D-02-0.482D-02-0.487D-02 0.111D-01
Coeff: 0.478D-01-0.828D-02-0.132D+00-0.131D+00 0.487D+00 0.736D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.34D-09 MaxDP=2.11D-07 DE=-1.00D-11 OVMax= 5.85D-07

SCF Done: E(RwB97XD) = -608.981534046 A.U. after 12 cycles
NFock= 12 Conv=0.53D-08 -V/T= 2.0045
KE= 6.062426096206D+02 PE=-2.846274015989D+03 EE= 9.134132413882D+02
Leave Link 502 at Fri Aug 21 20:05:08 2026, MaxMem= 805306368 cpu: 3122.5 elap: 520.6
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33578.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Aug 21 20:05:08 2026, MaxMem= 805306368 cpu: 2.3 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 20:05:09 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Supporting Information file

```
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=         800
       NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=      2527 IOpCl=  0 I1Cent=          0 NGrid=          0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 Leave Link  703 at Fri Aug 21 20:12:29 2026, MaxMem=    805306368 cpu:             2641.9 elap:
440.4
 (Enter /home/user/gauss16/g16/l716.exe)
 Dipole        = 1.51933063D+00-2.59526006D-03-4.54353626D-04
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number           X              Y              Z
 -------------------------------------------------------------------
     1        6          0.000014453   -0.000076431   -0.000281433
     2        6          0.000057539   -0.000000858    0.000364959
     3        6          0.000076187    0.000092428    0.000284321
     4        6         -0.000034635   -0.000054553   -0.000419566
     5        6          0.000011496   -0.000035296   -0.000375863
     6        6          0.000021507    0.000022913    0.000350701
     7        6         -0.000013825    0.000094932    0.000438757
     8        6         -0.000010571   -0.000053761   -0.000258083
     9        6          0.000017045   -0.000051870   -0.000365379
    10        6         -0.000045238    0.000025222    0.000216794
    11        6         -0.000012636    0.000065345    0.000250789
    12        6          0.000170463    0.000045910   -0.000017219
    13        6         -0.000038542   -0.000028629   -0.000201681
    14        6          0.000160635   -0.000049319    0.000011899
    15        6         -0.000181603    0.000278616    0.000242923
    16        6         -0.000192274   -0.000274650   -0.000241917
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000438757 RMS     0.000189954
 Leave Link  716 at Fri Aug 21 20:12:29 2026, MaxMem=    805306368 cpu:               0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000303081 RMS     0.000072937
 Search for a local minimum.
 Step number   9 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
```

Supporting Information file

```
 RMS Force = .72937D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                                      6    7    8    9
 DE= -3.16D-06 DEPred=-1.95D-06 R= 1.62D+00
 TightC=F SS=  1.41D+00  RLast= 1.64D-02 DXNew= 8.4853D-01 4.9113D-02
 Trust test= 1.62D+00 RLast= 1.64D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  1  1  1  1  0
    Eigenvalues ---    0.00419   0.01290   0.01571   0.01731   0.02291
    Eigenvalues ---    0.02625   0.02821   0.03355   0.03422   0.03926
    Eigenvalues ---    0.04047   0.06567   0.08079   0.08436   0.09389
    Eigenvalues ---    0.13340   0.23546   0.24440   0.24712   0.24988
    Eigenvalues ---    0.24995   0.24996   0.25000   0.25000   0.25004
    Eigenvalues ---    0.25099   0.28166   0.33023   0.33856   0.44130
    Eigenvalues ---    0.51321   0.54180   0.57379   0.58091   0.58166
    Eigenvalues ---    0.58218   0.78667   0.79284   0.79696   0.81395
    Eigenvalues ---    0.82168   0.97740
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:     9    8    7    6    5    4
 RFO step:  Lambda=-5.44266118D-06.
 NNeg= 0 NGDIIS= 6 SimSw=  2.50D-01 Rises=F DC= -3.16D-06 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.3713657610D-02 NUsed= 6 OKEnD=F EnDIS=F
 InvSVX:  RCond= 7.49D-08 Info=          0 Equed=N FErr=  9.81D-12 BErr=  4.13D-17
 DIIS inversion failure, remove point   6.
 InvSVX:  RCond= 9.04D-08 Info=          0 Equed=N FErr=  7.74D-12 BErr=  2.72D-17
 DIIS inversion failure, remove point   5.
 InvSVX:  RCond= 1.19D-07 Info=          0 Equed=N FErr=  5.07D-12 BErr=  3.67D-17
 Old DIIS coefficients:      3.33103     -2.83973      0.49672      0.01198      0.00000
 Old DIIS coefficients:      0.00000
 RFO-DIIS uses    4 points instead of    6
 DidBck=F Rises=F RFO-DIIS coefs:    2.60255   -2.00000    0.38809    0.00936    0.00000
              RFO-DIIS coefs:    0.00000
 Iteration  1 RMS(Cart)=  0.00175225 RMS(Int)=  0.00000613
 Iteration  2 RMS(Cart)=  0.00000487 RMS(Int)=  0.00000363
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000363
  ITry=  1  IFail=0  DXMaxC=  5.97D-03  DCOld=  1.00D+10  DXMaxT=  5.05D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)    (Quad)   (Total)
    R1        2.30692   0.00006   0.00036  -0.00033   0.00003   2.30694
    R2        2.54851   0.00012  -0.00029   0.00018  -0.00011   2.54840
    R3        2.54788   0.00010  -0.00031   0.00013  -0.00017   2.54771
    R4        2.30689   0.00006   0.00036  -0.00033   0.00003   2.30692
    R5        2.30299   0.00005   0.00031  -0.00031  -0.00000   2.30299
    R6        2.54799   0.00009  -0.00032   0.00012  -0.00020   2.54779
    R7        2.55066   0.00007  -0.00022   0.00006  -0.00016   2.55050
    R8        2.30295   0.00005   0.00032  -0.00031   0.00001   2.30296
```

R9	2.29562	0.00007	0.00027	-0.00024	0.00003	2.29565
R10	2.55073	0.00007	-0.00023	0.00005	-0.00018	2.55055
R11	2.61604	0.00003	-0.00027	0.00003	-0.00024	2.61579
R12	2.29562	0.00007	0.00027	-0.00024	0.00003	2.29565
R13	2.64643	-0.00008	0.00064	-0.00063	0.00001	2.64643
R14	2.73866	0.00017	0.00004	0.00049	0.00053	2.73919
R15	2.61602	0.00004	-0.00027	0.00004	-0.00023	2.61579
R16	2.73857	0.00017	0.00011	0.00050	0.00061	2.73917
R17	2.74130	-0.00030	-0.00080	-0.00138	-0.00217	2.73912
A1	2.61251	-0.00002	-0.00024	-0.00004	-0.00028	2.61223
A2	2.64436	-0.00002	-0.00006	-0.00008	-0.00015	2.64422
A3	2.61523	-0.00006	-0.00072	-0.00035	-0.00107	2.61416
A4	2.71593	0.00002	-0.00009	0.00006	-0.00004	2.71589
A5	2.64193	0.00002	0.00036	0.00020	0.00056	2.64248
A6	2.78042	0.00004	0.00069	0.00023	0.00091	2.78133
A7	2.71785	-0.00001	-0.00044	-0.00016	-0.00061	2.71725
A8	2.77909	0.00006	0.00092	0.00038	0.00129	2.78038
A9	2.83220	-0.00004	-0.00005	-0.00025	-0.00031	2.83189
A10	2.30643	0.00002	-0.00085	0.00006	-0.00080	2.30563
A11	2.51858	0.00002	0.00099	0.00008	0.00107	2.51965
A12	1.45763	-0.00004	-0.00016	-0.00014	-0.00030	1.45733
A13	2.83152	-0.00003	0.00008	-0.00017	-0.00009	2.83143
A14	2.30677	0.00002	-0.00092	0.00001	-0.00092	2.30585
A15	1.45742	-0.00004	-0.00010	-0.00010	-0.00020	1.45722
A16	2.51849	0.00002	0.00099	0.00008	0.00107	2.51956
A17	1.42701	0.00004	0.00038	0.00015	0.00053	1.42754
A18	1.42728	0.00003	0.00027	0.00011	0.00038	1.42766
A19	2.88024	-0.00000	-0.00015	-0.00020	-0.00035	2.87989
A20	2.88101	-0.00001	-0.00028	-0.00030	-0.00059	2.88042
A21	3.13859	0.00008	0.00038	0.00097	0.00136	3.13995
A22	3.13855	0.00008	0.00045	0.00088	0.00132	3.13988
D1	0.07345	0.00006	0.00321	0.00256	0.00577	0.07922
D2	-0.06716	-0.00002	-0.00330	-0.00233	-0.00562	-0.07278
D3	-0.06451	-0.00005	-0.00598	-0.00342	-0.00939	-0.07391
D4	0.07316	0.00006	0.00340	0.00261	0.00601	0.07916
D5	0.09692	0.00007	0.00660	0.00400	0.01060	0.10752
D6	-0.06353	-0.00006	-0.00630	-0.00360	-0.00990	-0.07343
D7	0.08966	-0.00002	0.00395	0.00065	0.00460	0.09426
D8	0.09589	0.00008	0.00689	0.00419	0.01108	0.10697
D9	0.09113	-0.00002	0.00378	0.00051	0.00430	0.09543
D10	-0.62492	-0.00005	-0.00817	-0.00317	-0.01134	-0.63626
D11	2.56659	-0.00003	-0.00695	-0.00296	-0.00990	2.55669
D12	0.74975	-0.00005	0.00116	0.00005	0.00121	0.75096
D13	-2.42047	-0.00006	0.00024	-0.00020	0.00004	-2.42043
D14	-2.42115	-0.00006	0.00048	-0.00007	0.00041	-2.42074
D15	0.69182	-0.00007	-0.00043	-0.00032	-0.00076	0.69106
D16	2.41010	-0.00008	-0.00072	-0.00038	-0.00110	2.40900
D17	-0.69425	-0.00006	0.00022	-0.00022	-0.00000	-0.69426

D18 -0.62689 -0.00005 -0.00803 -0.00303 -0.01107 -0.63795
D19 2.56346 -0.00002 -0.00640 -0.00260 -0.00900 2.55445
D20 -0.69427 -0.00006 0.00023 -0.00022 0.00001 -0.69426
D21 2.41096 -0.00008 -0.00101 -0.00054 -0.00156 2.40940
D22 0.66965 -0.00002 -0.00009 -0.00015 -0.00024 0.66941

Item	Value	Threshold	Converged?
Maximum Force	0.000303	0.000450	YES
RMS Force	0.000073	0.000300	YES
Maximum Displacement	0.005971	0.001800	NO
RMS Displacement	0.001752	0.001200	NO

Predicted change in Energy=-2.546054D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 20:12:29 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.622483	-0.673185	0.012360
2	6	0	3.007218	-1.726778	0.053555
3	6	0	3.621458	0.675154	-0.011833
4	6	0	1.854872	-2.426569	0.056876
5	6	0	3.006639	1.728988	-0.053240
6	6	0	0.644974	-2.572529	0.063471
7	6	0	1.853331	2.427268	-0.056935
8	6	0	-0.665890	-2.253908	0.022075
9	6	0	0.643452	2.573256	-0.063764
10	6	0	-1.731113	-1.671677	-0.023246
11	6	0	-0.667151	2.253408	-0.022641
12	6	0	-2.686879	-0.680793	-0.167209
13	6	0	-1.732150	1.670754	0.022532
14	6	0	-2.687122	0.679179	0.166986
15	6	0	-4.042240	-0.405414	-0.601099
16	6	0	-4.041883	0.402845	0.602112

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220781	0.000000			
3	C	1.348556	2.480090	0.000000		
4	C	2.490138	1.348191	3.570187	0.000000	
5	C	2.480726	3.457416	1.220772	4.313624	0.000000
6	C	3.532093	2.509101	4.405970	1.218688	4.908577
7	C	3.570365	4.312744	2.489621	4.855172	1.348231

```
  8  C    4.570441   3.710873   5.192486   2.526908   5.418173
  9  C    4.406790   4.908304   3.531856   5.145906   2.509492
 10  C    5.446031   4.739274   5.844465   3.665457   5.831956
 11  C    5.192989   5.417442   4.569811   5.316871   3.711157
 12  C    6.311921   5.793579   6.454289   4.870878   6.183540
 13  C    5.845190   5.831449   5.445505   5.445729   4.739752
 14  C    6.454759   6.182799   6.311115   5.503409   5.793920
 15  C    7.693895   7.202044   7.761903   6.268487   7.385290
 16  C    7.761968   7.384174   7.692716   6.563123   7.202069
                6          7          8          9         10
  6  C    0.000000
  7  C    5.145152   0.000000
  8  C    1.349666   5.316590   0.000000
  9  C    5.147358   1.218674   5.002325   0.000000
 10  C    2.542606   5.445247   1.214804   4.864119   0.000000
 11  C    5.001876   2.526704   4.507538   1.349694   4.066732
 12  C    3.838375   5.503245   2.568056   4.657321   1.384219
 13  C    4.863933   3.665283   4.066925   2.542723   3.342744
 14  C    4.656950   4.870489   3.565022   3.838423   2.544929
 15  C    5.206536   6.563380   3.899361   5.578254   2.697896
 16  C    5.577599   6.267868   4.334986   5.206384   3.167707
               11         12         13         14         15
 11  C    0.000000
 12  C    3.565072   0.000000
 13  C    1.214804   2.545050   0.000000
 14  C    2.567963   1.400433   1.384218   0.000000
 15  C    4.335341   1.449517   3.167950   1.898063   0.000000
 16  C    3.899194   1.897936   2.697846   1.449507   1.449482
               16
 16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 5.38D-05
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.622268   -0.674369    0.010709
    2          6           0        3.006667   -1.727862    0.049387
    3          6           0        3.621674    0.674024   -0.010255
    4          6           0        1.854098   -2.427291    0.051045
    5          6           0        3.007190    1.728150   -0.049131
    6          6           0        0.644153   -2.572880    0.057303
```

```
     7        6        0        1.854105    2.426805   -0.051141
     8        6        0       -0.666610   -2.253742    0.016684
     9        6        0        0.644273    2.573196   -0.057608
    10        6        0       -1.731647   -1.671063   -0.027231
    11        6        0       -0.666432    2.253669   -0.017237
    12        6        0       -2.687097   -0.679533   -0.168810
    13        6        0       -1.731616    1.671248    0.026552
    14        6        0       -2.686903    0.679636    0.168641
    15        6        0       -4.042375   -0.402683   -0.602025
    16        6        0       -4.041748    0.402693    0.603118
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8474306           0.3942233           0.2718438
 Leave Link  202 at Fri Aug 21 20:12:29 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.6774361154 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0074931591 Hartrees.
 Nuclear repulsion after empirical dispersion term =      717.6699429562 Hartrees.
 Leave Link  301 at Fri Aug 21 20:12:29 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33582.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  4.29D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
```

Supporting Information file

IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 562 562 562 562 562 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 20:12:30 2026, MaxMem= 805306368 cpu: 3.3 elap: 0.6
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 20:12:30 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000019 0.000002 -0.000003 Ang= 0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 20:12:30 2026, MaxMem= 805306368 cpu: 1.9 elap: 0.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981514296594
DIIS: error= 2.70D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981514296594 IErMin= 1 ErrMin= 2.70D-04
ErrMax= 2.70D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.45D-05 BMatP= 5.45D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 2.70D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=6.38D-05 MaxDP=1.65D-03 OVMax= 7.06D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.15D-05 CP: 9.98D-01
E= -608.981536952752 Delta-E= -0.000022656157 Rises=F Damp=F
DIIS: error= 2.75D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981536952752 IErMin= 2 ErrMin= 2.75D-05
ErrMax= 2.75D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.33D-07 BMatP= 5.45D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.297D-01 0.103D+01
Coeff: -0.297D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=7.97D-06 MaxDP=2.28D-04 DE=-2.27D-05 OVMax= 3.44D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 4.95D-06 CP: 9.98D-01 1.10D+00
E= -608.981537837741 Delta-E= -0.000000884990 Rises=F Damp=F
DIIS: error= 2.13D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981537837741 IErMin= 3 ErrMin= 2.13D-05
ErrMax= 2.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.35D-07 BMatP= 4.33D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.177D-01 0.420D+00 0.598D+00
Coeff: -0.177D-01 0.420D+00 0.598D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.40D-06 MaxDP=8.27D-05 DE=-8.85D-07 OVMax= 1.67D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 2.22D-06 CP: 9.98D-01 1.10D+00 9.29D-01
E= -608.981538105512 Delta-E= -0.000000267770 Rises=F Damp=F
DIIS: error= 1.69D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981538105512 IErMin= 4 ErrMin= 1.69D-05
ErrMax= 1.69D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.75D-08 BMatP= 2.35D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.123D-02-0.135D+00 0.279D+00 0.856D+00
Coeff: 0.123D-02-0.135D+00 0.279D+00 0.856D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.53D-06 MaxDP=4.63D-05 DE=-2.68D-07 OVMax= 1.72D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 8.09D-07 CP: 9.98D-01 1.12D+00 1.12D+00 1.18D+00
E= -608.981538226637 Delta-E= -0.000000121125 Rises=F Damp=F
DIIS: error= 7.96D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981538226637 IErMin= 5 ErrMin= 7.96D-06
ErrMax= 7.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-08 BMatP= 5.75D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.279D-02-0.124D+00 0.875D-01 0.477D+00 0.557D+00
Coeff: 0.279D-02-0.124D+00 0.875D-01 0.477D+00 0.557D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.43D-07 MaxDP=1.87D-05 DE=-1.21D-07 OVMax= 8.51D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.93D-07 CP: 9.98D-01 1.12D+00 1.19D+00 1.20D+00 1.11D+00
E= -608.981538259018 Delta-E= -0.000000032381 Rises=F Damp=F
DIIS: error= 5.82D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981538259018 IErMin= 6 ErrMin= 5.82D-06
ErrMax= 5.82D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-09 BMatP= 1.45D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.121D-03 0.225D-01-0.745D-01-0.204D+00 0.102D+00 0.115D+01
Coeff: 0.121D-03 0.225D-01-0.745D-01-0.204D+00 0.102D+00 0.115D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.26D-07 MaxDP=1.95D-05 DE=-3.24D-08 OVMax= 1.08D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.19D-07 CP: 9.98D-01 1.12D+00 1.22D+00 1.32D+00 1.46D+00
CP: 1.40D+00
E= -608.981538278401 Delta-E= -0.000000019383 Rises=F Damp=F
DIIS: error= 3.14D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981538278401 IErMin= 7 ErrMin= 3.14D-06
ErrMax= 3.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.92D-10 BMatP= 2.16D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.768D-03 0.412D-01-0.447D-01-0.196D+00-0.135D+00 0.325D+00
Coeff-Com: 0.101D+01
Coeff: -0.768D-03 0.412D-01-0.447D-01-0.196D+00-0.135D+00 0.325D+00
Coeff: 0.101D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.07D-07 MaxDP=8.48D-06 DE=-1.94D-08 OVMax= 7.10D-05

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.20D-07 CP: 9.98D-01 1.12D+00 1.24D+00 1.33D+00 1.65D+00
CP: 1.76D+00 1.57D+00
E= -608.981538284068 Delta-E= -0.000000005668 Rises=F Damp=F
DIIS: error= 1.32D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -608.981538284068 IErMin= 8 ErrMin= 1.32D-06
ErrMax= 1.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-10 BMatP= 5.92D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.401D-03 0.144D-01-0.508D-02-0.475D-01-0.846D-01-0.974D-01
Coeff-Com: 0.453D+00 0.767D+00
Coeff: -0.401D-03 0.144D-01-0.508D-02-0.475D-01-0.846D-01-0.974D-01
Coeff: 0.453D+00 0.767D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.17D-07 MaxDP=2.62D-06 DE=-5.67D-09 OVMax= 2.99D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.87D-08 CP: 9.98D-01 1.12D+00 1.25D+00 1.33D+00 1.67D+00
CP: 1.87D+00 1.95D+00 1.26D+00
E= -608.981538285120 Delta-E= -0.000000001051 Rises=F Damp=F
DIIS: error= 7.66D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -608.981538285120 IErMin= 9 ErrMin= 7.66D-07
ErrMax= 7.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.20D-11 BMatP= 1.80D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.246D-04-0.263D-02 0.852D-02 0.237D-01-0.126D-01-0.136D+00
Coeff-Com: -0.113D-01 0.406D+00 0.725D+00
Coeff: -0.246D-04-0.263D-02 0.852D-02 0.237D-01-0.126D-01-0.136D+00
Coeff: -0.113D-01 0.406D+00 0.725D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=6.63D-08 MaxDP=1.98D-06 DE=-1.05D-09 OVMax= 1.32D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.53D-08 CP: 9.98D-01 1.12D+00 1.25D+00 1.32D+00 1.67D+00
CP: 1.90D+00 2.12D+00 1.55D+00 1.29D+00
E= -608.981538285392 Delta-E= -0.000000000272 Rises=F Damp=F
DIIS: error= 2.80D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981538285392 IErMin=10 ErrMin= 2.80D-07
ErrMax= 2.80D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-11 BMatP= 6.20D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.131D-03-0.628D-02 0.560D-02 0.282D-01 0.275D-01-0.260D-01
Coeff-Com: -0.186D+00-0.880D-01 0.339D+00 0.906D+00
Coeff: 0.131D-03-0.628D-02 0.560D-02 0.282D-01 0.275D-01-0.260D-01
Coeff: -0.186D+00-0.880D-01 0.339D+00 0.906D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=5.49D-08 MaxDP=2.16D-06 DE=-2.72D-10 OVMax= 8.49D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.72D-08 CP: 9.98D-01 1.12D+00 1.25D+00 1.31D+00 1.65D+00
CP: 1.93D+00 2.22D+00 1.73D+00 1.63D+00 1.55D+00
E= -608.981538285468 Delta-E= -0.000000000076 Rises=F Damp=F
DIIS: error= 8.78D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981538285468 IErMin=11 ErrMin= 8.78D-08
ErrMax= 8.78D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-12 BMatP= 1.46D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.211D-04-0.469D-03-0.554D-03 0.973D-04 0.696D-02 0.190D-01
Coeff-Com: -0.296D-01-0.816D-01-0.583D-01 0.185D+00 0.959D+00
Coeff: 0.211D-04-0.469D-03-0.554D-03 0.973D-04 0.696D-02 0.190D-01
Coeff: -0.296D-01-0.816D-01-0.583D-01 0.185D+00 0.959D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.64D-08 MaxDP=8.92D-07 DE=-7.59D-11 OVMax= 2.01D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 7.36D-09 CP: 9.98D-01 1.12D+00 1.25D+00 1.31D+00 1.65D+00
CP: 1.93D+00 2.22D+00 1.76D+00 1.75D+00 1.91D+00
CP: 1.34D+00
E= -608.981538285479 Delta-E= -0.000000000011 Rises=F Damp=F
DIIS: error= 4.99D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981538285479 IErMin=12 ErrMin= 4.99D-08
ErrMax= 4.99D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.53D-13 BMatP= 1.54D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.191D-04 0.116D-02-0.150D-02-0.629D-02-0.263D-02 0.162D-01

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 Coeff-Com:  0.244D-01-0.222D-01-0.978D-01-0.104D+00 0.457D+00 0.735D+00
 Coeff:     -0.191D-04 0.116D-02-0.150D-02-0.629D-02-0.263D-02 0.162D-01
 Coeff:      0.244D-01-0.222D-01-0.978D-01-0.104D+00 0.457D+00 0.735D+00
 Gap=     0.247 Goal=   None    Shift=    0.000
 RMSDP=8.04D-09 MaxDP=4.31D-07 DE=-1.14D-11 OVMax= 9.20D-07

 SCF Done:  E(RwB97XD) =  -608.981538285     A.U. after   12 cycles
          NFock= 12  Conv=0.80D-08     -V/T= 2.0045
 KE= 6.062447872355D+02 PE=-2.846341858416D+03 EE= 9.134455899387D+02
 Leave Link  502 at Fri Aug 21 20:22:34 2026, MaxMem=    805306368 cpu:             3620.5 elap:
603.6
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33582.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 Leave Link  701 at Fri Aug 21 20:22:34 2026, MaxMem=    805306368 cpu:                4.2 elap:
0.7
 (Enter /home/user/gauss16/g16/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link  702 at Fri Aug 21 20:22:35 2026, MaxMem=    805306368 cpu:                0.3 elap:
0.1
 (Enter /home/user/gauss16/g16/l703.exe)
 Integral derivatives from FoFJK, PRISM(SPDF).
 Compute integral first derivatives, UseDBF=F ICtDFT=          0.
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=         800
        NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
        wScrn=  0.000000 ICntrl=      2527 IOpCl=  0 I1Cent=          0 NGrid=          0
        NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 Leave Link  703 at Fri Aug 21 20:30:25 2026, MaxMem=    805306368 cpu:             2822.9 elap:
470.5
 (Enter /home/user/gauss16/g16/l716.exe)
 Dipole        = 1.51754080D+00-1.89892547D-03-3.05358975D-04
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
     1        6          0.000021870   -0.000090482   -0.000240125
     2        6          0.000102458   -0.000007855    0.000269207
     3        6          0.000066036    0.000102335    0.000240202
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     4        6       -0.000029972   -0.000057410   -0.000272002
     5        6        0.000069323   -0.000018003   -0.000272452
     6        6       -0.000019026   -0.000047678    0.000254688
     7        6       -0.000016049    0.000086206    0.000281359
     8        6        0.000031974   -0.000016601   -0.000135226
     9        6       -0.000020969    0.000026426   -0.000265317
    10        6       -0.000140932   -0.000062026   -0.000008948
    11        6        0.000030412    0.000023565    0.000132523
    12        6        0.000212045    0.000202252    0.000194385
    13        6       -0.000137323    0.000059898    0.000024268
    14        6        0.000202828   -0.000200725   -0.000200428
    15        6       -0.000188190    0.000050152   -0.000060347
    16        6       -0.000184484   -0.000050053    0.000058212
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000281359 RMS     0.000145596
 Leave Link  716 at Fri Aug 21 20:30:25 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000183572 RMS     0.000074995
 Search for a local minimum.
 Step number  10 out of a maximum of   71
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .74995D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4    5
                                      6    7    8    9   10
 DE= -4.24D-06 DEPred=-2.55D-06 R= 1.66D+00
 TightC=F SS=  1.41D+00  RLast= 3.19D-02 DXNew= 8.4853D-01 9.5654D-02
 Trust test= 1.66D+00 RLast= 3.19D-02 DXMaxT set to 5.05D-01
 ITU=  1  1  1  1  1  1  1  1  1  0
    Eigenvalues ---    0.00330   0.01290   0.01570   0.01731   0.02119
    Eigenvalues ---    0.02626   0.02785   0.03335   0.03422   0.03926
    Eigenvalues ---    0.04047   0.06915   0.08126   0.08439   0.09397
    Eigenvalues ---    0.10628   0.24385   0.24426   0.24687   0.24988
    Eigenvalues ---    0.24994   0.24995   0.25000   0.25000   0.25012
    Eigenvalues ---    0.25650   0.28166   0.32710   0.36018   0.43155
    Eigenvalues ---    0.51320   0.54132   0.57377   0.58118   0.58172
    Eigenvalues ---    0.58400   0.78666   0.79237   0.79695   0.81366
    Eigenvalues ---    0.82167   0.92886
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    10    9    8    7    6    5    4
 RFO step:  Lambda=-2.27660351D-06.
 NNeg= 0 NGDIIS= 7 SimSw=  2.50D-01 Rises=F DC= -4.24D-06 SmlDif=  1.00D-05
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Supporting Information file

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 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.2276392689D-02 NUsed= 7 OKEnD=F EnDIS=F
 InvSVX:  RCond= 1.08D-08 Info=          0 Equed=N FErr=  7.70D-11 BErr=  4.84D-17
 DIIS inversion failure, remove point   7.
 InvSVX:  RCond= 1.77D-08 Info=          0 Equed=N FErr=  5.46D-11 BErr=  2.97D-17
 DIIS inversion failure, remove point   6.
 InvSVX:  RCond= 2.76D-08 Info=          0 Equed=N FErr=  3.59D-11 BErr=  3.38D-17
 DIIS inversion failure, remove point   5.
 InvSVX:  RCond= 5.72D-08 Info=          0 Equed=N FErr=  1.99D-11 BErr=  5.59D-17
 DIIS inversion failure, remove point   4.
 InvSVX:  RCond= 2.50D-07 Info=          0 Equed=N FErr=  3.36D-12 BErr=  5.42D-17
 RFO-DIIS uses    3 points instead of    7
 DidBck=F Rises=F RFO-DIIS coefs:    1.94016   -1.67111    0.73095    0.00000    0.00000
              RFO-DIIS coefs:    0.00000    0.00000
 Iteration  1 RMS(Cart)=  0.00071248 RMS(Int)=  0.00000254
 Iteration  2 RMS(Cart)=  0.00000137 RMS(Int)=  0.00000144
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000144
  ITry=  1  IFail=0  DXMaxC=  2.59D-03  DCOld=  1.00D+10  DXMaxT=  5.05D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)    (Quad)   (Total)
   R1        2.30694   0.00010  -0.00004   0.00015   0.00011   2.30705
   R2        2.54840   0.00018   0.00017   0.00006   0.00023   2.54863
   R3        2.54771   0.00016   0.00010   0.00006   0.00016   2.54787
   R4        2.30692   0.00010  -0.00004   0.00015   0.00011   2.30704
   R5        2.30299   0.00011  -0.00005   0.00016   0.00011   2.30310
   R6        2.54779   0.00015   0.00008   0.00005   0.00013   2.54792
   R7        2.55050   0.00009   0.00004   0.00000   0.00005   2.55055
   R8        2.30296   0.00011  -0.00004   0.00016   0.00012   2.30308
   R9        2.29565   0.00012  -0.00000   0.00015   0.00015   2.29580
  R10        2.55055   0.00009   0.00003   0.00000   0.00003   2.55059
  R11        2.61579   0.00005  -0.00003  -0.00003  -0.00007   2.61573
  R12        2.29565   0.00012  -0.00000   0.00015   0.00015   2.29579
  R13        2.64643  -0.00010  -0.00030  -0.00033  -0.00063   2.64580
  R14        2.73919   0.00018   0.00068   0.00052   0.00120   2.74039
  R15        2.61579   0.00005  -0.00002  -0.00004  -0.00006   2.61573
  R16        2.73917   0.00018   0.00072   0.00051   0.00123   2.74040
  R17        2.73912  -0.00002  -0.00157  -0.00013  -0.00169   2.73743
   A1        2.61223   0.00003  -0.00013   0.00017   0.00004   2.61227
   A2        2.64422  -0.00001  -0.00011  -0.00004  -0.00016   2.64406
   A3        2.61416  -0.00000  -0.00062   0.00009  -0.00054   2.61362
   A4        2.71589   0.00000   0.00002   0.00001   0.00003   2.71592
   A5        2.64248   0.00001   0.00033   0.00003   0.00036   2.64284
   A6        2.78133  -0.00004   0.00048  -0.00026   0.00022   2.78155
   A7        2.71725  -0.00002  -0.00033  -0.00005  -0.00037   2.71687
   A8        2.78038  -0.00002   0.00072  -0.00023   0.00049   2.78088
   A9        2.83189  -0.00006  -0.00028  -0.00019  -0.00048   2.83141
  A10        2.30563   0.00009  -0.00026   0.00047   0.00020   2.30583
```

A11	2.51965	-0.00010	0.00048	-0.00047	0.00001	2.51966
A12	1.45733	0.00000	-0.00024	0.00001	-0.00022	1.45711
A13	2.83143	-0.00005	-0.00015	-0.00018	-0.00033	2.83109
A14	2.30585	0.00009	-0.00034	0.00046	0.00013	2.30597
A15	1.45722	0.00001	-0.00017	0.00001	-0.00016	1.45705
A16	2.51956	-0.00010	0.00048	-0.00046	0.00002	2.51958
A17	1.42754	-0.00002	0.00025	-0.00005	0.00020	1.42774
A18	1.42766	-0.00002	0.00017	-0.00004	0.00013	1.42779
A19	2.87989	-0.00000	-0.00032	0.00004	-0.00028	2.87961
A20	2.88042	-0.00001	-0.00047	0.00004	-0.00043	2.87999
A21	3.13995	0.00009	0.00167	-0.00028	0.00139	3.14134
A22	3.13988	0.00009	0.00161	0.00003	0.00164	3.14152
D1	0.07922	0.00006	0.00392	0.00087	0.00480	0.08402
D2	-0.07278	-0.00001	-0.00326	-0.00120	-0.00446	-0.07724
D3	-0.07391	-0.00003	-0.00552	-0.00079	-0.00630	-0.08021
D4	0.07916	0.00006	0.00404	0.00085	0.00490	0.08406
D5	0.10752	0.00003	0.00648	0.00080	0.00728	0.11480
D6	-0.07343	-0.00003	-0.00582	-0.00078	-0.00660	-0.08003
D7	0.09426	-0.00004	0.00149	-0.00068	0.00081	0.09506
D8	0.10697	0.00003	0.00677	0.00084	0.00761	0.11458
D9	0.09543	-0.00004	0.00128	-0.00078	0.00050	0.09592
D10	-0.63626	-0.00000	-0.00623	0.00112	-0.00511	-0.64137
D11	2.55669	-0.00002	-0.00543	0.00065	-0.00479	2.55190
D12	0.75096	-0.00002	0.00071	-0.00064	0.00007	0.75102
D13	-2.42043	-0.00002	0.00005	-0.00031	-0.00026	-2.42069
D14	-2.42074	-0.00002	0.00026	-0.00038	-0.00012	-2.42086
D15	0.69106	-0.00001	-0.00040	-0.00005	-0.00045	0.69061
D16	2.40900	-0.00004	-0.00085	0.00022	-0.00063	2.40836
D17	-0.69426	-0.00005	-0.00025	-0.00015	-0.00040	-0.69466
D18	-0.63795	0.00000	-0.00604	0.00130	-0.00474	-0.64269
D19	2.55445	-0.00001	-0.00488	0.00069	-0.00419	2.55027
D20	-0.69426	-0.00005	-0.00024	-0.00015	-0.00039	-0.69465
D21	2.40940	-0.00004	-0.00112	0.00032	-0.00080	2.40860
D22	0.66941	-0.00003	-0.00010	-0.00009	-0.00020	0.66921

Item	Value	Threshold	Converged?
Maximum Force	0.000184	0.000450	YES
RMS Force	0.000075	0.000300	YES
Maximum Displacement	0.002588	0.001800	NO
RMS Displacement	0.000713	0.001200	YES

Predicted change in Energy=-1.023448D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 20:30:25 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Supporting Information file

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.622838	-0.673225	0.011716
2	6	0	3.007490	-1.726810	0.053562
3	6	0	3.621999	0.675252	-0.011480
4	6	0	1.854973	-2.426482	0.055949
5	6	0	3.006776	1.728897	-0.053436
6	6	0	0.645010	-2.572333	0.063750
7	6	0	1.853460	2.427305	-0.055958
8	6	0	-0.665950	-2.254040	0.022016
9	6	0	0.643485	2.572960	-0.063840
10	6	0	-1.731260	-1.671693	-0.021876
11	6	0	-0.667229	2.253563	-0.022166
12	6	0	-2.686802	-0.680760	-0.166639
13	6	0	-1.732278	1.670718	0.021456
14	6	0	-2.687114	0.679138	0.166459
15	6	0	-4.042735	-0.405345	-0.600841
16	6	0	-4.042663	0.402855	0.601329

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220838	0.000000			
3	C	1.348676	2.480273	0.000000		
4	C	2.490224	1.348274	3.570390	0.000000	
5	C	2.480719	3.457363	1.220831	4.313443	0.000000
6	C	3.532248	2.509248	4.406237	1.218746	4.908385
7	C	3.570513	4.312825	2.489860	4.855077	1.348302
8	C	4.570862	3.711216	5.193108	2.527041	5.418338
9	C	4.406809	4.908190	3.532079	5.145530	2.509521
10	C	5.446506	4.739671	5.845138	3.665628	5.832151
11	C	5.193449	5.417810	4.570411	5.316994	3.711410
12	C	6.312164	5.793762	6.454751	4.870812	6.183534
13	C	5.845633	5.831778	5.446129	5.445788	4.740002
14	C	6.455101	6.183030	6.311624	5.503421	5.794026
15	C	7.694673	7.202791	7.762937	6.268917	7.385814
16	C	7.763085	7.385133	7.693945	6.563893	7.202895

		6	7	8	9	10
6	C	0.000000				
7	C	5.145003	0.000000			
8	C	1.349692	5.316812	0.000000		
9	C	5.146875	1.218736	5.002191	0.000000	
10	C	2.542665	5.445472	1.214883	4.863975	0.000000
11	C	5.001861	2.526896	4.507819	1.349713	4.066914
12	C	3.838241	5.503299	2.568003	4.657046	1.384184
13	C	4.863822	3.665506	4.067035	2.542748	3.342692
14	C	4.656787	4.870562	3.565039	3.838293	2.544707

```
  15  C    5.206964   6.563987   3.899782   5.578471   2.698473
  16  C    5.578083   6.268548   4.335537   5.206899   3.167762
             11         12         13         14         15
  11  C    0.000000
  12  C    3.565080   0.000000
  13  C    1.214882   2.544788   0.000000
  14  C    2.567942   1.400099   1.384185   0.000000
  15  C    4.335746   1.450152   3.167886   1.898041   0.000000
  16  C    3.899669   1.897987   2.698446   1.450157   1.448586
             16
  16  C    0.000000
 Stoichiometry    C16
 Framework group  C1[X(C16)]
 Deg. of freedom    42
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 1.19D-05
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.622628   -0.674380    0.010077
     2          6           0        3.006952   -1.727871    0.049402
     3          6           0        3.622209    0.674148   -0.009889
     4          6           0        1.854217   -2.427187    0.050122
     5          6           0        3.007314    1.728083   -0.049316
     6          6           0        0.644209   -2.572679    0.057583
     7          6           0        1.854216    2.426854   -0.050156
     8          6           0       -0.666652   -2.253878    0.016621
     9          6           0        0.644287    2.572905   -0.057680
    10          6           0       -1.731781   -1.671096   -0.025869
    11          6           0       -0.666527    2.253817   -0.016762
    12          6           0       -2.687015   -0.679522   -0.168250
    13          6           0       -1.731757    1.671202    0.025471
    14          6           0       -2.686902    0.679575    0.168105
    15          6           0       -4.042865   -0.402644   -0.601781
    16          6           0       -4.042533    0.402673    0.602322
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8474928           0.3941534           0.2718102
 Leave Link  202 at Fri Aug 21 20:30:25 2026, MaxMem=    805306368 cpu:                 0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
```

```
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.6511336511 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0074926751 Hartrees.
 Nuclear repulsion after empirical dispersion term =      717.6436409760 Hartrees.
 Leave Link  301 at Fri Aug 21 20:30:25 2026, MaxMem=    805306368 cpu:                 0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33580.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   496 RedAO= T EigKep=  4.36D-06  NBF=   496
 NBsUse=   496 1.00D-06 EigRej= -1.00D+00 NBFU=   496
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=         32
 NSgBfM=   564   564   564   564   564 MxSgAt=    16 MxSgA2=    16.
 Leave Link  302 at Fri Aug 21 20:30:26 2026, MaxMem=    805306368 cpu:                 3.4 elap:
0.6
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Aug 21 20:30:26 2026, MaxMem=    805306368 cpu:                 0.5 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca.chk"
 B after Tr=     0.000000    0.000000    0.000000
       Rot=    1.000000   -0.000000    0.000002   -0.000004 Ang=  -0.00 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Leave Link  401 at Fri Aug 21 20:30:26 2026, MaxMem=    805306368 cpu:                 2.0 elap:
0.3
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
```

Supporting Information file

Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981532932494
DIIS: error= 1.42D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981532932494 IErMin= 1 ErrMin= 1.42D-04
ErrMax= 1.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-05 BMatP= 1.42D-05
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.42D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.960 Goal= None Shift= 0.000
RMSDP=4.81D-05 MaxDP=1.23D-03 OVMax= 4.38D-04

Cycle 2 Pass 1 IDiag 1:
RMSU= 4.61D-05 CP: 9.98D-01
E= -608.981539607835 Delta-E= -0.000006675341 Rises=F Damp=F
DIIS: error= 1.71D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -608.981539607835 IErMin= 2 ErrMin= 1.71D-05
ErrMax= 1.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-07 BMatP= 1.42D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.327D-01 0.103D+01
Coeff: -0.327D-01 0.103D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=4.47D-06 MaxDP=1.35D-04 DE=-6.68D-06 OVMax= 3.09D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 2.67D-06 CP: 9.98D-01 1.08D+00
E= -608.981540007872 Delta-E= -0.000000400037 Rises=F Damp=F
DIIS: error= 1.14D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -608.981540007872 IErMin= 3 ErrMin= 1.14D-05
ErrMax= 1.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.49D-08 BMatP= 1.45D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.171D-01 0.324D+00 0.693D+00

Coeff: -0.171D-01 0.324D+00 0.693D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.48D-06 MaxDP=5.38D-05 DE=-4.00D-07 OVMax= 1.24D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 1.40D-06 CP: 9.98D-01 1.08D+00 9.08D-01
E= -608.981540105893 Delta-E= -0.000000098021 Rises=F Damp=F
DIIS: error= 8.95D-06 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -608.981540105893 IErMin= 4 ErrMin= 8.95D-06
ErrMax= 8.95D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.94D-08 BMatP= 5.49D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.349D-02-0.203D+00 0.317D+00 0.882D+00
Coeff: 0.349D-02-0.203D+00 0.317D+00 0.882D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=9.79D-07 MaxDP=4.81D-05 DE=-9.80D-08 OVMax= 1.35D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 5.81D-07 CP: 9.98D-01 1.08D+00 1.19D+00 1.01D+00
E= -608.981540169085 Delta-E= -0.000000063191 Rises=F Damp=F
DIIS: error= 5.47D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -608.981540169085 IErMin= 5 ErrMin= 5.47D-06
ErrMax= 5.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-09 BMatP= 1.94D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.288D-02-0.936D-01 0.219D-01 0.238D+00 0.831D+00
Coeff: 0.288D-02-0.936D-01 0.219D-01 0.238D+00 0.831D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.84D-07 MaxDP=1.12D-05 DE=-6.32D-08 OVMax= 7.69D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.22D-07 CP: 9.98D-01 1.08D+00 1.27D+00 1.09D+00 1.31D+00
E= -608.981540183043 Delta-E= -0.000000013958 Rises=F Damp=F
DIIS: error= 4.51D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -608.981540183043 IErMin= 6 ErrMin= 4.51D-06
ErrMax= 4.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-09 BMatP= 2.45D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.354D-03 0.285D-01-0.127D+00-0.246D+00 0.536D+00 0.807D+00
Coeff: 0.354D-03 0.285D-01-0.127D+00-0.246D+00 0.536D+00 0.807D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=3.43D-07 MaxDP=1.13D-05 DE=-1.40D-08 OVMax= 6.94D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.56D-07 CP: 9.98D-01 1.09D+00 1.32D+00 1.20D+00 1.62D+00
CP: 1.47D+00
E= -608.981540191591 Delta-E= -0.000000008548 Rises=F Damp=F
DIIS: error= 1.92D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -608.981540191591 IErMin= 7 ErrMin= 1.92D-06
ErrMax= 1.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.59D-10 BMatP= 1.54D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.955D-03 0.443D-01-0.493D-01-0.166D+00-0.124D+00 0.271D+00
Coeff-Com: 0.102D+01
Coeff: -0.955D-03 0.443D-01-0.493D-01-0.166D+00-0.124D+00 0.271D+00
Coeff: 0.102D+01
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=2.35D-07 MaxDP=6.86D-06 DE=-8.55D-09 OVMax= 5.00D-05

Cycle   8 Pass 1 IDiag 1:
RMSU= 8.78D-08   CP: 9.98D-01 1.09D+00 1.36D+00 1.21D+00 1.79D+00
               CP: 1.96D+00 1.53D+00
E= -608.981540193959   Delta-E=   -0.000000002368 Rises=F Damp=F
DIIS: error= 6.79D-07 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -608.981540193959   IErMin= 8 ErrMin= 6.79D-07
ErrMax= 6.79D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.20D-11 BMatP= 2.59D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.434D-03 0.137D-01-0.324D-02-0.338D-01-0.115D+00 0.358D-02
Coeff-Com: 0.375D+00 0.760D+00
Coeff: -0.434D-03 0.137D-01-0.324D-02-0.338D-01-0.115D+00 0.358D-02
Coeff: 0.375D+00 0.760D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=7.44D-08 MaxDP=2.39D-06 DE=-2.37D-09 OVMax= 1.36D-05

Cycle   9 Pass 1 IDiag 1:
RMSU= 3.57D-08   CP: 9.98D-01 1.09D+00 1.36D+00 1.21D+00 1.80D+00
               CP: 2.12D+00 1.72D+00 1.28D+00
E= -608.981540194243   Delta-E=   -0.000000000284 Rises=F Damp=F
DIIS: error= 3.63D-07 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -608.981540194243   IErMin= 9 ErrMin= 3.63D-07
ErrMax= 3.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-11 BMatP= 5.20D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.884D-04-0.793D-02 0.145D-01 0.383D-01-0.139D-01-0.929D-01
Coeff-Com: -0.172D+00 0.411D+00 0.823D+00
Coeff: 0.884D-04-0.793D-02 0.145D-01 0.383D-01-0.139D-01-0.929D-01
Coeff: -0.172D+00 0.411D+00 0.823D+00
Gap=   0.247 Goal=   None   Shift=   0.000
RMSDP=5.22D-08 MaxDP=1.85D-06 DE=-2.84D-10 OVMax= 8.82D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.24D-08   CP: 9.98D-01 1.09D+00 1.37D+00 1.20D+00 1.79D+00
               CP: 2.20D+00 1.86D+00 1.55D+00 1.30D+00
E= -608.981540194354   Delta-E=   -0.000000000111 Rises=F Damp=F
DIIS: error= 1.45D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -608.981540194354   IErMin=10 ErrMin= 1.45D-07
ErrMax= 1.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.06D-12 BMatP= 2.23D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.141D-03-0.674D-02 0.687D-02 0.248D-01 0.271D-01-0.440D-01
Coeff-Com: -0.181D+00-0.756D-02 0.384D+00 0.796D+00
Coeff: 0.141D-03-0.674D-02 0.687D-02 0.248D-01 0.271D-01-0.440D-01

Coeff: -0.181D+00-0.756D-02 0.384D+00 0.796D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.34D-08 MaxDP=1.03D-06 DE=-1.11D-10 OVMax= 3.70D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 8.33D-09 CP: 9.98D-01 1.09D+00 1.37D+00 1.19D+00 1.79D+00
CP: 2.22D+00 1.89D+00 1.65D+00 1.58D+00 1.46D+00
E= -608.981540194374 Delta-E= -0.000000000020 Rises=F Damp=F
DIIS: error= 5.34D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -608.981540194374 IErMin=11 ErrMin= 5.34D-08
ErrMax= 5.34D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.97D-13 BMatP= 5.06D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.204D-04-0.139D-03-0.142D-02-0.180D-02 0.148D-01 0.877D-02
Coeff-Com: -0.231D-01-0.110D+00-0.596D-01 0.308D+00 0.865D+00
Coeff: 0.204D-04-0.139D-03-0.142D-02-0.180D-02 0.148D-01 0.877D-02
Coeff: -0.231D-01-0.110D+00-0.596D-01 0.308D+00 0.865D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=1.26D-08 MaxDP=6.10D-07 DE=-2.05D-11 OVMax= 1.53D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.69D-09 CP: 9.98D-01 1.09D+00 1.37D+00 1.19D+00 1.79D+00
CP: 2.21D+00 1.88D+00 1.67D+00 1.77D+00 1.75D+00
CP: 1.40D+00
E= -608.981540194379 Delta-E= -0.000000000005 Rises=F Damp=F
DIIS: error= 3.00D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -608.981540194379 IErMin=12 ErrMin= 3.00D-08
ErrMax= 3.00D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.90D-13 BMatP= 9.97D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.220D-04 0.143D-02-0.219D-02-0.669D-02 0.221D-02 0.145D-01
Coeff-Com: 0.258D-01-0.534D-01-0.109D+00-0.150D-01 0.432D+00 0.710D+00
Coeff: -0.220D-04 0.143D-02-0.219D-02-0.669D-02 0.221D-02 0.145D-01
Coeff: 0.258D-01-0.534D-01-0.109D+00-0.150D-01 0.432D+00 0.710D+00
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=6.40D-09 MaxDP=2.78D-07 DE=-5.00D-12 OVMax= 6.68D-07

SCF Done: E(RwB97XD) = -608.981540194 A.U. after 12 cycles
NFock= 12 Conv=0.64D-08 -V/T= 2.0045
KE= 6.062420690731D+02 PE=-2.846286594698D+03 EE= 9.134193444550D+02
Leave Link 502 at Fri Aug 21 20:38:11 2026, MaxMem= 805306368 cpu: 2786.4 elap: 464.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 7 Len= 274

Leave Link 701 at Fri Aug 21 20:38:11 2026, MaxMem= 805306368 cpu: 2.1 elap: 0.4
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 20:38:11 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 2462.4 elap: 410.4
(Enter /home/user/gauss16/g16/l716.exe)
Dipole = 1.51648605D+00-1.36620676D-03-1.34471627D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000026695	-0.000040585	-0.000199513
2	6	0.000064794	0.000017116	0.000201414
3	6	0.000005232	0.000048433	0.000198632
4	6	-0.000029035	-0.000005914	-0.000184797
5	6	0.000041019	-0.000035041	-0.000201661
6	6	0.000000939	-0.000053202	0.000163728
7	6	-0.000017699	0.000026579	0.000189342
8	6	0.000014154	0.000044764	-0.000031415
9	6	-0.000002106	0.000037122	-0.000162680
10	6	-0.000075257	-0.000105408	-0.000118629
11	6	0.000014127	-0.000038161	0.000013713
12	6	0.000110816	0.000188858	0.000193858
13	6	-0.000074866	0.000102600	0.000136547
14	6	0.000105351	-0.000185022	-0.000193038
15	6	-0.000070758	-0.000082644	-0.000131243
16	6	-0.000060019	0.000080508	0.000125743

Cartesian Forces: Max 0.000201661 RMS 0.000111407
Leave Link 716 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

Supporting Information file

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000108465 RMS 0.000041757
Search for a local minimum.
Step number 11 out of a maximum of 71
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .41757D-04 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 1 2 3 4 5
6 7 8 9 10
11
DE= -1.91D-06 DEPred=-1.02D-06 R= 1.87D+00
TightC=F SS= 1.41D+00 RLast= 1.91D-02 DXNew= 8.4853D-01 5.7341D-02
Trust test= 1.87D+00 RLast= 1.91D-02 DXMaxT set to 5.05D-01
ITU= 1 1 1 1 1 1 1 1 1 1 0
Eigenvalues --- 0.00288 0.01290 0.01565 0.01615 0.01735
Eigenvalues --- 0.02626 0.02770 0.03294 0.03422 0.03926
Eigenvalues --- 0.04057 0.07224 0.08044 0.08443 0.09471
Eigenvalues --- 0.10199 0.24404 0.24561 0.24696 0.24988
Eigenvalues --- 0.24993 0.24995 0.25000 0.25000 0.25020
Eigenvalues --- 0.26628 0.28165 0.31862 0.35533 0.40320
Eigenvalues --- 0.51320 0.53500 0.57376 0.57991 0.58167
Eigenvalues --- 0.58204 0.78666 0.79299 0.79695 0.81379
Eigenvalues --- 0.82166 0.87958
En-DIIS/RFO-DIIS/Sim-DIIS IScMMF= -3 using points: 11 10 9 8 7 6 5 4
RFO step: Lambda=-1.17424508D-06.
NNeg= 0 NGDIIS= 8 SimSw= 2.50D-01 Rises=F DC= -1.91D-06 SmlDif= 1.00D-05
NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj= 3.0
RMS Error= 0.1583635339D-02 NUsed= 8 OKEnD=F EnDIS=F
InvSVX: RCond= 7.43D-09 Info= 0 Equed=N FErr= 6.55D-11 BErr= 1.42D-17
DIIS inversion failure, remove point 8.
InvSVX: RCond= 9.29D-09 Info= 0 Equed=N FErr= 5.13D-11 BErr= 5.12D-17
DIIS inversion failure, remove point 7.
InvSVX: RCond= 1.39D-08 Info= 0 Equed=N FErr= 3.39D-11 BErr= 8.73D-17
DIIS inversion failure, remove point 6.
InvSVX: RCond= 1.66D-08 Info= 0 Equed=N FErr= 3.13D-11 BErr= 8.65D-17
DIIS inversion failure, remove point 5.
InvSVX: RCond= 5.70D-08 Info= 0 Equed=N FErr= 9.36D-12 BErr= 5.34D-17
DIIS inversion failure, remove point 4.
InvSVX: RCond= 6.27D-07 Info= 0 Equed=N FErr= 4.75D-13 BErr= 3.70D-17
RFO-DIIS uses 3 points instead of 8
DidBck=F Rises=F RFO-DIIS coefs: 2.48602 -1.99894 0.51292 0.00000 0.00000
RFO-DIIS coefs: 0.00000 0.00000 0.00000
Iteration 1 RMS(Cart)= 0.00060599 RMS(Int)= 0.00000187

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Iteration 2 RMS(Cart)= 0.00000083 RMS(Int)= 0.00000158
ITry= 1 IFail=0 DXMaxC= 1.75D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.30705	0.00001	0.00015	-0.00015	-0.00000	2.30705
R2	2.54863	0.00005	0.00039	-0.00025	0.00014	2.54877
R3	2.54787	0.00006	0.00032	-0.00019	0.00013	2.54800
R4	2.30704	0.00001	0.00015	-0.00014	0.00000	2.30704
R5	2.30310	0.00002	0.00016	-0.00014	0.00003	2.30312
R6	2.54792	0.00005	0.00030	-0.00019	0.00011	2.54804
R7	2.55055	0.00003	0.00015	-0.00011	0.00004	2.55059
R8	2.30308	0.00002	0.00017	-0.00013	0.00004	2.30311
R9	2.29580	0.00002	0.00021	-0.00016	0.00005	2.29584
R10	2.55059	0.00002	0.00014	-0.00011	0.00003	2.55062
R11	2.61573	0.00002	0.00002	-0.00001	0.00001	2.61574
R12	2.29579	0.00002	0.00020	-0.00015	0.00005	2.29584
R13	2.64580	-0.00007	-0.00094	0.00021	-0.00073	2.64508
R14	2.74039	0.00007	0.00151	-0.00065	0.00086	2.74125
R15	2.61573	0.00002	0.00003	-0.00002	0.00001	2.61574
R16	2.74040	0.00006	0.00151	-0.00068	0.00084	2.74124
R17	2.73743	0.00009	-0.00140	0.00078	-0.00063	2.73680
A1	2.61227	0.00005	0.00020	0.00016	0.00036	2.61263
A2	2.64406	-0.00001	-0.00016	-0.00000	-0.00016	2.64389
A3	2.61362	0.00003	-0.00025	0.00013	-0.00013	2.61350
A4	2.71592	-0.00001	0.00007	-0.00010	-0.00003	2.71589
A5	2.64284	0.00001	0.00024	0.00003	0.00028	2.64312
A6	2.78155	-0.00007	-0.00014	-0.00024	-0.00038	2.78118
A7	2.71687	-0.00002	-0.00024	-0.00012	-0.00036	2.71651
A8	2.78088	-0.00006	0.00007	-0.00021	-0.00014	2.78074
A9	2.83141	-0.00004	-0.00055	0.00004	-0.00050	2.83090
A10	2.30583	0.00008	0.00071	-0.00001	0.00071	2.30654
A11	2.51966	-0.00011	-0.00053	-0.00013	-0.00066	2.51900
A12	1.45711	0.00002	-0.00018	0.00014	-0.00004	1.45707
A13	2.83109	-0.00004	-0.00045	0.00005	-0.00039	2.83070
A14	2.30597	0.00008	0.00066	-0.00000	0.00066	2.30663
A15	1.45705	0.00002	-0.00014	0.00012	-0.00002	1.45703
A16	2.51958	-0.00010	-0.00051	-0.00011	-0.00063	2.51895
A17	1.42774	-0.00003	0.00003	-0.00008	-0.00005	1.42769
A18	1.42779	-0.00002	-0.00001	-0.00004	-0.00005	1.42774
A19	2.87961	0.00000	-0.00023	0.00021	-0.00002	2.87959
A20	2.87999	-0.00000	-0.00034	0.00013	-0.00020	2.87979
A21	3.14134	0.00005	0.00137	0.00021	0.00158	3.14292
A22	3.14152	0.00004	0.00176	-0.00096	0.00080	3.14231
D1	0.08402	0.00004	0.00417	0.00040	0.00457	0.08859
D2	-0.07724	-0.00002	-0.00374	-0.00062	-0.00435	-0.08159
D3	-0.08021	-0.00003	-0.00455	-0.00048	-0.00503	-0.08524
D4	0.08406	0.00004	0.00419	0.00042	0.00461	0.08867

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D5	0.11480	0.00002	0.00538	0.00026	0.00563	0.12043
D6	-0.08003	-0.00003	-0.00472	-0.00048	-0.00520	-0.08523
D7	0.09506	-0.00003	-0.00116	-0.00022	-0.00138	0.09368
D8	0.11458	0.00002	0.00563	0.00028	0.00592	0.12050
D9	0.09592	-0.00003	-0.00147	-0.00032	-0.00179	0.09413
D10	-0.64137	0.00002	-0.00178	0.00071	-0.00107	-0.64244
D11	2.55190	0.00000	-0.00203	0.00043	-0.00160	2.55030
D12	0.75102	-0.00000	-0.00052	-0.00007	-0.00059	0.75043
D13	-2.42069	0.00001	-0.00040	-0.00000	-0.00041	-2.42109
D14	-2.42086	0.00001	-0.00039	0.00009	-0.00031	-2.42117
D15	0.69061	0.00002	-0.00028	0.00015	-0.00012	0.69049
D16	2.40836	0.00001	-0.00038	0.00048	0.00010	2.40846
D17	-0.69466	-0.00001	-0.00059	0.00027	-0.00033	-0.69498
D18	-0.64269	0.00003	-0.00137	0.00062	-0.00075	-0.64344
D19	2.55027	0.00000	-0.00160	0.00049	-0.00111	2.54916
D20	-0.69465	-0.00002	-0.00059	0.00026	-0.00033	-0.69498
D21	2.40860	0.00000	-0.00040	0.00036	-0.00004	2.40856
D22	0.66921	-0.00002	-0.00017	0.00002	-0.00015	0.66907

Item	Value	Threshold	Converged?
Maximum Force	0.000108	0.000450	YES
RMS Force	0.000042	0.000300	YES
Maximum Displacement	0.001755	0.001800	YES
RMS Displacement	0.000606	0.001200	YES

Predicted change in Energy=-4.279991D-07
Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.2208	-DE/DX = 0.0
R2	R(1,3)	1.3487	-DE/DX = 0.0001
R3	R(2,4)	1.3483	-DE/DX = 0.0001
R4	R(3,5)	1.2208	-DE/DX = 0.0
R5	R(4,6)	1.2187	-DE/DX = 0.0
R6	R(5,7)	1.3483	-DE/DX = 0.0001
R7	R(6,8)	1.3497	-DE/DX = 0.0
R8	R(7,9)	1.2187	-DE/DX = 0.0
R9	R(8,10)	1.2149	-DE/DX = 0.0
R10	R(9,11)	1.3497	-DE/DX = 0.0
R11	R(10,12)	1.3842	-DE/DX = 0.0
R12	R(11,13)	1.2149	-DE/DX = 0.0
R13	R(12,14)	1.4001	-DE/DX = -0.0001
R14	R(12,15)	1.4502	-DE/DX = 0.0001
R15	R(13,14)	1.3842	-DE/DX = 0.0
R16	R(14,16)	1.4502	-DE/DX = 0.0001

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! R17   R(15,16)            1.4486        -DE/DX =    0.0001           !
! A1    A(2,1,3)           149.6721        -DE/DX =    0.0001           !
! A2    A(1,2,4)           151.4933        -DE/DX =    0.0              !
! A3    A(1,3,5)           149.7496        -DE/DX =    0.0              !
! A4    A(2,4,6)           155.611        -DE/DX =    0.0              !
! A5    A(3,5,7)           151.4236        -DE/DX =    0.0              !
! A6    A(4,6,8)           159.3713        -DE/DX =   -0.0001           !
! A7    A(5,7,9)           155.6653        -DE/DX =    0.0              !
! A8    A(7,9,11)          159.3325        -DE/DX =   -0.0001           !
! A9    A(8,10,12)         162.2277        -DE/DX =    0.0              !
! A10   A(10,12,14)        132.1145        -DE/DX =    0.0001           !
! A11   A(10,12,15)        144.366         -DE/DX =   -0.0001           !
! A12   A(14,12,15)        83.4862         -DE/DX =    0.0              !
! A13   A(11,13,14)        162.2098        -DE/DX =    0.0              !
! A14   A(12,14,13)        132.1225        -DE/DX =    0.0001           !
! A15   A(12,14,16)        83.4831         -DE/DX =    0.0              !
! A16   A(13,14,16)        144.3616        -DE/DX =   -0.0001           !
! A17   A(12,15,16)        81.8034         -DE/DX =    0.0              !
! A18   A(14,16,15)        81.8061         -DE/DX =    0.0              !
! A19   L(6,8,10,7,-1)     164.9895        -DE/DX =    0.0              !
! A20   L(9,11,13,4,-1)    165.0111        -DE/DX =    0.0              !
! A21   L(6,8,10,7,-2)     179.9856        -DE/DX =    0.0001           !
! A22   L(9,11,13,4,-2)    179.9957        -DE/DX =    0.0              !
! D1    D(3,1,2,4)          4.8138        -DE/DX =    0.0              !
! D2    D(2,1,3,5)         -4.4253        -DE/DX =    0.0              !
! D3    D(1,2,4,6)         -4.5956        -DE/DX =    0.0              !
! D4    D(1,3,5,7)          4.8162        -DE/DX =    0.0              !
! D5    D(2,4,6,8)          6.5774        -DE/DX =    0.0              !
! D6    D(3,5,7,9)         -4.5852        -DE/DX =    0.0              !
! D7    D(4,6,10,12)        5.4468        -DE/DX =    0.0              !
! D8    D(5,7,9,11)         6.5651        -DE/DX =    0.0              !
! D9    D(7,9,13,14)        5.496         -DE/DX =    0.0              !
! D10   D(8,10,12,14)      -36.7476        -DE/DX =    0.0              !
! D11   D(8,10,12,15)      146.2131        -DE/DX =    0.0              !
! D12   D(10,12,14,13)      43.0305        -DE/DX =    0.0              !
! D13   D(10,12,14,16)     -138.695        -DE/DX =    0.0              !
! D14   D(15,12,14,13)     -138.7051        -DE/DX =    0.0              !
! D15   D(15,12,14,16)      39.5693        -DE/DX =    0.0              !
! D16   D(10,12,15,16)      137.989        -DE/DX =    0.0              !
! D17   D(14,12,15,16)     -39.8008        -DE/DX =    0.0              !
! D18   D(11,13,14,12)     -36.8236        -DE/DX =    0.0              !
! D19   D(11,13,14,16)      146.1196        -DE/DX =    0.0              !
! D20   D(12,14,16,15)     -39.8006        -DE/DX =    0.0              !
! D21   D(13,14,16,15)      138.0026        -DE/DX =    0.0              !
! D22   D(12,15,16,14)       38.343        -DE/DX =    0.0              !
--------------------------------------------------------------------------------
Lowest energy point so far.  Saving SCF results.
Largest change from initial coordinates is atom   15       0.102 Angstoms.
```

Supporting Information file

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.622838	-0.673225	0.011716
2	6	0	3.007490	-1.726810	0.053562
3	6	0	3.621999	0.675252	-0.011480
4	6	0	1.854973	-2.426482	0.055949
5	6	0	3.006776	1.728897	-0.053436
6	6	0	0.645010	-2.572333	0.063750
7	6	0	1.853460	2.427305	-0.055958
8	6	0	-0.665950	-2.254040	0.022016
9	6	0	0.643485	2.572960	-0.063840
10	6	0	-1.731260	-1.671693	-0.021876
11	6	0	-0.667229	2.253563	-0.022166
12	6	0	-2.686802	-0.680760	-0.166639
13	6	0	-1.732278	1.670718	0.021456
14	6	0	-2.687114	0.679138	0.166459
15	6	0	-4.042735	-0.405345	-0.600841
16	6	0	-4.042663	0.402855	0.601329

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.220838	0.000000			
3	C	1.348676	2.480273	0.000000		
4	C	2.490224	1.348274	3.570390	0.000000	
5	C	2.480719	3.457363	1.220831	4.313443	0.000000
6	C	3.532248	2.509248	4.406237	1.218746	4.908385
7	C	3.570513	4.312825	2.489860	4.855077	1.348302
8	C	4.570862	3.711216	5.193108	2.527041	5.418338
9	C	4.406809	4.908190	3.532079	5.145530	2.509521
10	C	5.446506	4.739671	5.845138	3.665628	5.832151
11	C	5.193449	5.417810	4.570411	5.316994	3.711410
12	C	6.312164	5.793762	6.454751	4.870812	6.183534
13	C	5.845633	5.831778	5.446129	5.445788	4.740002
14	C	6.455101	6.183030	6.311624	5.503421	5.794026
15	C	7.694673	7.202791	7.762937	6.268917	7.385814
16	C	7.763085	7.385133	7.693945	6.563893	7.202895

		6	7	8	9	10
6	C	0.000000				
7	C	5.145003	0.000000			

```
 8  C    1.349692   5.316812   0.000000
 9  C    5.146875   1.218736   5.002191   0.000000
10  C    2.542665   5.445472   1.214883   4.863975   0.000000
11  C    5.001861   2.526896   4.507819   1.349713   4.066914
12  C    3.838241   5.503299   2.568003   4.657046   1.384184
13  C    4.863822   3.665506   4.067035   2.542748   3.342692
14  C    4.656787   4.870562   3.565039   3.838293   2.544707
15  C    5.206964   6.563987   3.899782   5.578471   2.698473
16  C    5.578083   6.268548   4.335537   5.206899   3.167762
            11         12         13         14         15
11  C    0.000000
12  C    3.565080   0.000000
13  C    1.214882   2.544788   0.000000
14  C    2.567942   1.400099   1.384185   0.000000
15  C    4.335746   1.450152   3.167886   1.898041   0.000000
16  C    3.899669   1.897987   2.698446   1.450157   1.448586
            16
16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 2.37D-16
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.622628   -0.674380    0.010077
    2          6           0        3.006952   -1.727871    0.049402
    3          6           0        3.622209    0.674148   -0.009889
    4          6           0        1.854217   -2.427187    0.050122
    5          6           0        3.007314    1.728083   -0.049316
    6          6           0        0.644209   -2.572679    0.057583
    7          6           0        1.854216    2.426854   -0.050156
    8          6           0       -0.666652   -2.253878    0.016621
    9          6           0        0.644287    2.572905   -0.057680
   10          6           0       -1.731781   -1.671096   -0.025869
   11          6           0       -0.666527    2.253817   -0.016762
   12          6           0       -2.687015   -0.679522   -0.168250
   13          6           0       -1.731757    1.671202    0.025471
   14          6           0       -2.686902    0.679575    0.168105
   15          6           0       -4.042865   -0.402644   -0.601781
   16          6           0       -4.042533    0.402673    0.602322
---------------------------------------------------------------------
Rotational constants (GHZ):           0.8474928           0.3941534           0.2718102
```

Supporting Information file

Leave Link 202 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

****

Population analysis using the SCF Density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -10.40290 -10.40234 -10.36614 -10.36566 -10.36544
Alpha occ. eigenvalues -- -10.36529 -10.36405 -10.36403 -10.36298 -10.36284
Alpha occ. eigenvalues -- -10.36095 -10.36086 -10.36059 -10.36016 -10.35396
Alpha occ. eigenvalues -- -10.35389 -1.09543 -0.98450 -0.96923 -0.95287
Alpha occ. eigenvalues -- -0.93288 -0.90789 -0.88055 -0.83369 -0.81518
Alpha occ. eigenvalues -- -0.78453 -0.75191 -0.72291 -0.69613 -0.67340
Alpha occ. eigenvalues -- -0.65377 -0.64116 -0.53785 -0.53390 -0.52300
Alpha occ. eigenvalues -- -0.52137 -0.50854 -0.50302 -0.46892 -0.46765
Alpha occ. eigenvalues -- -0.44455 -0.43078 -0.39179 -0.38998 -0.35360
Alpha occ. eigenvalues -- -0.33202 -0.32643 -0.32137
Alpha virt. eigenvalues -- -0.07459 -0.07451 -0.05079 -0.02464 0.01006
Alpha virt. eigenvalues -- 0.03001 0.04417 0.05669 0.07664 0.10061
Alpha virt. eigenvalues -- 0.10853 0.11107 0.12094 0.12326 0.12804
Alpha virt. eigenvalues -- 0.15818 0.17145 0.19752 0.21010 0.21648
Alpha virt. eigenvalues -- 0.22475 0.23038 0.23232 0.24300 0.25409
Alpha virt. eigenvalues -- 0.26086 0.26988 0.27033 0.28599 0.28782
Alpha virt. eigenvalues -- 0.29464 0.30645 0.31347 0.31443 0.31854
Alpha virt. eigenvalues -- 0.31986 0.32968 0.33624 0.35286 0.35445
Alpha virt. eigenvalues -- 0.35703 0.36916 0.37285 0.38176 0.38189
Alpha virt. eigenvalues -- 0.39249 0.39377 0.39588 0.40449 0.41584
Alpha virt. eigenvalues -- 0.42331 0.43001 0.43642 0.44709 0.46023
Alpha virt. eigenvalues -- 0.46495 0.46639 0.47553 0.47694 0.48811
Alpha virt. eigenvalues -- 0.49117 0.50284 0.50725 0.50921 0.52249
Alpha virt. eigenvalues -- 0.52732 0.52984 0.53200 0.54297 0.54536
Alpha virt. eigenvalues -- 0.54926 0.55685 0.56069 0.56549 0.58161
Alpha virt. eigenvalues -- 0.58302 0.59013 0.59185 0.59368 0.60396
Alpha virt. eigenvalues -- 0.61116 0.63299 0.63574 0.63723 0.64293
Alpha virt. eigenvalues -- 0.65210 0.67191 0.67561 0.67944 0.68624
Alpha virt. eigenvalues -- 0.70914 0.71012 0.72044 0.72422 0.74301
Alpha virt. eigenvalues -- 0.75848 0.76815 0.77208 0.78800 0.79808
Alpha virt. eigenvalues -- 0.80557 0.84401 0.84818 0.85440 0.85915
Alpha virt. eigenvalues -- 0.86699 0.90213 0.91512 0.92663 0.92870
Alpha virt. eigenvalues -- 0.93592 0.95722 0.96684 0.98165 0.99140
Alpha virt. eigenvalues -- 1.01137 1.01981 1.02368 1.05797 1.07381
Alpha virt. eigenvalues -- 1.09301 1.09335 1.09879 1.12188 1.12432
Alpha virt. eigenvalues -- 1.13358 1.15262 1.15994 1.16387 1.18464
Alpha virt. eigenvalues -- 1.19675 1.22055 1.23127 1.23523 1.23875
Alpha virt. eigenvalues -- 1.26222 1.27253 1.27711 1.27775 1.30100
Alpha virt. eigenvalues -- 1.31458 1.33407 1.34466 1.35849 1.36137
Alpha virt. eigenvalues -- 1.37502 1.38475 1.39202 1.39243 1.40757
Alpha virt. eigenvalues -- 1.41670 1.42611 1.43166 1.43339 1.43747

Alpha virt. eigenvalues --	1.45417	1.46011	1.47089	1.48236	1.48834
Alpha virt. eigenvalues --	1.49155	1.49688	1.49957	1.50561	1.50861
Alpha virt. eigenvalues --	1.51264	1.53178	1.54048	1.54566	1.57963
Alpha virt. eigenvalues --	1.59431	1.61318	1.61735	1.62193	1.62991
Alpha virt. eigenvalues --	1.63954	1.64765	1.65752	1.67667	1.69594
Alpha virt. eigenvalues --	1.69727	1.71038	1.71633	1.72894	1.72985
Alpha virt. eigenvalues --	1.74463	1.76303	1.77824	1.77871	1.78794
Alpha virt. eigenvalues --	1.79143	1.81311	1.82715	1.84830	1.85724
Alpha virt. eigenvalues --	1.85892	1.86104	1.90730	1.92761	1.97301
Alpha virt. eigenvalues --	1.97394	1.98529	2.00087	2.00338	2.03215
Alpha virt. eigenvalues --	2.06572	2.10393	2.10749	2.11554	2.15349
Alpha virt. eigenvalues --	2.16006	2.16253	2.20506	2.22128	2.22994
Alpha virt. eigenvalues --	2.25084	2.26037	2.34826	2.36193	2.39105
Alpha virt. eigenvalues --	2.39541	2.40646	2.43305	2.43825	2.45271
Alpha virt. eigenvalues --	2.45641	2.46458	2.48206	2.48369	2.48652
Alpha virt. eigenvalues --	2.49877	2.49972	2.50630	2.52333	2.52909
Alpha virt. eigenvalues --	2.54337	2.55896	2.57415	2.59904	2.60059
Alpha virt. eigenvalues --	2.61447	2.62912	2.63001	2.63543	2.63877
Alpha virt. eigenvalues --	2.65023	2.65556	2.66665	2.69415	2.72825
Alpha virt. eigenvalues --	2.72966	2.73587	2.73969	2.74220	2.75500
Alpha virt. eigenvalues --	2.76290	2.78373	2.79430	2.80787	2.81160
Alpha virt. eigenvalues --	2.81927	2.82119	2.82687	2.83545	2.84161
Alpha virt. eigenvalues --	2.84257	2.85323	2.85747	2.86362	2.86737
Alpha virt. eigenvalues --	2.87626	2.87915	2.88434	2.89145	2.89823
Alpha virt. eigenvalues --	2.90026	2.90920	2.91331	2.92171	2.93036
Alpha virt. eigenvalues --	2.93049	2.96180	2.97117	2.97353	2.98234
Alpha virt. eigenvalues --	2.99198	2.99330	3.00503	3.01157	3.02464
Alpha virt. eigenvalues --	3.03691	3.04173	3.05115	3.05290	3.06112
Alpha virt. eigenvalues --	3.06968	3.09380	3.10536	3.11850	3.12890
Alpha virt. eigenvalues --	3.13088	3.14267	3.15253	3.15528	3.16162
Alpha virt. eigenvalues --	3.17364	3.19726	3.20239	3.20541	3.22443
Alpha virt. eigenvalues --	3.22585	3.25884	3.26203	3.26424	3.26889
Alpha virt. eigenvalues --	3.27539	3.28972	3.30006	3.31788	3.31805
Alpha virt. eigenvalues --	3.32125	3.34004	3.34047	3.35084	3.36171
Alpha virt. eigenvalues --	3.36488	3.36557	3.37888	3.40448	3.40497
Alpha virt. eigenvalues --	3.41377	3.42553	3.43457	3.43521	3.44323
Alpha virt. eigenvalues --	3.48510	3.48779	3.49564	3.49721	3.52594
Alpha virt. eigenvalues --	3.54345	3.54886	3.55158	3.55931	3.57777
Alpha virt. eigenvalues --	3.58282	3.63219	3.63308	3.64243	3.66162
Alpha virt. eigenvalues --	3.66642	3.70949	3.71954	3.75863	3.76958
Alpha virt. eigenvalues --	3.79693	3.82502	3.83022	3.86054	3.87574
Alpha virt. eigenvalues --	3.88441	3.89760	3.91625	3.94769	3.96338
Alpha virt. eigenvalues --	3.98359	4.04724	4.04935	4.06137	4.08851
Alpha virt. eigenvalues --	4.09491	4.10420	4.10655	4.16563	4.16906
Alpha virt. eigenvalues --	4.19249	4.21263	4.22009	4.25228	4.30376
Alpha virt. eigenvalues --	4.31725	4.38658	4.40094	4.41147	4.48289
Alpha virt. eigenvalues --	4.49793	4.51308	4.53702	4.57236	4.58556
Alpha virt. eigenvalues --	4.61495	4.67897	4.73076	4.75597	4.76838

Supporting Information file

Alpha virt. eigenvalues -- 4.77724 4.78139 4.79230 4.89536 4.90163
Alpha virt. eigenvalues -- 4.92645 4.96840 4.99803 5.03008 5.04347
Alpha virt. eigenvalues -- 5.05594 5.06108 5.08303 5.12228 5.14609
Alpha virt. eigenvalues -- 5.17477 5.18973 5.20311 5.21334 5.23774
Alpha virt. eigenvalues -- 5.23822 5.25105 5.28525 5.30983 5.32793
Alpha virt. eigenvalues -- 5.40418 5.40523 5.48109 5.55173 5.60214
Alpha virt. eigenvalues -- 5.62385 5.76190 5.82830 5.99685 6.02968
Alpha virt. eigenvalues -- 6.14446 6.22586 22.16659 22.23400 22.50352
Alpha virt. eigenvalues -- 22.84888 23.09533 23.23080 23.31108 23.42168
Alpha virt. eigenvalues -- 23.61197 23.69701 23.79969 23.83195 23.91931
Alpha virt. eigenvalues -- 23.94694 24.23848 24.29259

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.875929	0.884298	0.505163	-0.090050	-0.085682	-0.057731
2	C	0.884298	4.869911	-0.085968	0.525382	-0.051217	-0.093478
3	C	0.505163	-0.085968	4.877048	-0.013447	0.884280	-0.006946
4	C	-0.090050	0.525382	-0.013447	4.882921	-0.006879	0.919487
5	C	-0.085682	-0.051217	0.884280	-0.006879	4.868805	-0.002156
6	C	-0.057731	-0.093478	-0.006946	0.919487	-0.002156	4.996634
7	C	-0.013420	-0.006884	-0.090250	-0.001223	0.525000	-0.000513
8	C	-0.009837	-0.021991	-0.001051	-0.105374	-0.000494	0.513962
9	C	-0.006917	-0.002149	-0.057644	-0.000508	-0.093179	-0.000030
10	C	-0.002426	-0.009679	-0.000358	-0.077807	-0.000132	-0.206969
11	C	-0.001051	-0.000489	-0.009797	0.000209	-0.021911	0.001967
12	C	-0.000215	-0.000776	-0.000056	-0.007249	-0.000121	-0.031763
13	C	-0.000359	-0.000129	-0.002410	-0.000124	-0.009624	0.000372
14	C	-0.000057	-0.000121	-0.000213	-0.001250	-0.000770	-0.009122
15	C	-0.000002	-0.000016	0.000002	-0.000271	0.000006	-0.002747
16	C	0.000002	0.000006	-0.000002	0.000111	-0.000016	0.001037

		7	8	9	10	11	12
1	C	-0.013420	-0.009837	-0.006917	-0.002426	-0.001051	-0.000215
2	C	-0.006884	-0.021991	-0.002149	-0.009679	-0.000489	-0.000776
3	C	-0.090250	-0.001051	-0.057644	-0.000358	-0.009797	-0.000056
4	C	-0.001223	-0.105374	-0.000508	-0.077807	0.000209	-0.007249
5	C	0.525000	-0.000494	-0.093179	-0.000132	-0.021911	-0.000121
6	C	-0.000513	0.513962	-0.000030	-0.206969	0.001967	-0.031763
7	C	4.883748	0.000209	0.919368	-0.000122	-0.105232	-0.001243
8	C	0.000209	5.069291	0.001968	0.610821	0.013746	-0.159530
9	C	0.919368	0.001968	4.995279	0.000365	0.513482	-0.009099
10	C	-0.000122	0.610821	0.000365	5.493673	0.000349	0.491076
11	C	-0.105232	0.013746	0.513482	0.000349	5.068779	-0.075527
12	C	-0.001243	-0.159530	-0.009099	0.491076	-0.075527	5.217464
13	C	-0.077520	0.000351	-0.206536	0.003978	0.611039	-0.046164
14	C	-0.007204	-0.075562	-0.031555	-0.046324	-0.158943	0.364928
15	C	0.000111	-0.020940	0.001033	-0.093337	0.011950	0.036601
16	C	-0.000271	0.011952	-0.002738	0.010300	-0.020896	0.104612

		13	14	15	16
1	C	-0.000359	-0.000057	-0.000002	0.000002

2	C	-0.000129	-0.000121	-0.000016	0.000006
3	C	-0.002410	-0.000213	0.000002	-0.000002
4	C	-0.000124	-0.001250	-0.000271	0.000111
5	C	-0.009624	-0.000770	0.000006	-0.000016
6	C	0.000372	-0.009122	-0.002747	0.001037
7	C	-0.077520	-0.007204	0.000111	-0.000271
8	C	0.000351	-0.075562	-0.020940	0.011952
9	C	-0.206536	-0.031555	0.001033	-0.002738
10	C	0.003978	-0.046324	-0.093337	0.010300
11	C	0.611039	-0.158943	0.011950	-0.020896
12	C	-0.046164	0.364928	0.036601	0.104612
13	C	5.492106	0.490539	0.010203	-0.093142
14	C	0.490539	5.217036	0.104731	0.036670
15	C	0.010203	0.104731	5.913528	0.105640
16	C	-0.093142	0.036670	0.105640	5.913104

Mulliken charges:

		1
1	C	0.002356
2	C	-0.006702
3	C	0.001650
4	C	-0.023928
5	C	-0.005909
6	C	-0.022005
7	C	-0.024554
8	C	0.172479
9	C	-0.021142
10	C	-0.173407
11	C	0.172325
12	C	0.117063
13	C	-0.172581
14	C	0.117217
15	C	-0.066492
16	C	-0.066370

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.002356
2	C	-0.006702
3	C	0.001650
4	C	-0.023928
5	C	-0.005909
6	C	-0.022005
7	C	-0.024554
8	C	0.172479
9	C	-0.021142
10	C	-0.173407
11	C	0.172325
12	C	0.117063

13 C -0.172581
14 C 0.117217
15 C -0.066492
16 C -0.066370
Electronic spatial extent (au): <R**2>= 3544.7415
Charge= -0.0000 electrons
Dipole moment (field-independent basis, Debye):
X= 3.8545 Y= -0.0035 Z= -0.0003 Tot= 3.8545
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -103.3334 YY= -85.1444 ZZ= -90.9433
XY= -0.0031 XZ= 0.0018 YZ= -1.6871
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= -10.1930 YY= 7.9960 ZZ= 2.1971
XY= -0.0031 XZ= 0.0018 YZ= -1.6871
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= 121.5883 YYY= -0.0319 ZZZ= -0.0049 XYY= 4.1229
XXY= -0.0097 XXZ= -0.0023 XZZ= 17.3257 YZZ= -0.0021
YYZ= 0.0005 XYZ= 6.8734
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -4135.0365 YYYY= -1695.6462 ZZZZ= -137.2008 XXXY= -0.0650
XXXZ= -0.0015 YYYX= -0.0240 YYYZ= -3.3929 ZZZX= 0.0197
ZZZY= -4.0586 XXYY= -878.9386 XXZZ= -703.0480 YYZZ= -309.2486
XXYZ= -32.3114 YYXZ= 0.0000 ZZXY= 0.0033
N-N= 7.176436409760D+02 E-N=-2.846286593279D+03 KE= 6.062420690731D+02
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Fri Aug 21 20:45:02 2026, MaxMem= 805306368 cpu: 2.2 elap: 0.4
(Enter /home/user/gauss16/g16/l9999.exe)
Unable to Open any file for archive entry.
1\1\GINC-MAKCLUS\FOpt\RwB97XD\def2TZVP\C16\USER\21-Aug-2026\0\\#p opt freq wb97xd/Def2TZVP\\title card\\0,1\C,3.6228376463,-0.6732249818,0.0117161678\C,3.0074903508,-1.7268103129,0.053561589\C,3.6219990344,0.6752517291,-0.0114804595\C,1.8549727576,-2.4264821233,0.0559489129\C,3.0067757714,1.7288968719,-0.053435984\C,0.6450102379,-2.5723325127,0.0637503509\C,1.8534597591,2.4273050814,-0.0559576911\C,-0.6659496215,-2.2540395139,0.0220162976\C,0.64348505,2.5729602883,-0.0638397256\C,-1.7312599731,-1.6716930394,-0.0218764649\C,-0.6672294743,2.2535625776,-0.0221657635\C,-2.6868018486,-0.6807603584,-0.1666389885\C,-1.7322778476,1.6707178542,0.0214559206\C,-2.6871144989,0.6791381312,0.1664592453\C,-4.0427351084,-0.4053452265,-0.6008413095\C,-4.0426632352,0.4028545352,0.6013289025\\Version=ES64L-G16RevC.01\State=1-A\HF=-608.9815402\RMSD=6.404e-09\RMSF=1.114e-04\Dipole=1.5164864,-0.0008938,-0.0001213\Quadrupole=-7.5782732,5.9387743,1.6394989,-0.0065292,0.0016962,-1.2646285\PG=C01 [X(C16)]\\@
The archive entry for this job was punched.

Supporting Information file

```
 QUANTUM MECHANICS IS BOHRING -- M.S. GORDON
 Leave Link 9999 at Fri Aug 21 20:45:02 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.0
 Job cpu time:       0 days 17 hours 48 minutes 58.4 seconds.
 Elapsed time:       0 days  2 hours 58 minutes 12.7 seconds.
 File lengths (MBytes):  RWF=    155 Int=      0 D2E=      0 Chk=     19 Scr=      1
 Normal termination of Gaussian 16 at Fri Aug 21 20:45:02 2026.
 (Enter /home/user/gauss16/g16/l1.exe)
 Link1:  Proceeding to internal job step number  2.
 ----------------------------------------------------------------------
 #P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RwB97XD/def2TZVP Freq
 ----------------------------------------------------------------------
 1/10=4,29=7,30=1,38=1,40=1/1,3;
 2/12=2,40=1/2;
 3/5=44,7=101,11=2,14=-4,25=1,30=1,70=2,71=2,74=-58,116=1,140=1/1,2,3;
 4/5=101/1;
 5/5=2,38=6,98=1/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7/8=1,10=1,25=1/1,2,3,16;
 1/10=4,30=1/3;
 99//99;
 Leave Link     1 at Fri Aug 21 20:45:02 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.0
 (Enter /home/user/gauss16/g16/l101.exe)
 Structure from the checkpoint file:  "cdca.chk"
 ----------
 title card
 ----------
 Charge =  0 Multiplicity = 1
 Redundant internal coordinates found in file.  (old form).
 C,0,3.6228376463,-0.6732249818,0.0117161678
 C,0,3.0074903508,-1.7268103129,0.053561589
 C,0,3.6219990344,0.6752517291,-0.0114804595
 C,0,1.8549727576,-2.4264821233,0.0559489129
 C,0,3.0067757714,1.7288968719,-0.053435984
 C,0,0.6450102379,-2.5723325127,0.0637503509
 C,0,1.8534597591,2.4273050814,-0.0559576911
 C,0,-0.6659496215,-2.2540395139,0.0220162976
 C,0,0.64348505,2.5729602883,-0.0638397256
 C,0,-1.7312599731,-1.6716930394,-0.0218764649
 C,0,-0.6672294743,2.2535625776,-0.0221657635
 C,0,-2.6868018486,-0.6807603584,-0.1666389885
 C,0,-1.7322778476,1.6707178542,0.0214559206
 C,0,-2.6871144989,0.6791381312,0.1664592453
```

Supporting Information file

```
C,0,-4.0427351084,-0.4053452265,-0.6008413095
C,0,-4.0426632352,0.4028545352,0.6013289025
Recover connectivity data from disk.
ITRead=  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
MicOpt= -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
NAtoms=     16 NQM=       16 NQMF=       0 NMMI=      0 NMMIF=      0
            NMic=       0 NMicF=      0.
               Isotopes and Nuclear Properties:
(Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic moments (NMagM)
 in nuclear magnetons)

 Atom        1         2         3         4         5         6         7         8         9        10
IAtWgt=         12        12        12        12        12        12        12        12        12        12
 AtmWgt=    12.0000000  12.0000000  12.0000000  12.0000000  12.0000000  12.0000000
12.0000000  12.0000000  12.0000000  12.0000000
 NucSpn=          0         0         0         0         0         0         0         0         0         0
 AtZEff=    3.6000000  3.6000000  3.6000000  3.6000000  3.6000000  3.6000000  3.6000000
3.6000000  3.6000000  3.6000000
 NQMom=     0.0000000  0.0000000  0.0000000  0.0000000  0.0000000  0.0000000  0.0000000
0.0000000  0.0000000  0.0000000
 NMagM=     0.0000000  0.0000000  0.0000000  0.0000000  0.0000000  0.0000000  0.0000000
0.0000000  0.0000000  0.0000000
 AtZNuc=    6.0000000  6.0000000  6.0000000  6.0000000  6.0000000  6.0000000  6.0000000
6.0000000  6.0000000  6.0000000

 Atom       11        12        13        14        15        16
 IAtWgt=         12        12        12        12        12        12
 AtmWgt=  12.0000000  12.0000000  12.0000000  12.0000000  12.0000000  12.0000000
 NucSpn=          0         0         0         0         0         0
 AtZEff=    3.6000000  3.6000000  3.6000000  3.6000000  3.6000000  3.6000000
 NQMom=     0.0000000  0.0000000  0.0000000  0.0000000  0.0000000  0.0000000
 NMagM=     0.0000000  0.0000000  0.0000000  0.0000000  0.0000000  0.0000000
 AtZNuc=    6.0000000  6.0000000  6.0000000  6.0000000  6.0000000  6.0000000
 Leave Link  101 at Fri Aug 21 20:45:03 2026, MaxMem=    805306368 cpu:                2.1 elap:
0.4
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.
                      ----------------------------
                      !    Initial Parameters    !
                      ! (Angstroms and Degrees)  !
 --------------------------                  --------------------------
 ! Name  Definition              Value          Derivative Info.                !
 --------------------------------------------------------------------------------
 ! R1    R(1,2)                  1.2208         calculate D2E/DX2 analytically  !
 ! R2    R(1,3)                  1.3487         calculate D2E/DX2 analytically  !
```

```
! R3    R(2,4)              1.3483       calculate D2E/DX2 analytically  !
! R4    R(3,5)              1.2208       calculate D2E/DX2 analytically  !
! R5    R(4,6)              1.2187       calculate D2E/DX2 analytically  !
! R6    R(5,7)              1.3483       calculate D2E/DX2 analytically  !
! R7    R(6,8)              1.3497       calculate D2E/DX2 analytically  !
! R8    R(7,9)              1.2187       calculate D2E/DX2 analytically  !
! R9    R(8,10)             1.2149       calculate D2E/DX2 analytically  !
! R10   R(9,11)             1.3497       calculate D2E/DX2 analytically  !
! R11   R(10,12)            1.3842       calculate D2E/DX2 analytically  !
! R12   R(11,13)            1.2149       calculate D2E/DX2 analytically  !
! R13   R(12,14)            1.4001       calculate D2E/DX2 analytically  !
! R14   R(12,15)            1.4502       calculate D2E/DX2 analytically  !
! R15   R(13,14)            1.3842       calculate D2E/DX2 analytically  !
! R16   R(14,16)            1.4502       calculate D2E/DX2 analytically  !
! R17   R(15,16)            1.4486       calculate D2E/DX2 analytically  !
! A1    A(2,1,3)            149.6721     calculate D2E/DX2 analytically  !
! A2    A(1,2,4)            151.4933     calculate D2E/DX2 analytically  !
! A3    A(1,3,5)            149.7496     calculate D2E/DX2 analytically  !
! A4    A(2,4,6)            155.611      calculate D2E/DX2 analytically  !
! A5    A(3,5,7)            151.4236     calculate D2E/DX2 analytically  !
! A6    A(4,6,8)            159.3713     calculate D2E/DX2 analytically  !
! A7    A(5,7,9)            155.6653     calculate D2E/DX2 analytically  !
! A8    A(7,9,11)           159.3325     calculate D2E/DX2 analytically  !
! A9    A(8,10,12)          162.2277     calculate D2E/DX2 analytically  !
! A10   A(10,12,14)         132.1145     calculate D2E/DX2 analytically  !
! A11   A(10,12,15)         144.366      calculate D2E/DX2 analytically  !
! A12   A(14,12,15)         83.4862      calculate D2E/DX2 analytically  !
! A13   A(11,13,14)         162.2098     calculate D2E/DX2 analytically  !
! A14   A(12,14,13)         132.1225     calculate D2E/DX2 analytically  !
! A15   A(12,14,16)         83.4831      calculate D2E/DX2 analytically  !
! A16   A(13,14,16)         144.3616     calculate D2E/DX2 analytically  !
! A17   A(12,15,16)         81.8034      calculate D2E/DX2 analytically  !
! A18   A(14,16,15)         81.8061      calculate D2E/DX2 analytically  !
! A19   L(6,8,10,7,-1)      164.9895     calculate D2E/DX2 analytically  !
! A20   L(9,11,13,4,-1)     165.0111     calculate D2E/DX2 analytically  !
! A21   L(6,8,10,7,-2)      179.9856     calculate D2E/DX2 analytically  !
! A22   L(9,11,13,4,-2)     179.9957     calculate D2E/DX2 analytically  !
! D1    D(3,1,2,4)          4.8138       calculate D2E/DX2 analytically  !
! D2    D(2,1,3,5)          -4.4253      calculate D2E/DX2 analytically  !
! D3    D(1,2,4,6)          -4.5956      calculate D2E/DX2 analytically  !
! D4    D(1,3,5,7)          4.8162       calculate D2E/DX2 analytically  !
! D5    D(2,4,6,8)          6.5774       calculate D2E/DX2 analytically  !
! D6    D(3,5,7,9)          -4.5852      calculate D2E/DX2 analytically  !
! D7    D(4,6,10,12)        5.4468       calculate D2E/DX2 analytically  !
! D8    D(5,7,9,11)         6.5651       calculate D2E/DX2 analytically  !
! D9    D(7,9,13,14)        5.496        calculate D2E/DX2 analytically  !
! D10   D(8,10,12,14)       -36.7476     calculate D2E/DX2 analytically  !
! D11   D(8,10,12,15)       146.2131     calculate D2E/DX2 analytically  !
```

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```
 ! D12   D(10,12,14,13)       43.0305        calculate D2E/DX2 analytically  !
 ! D13   D(10,12,14,16)      -138.695         calculate D2E/DX2 analytically  !
 ! D14   D(15,12,14,13)      -138.7051        calculate D2E/DX2 analytically  !
 ! D15   D(15,12,14,16)       39.5693         calculate D2E/DX2 analytically  !
 ! D16   D(10,12,15,16)       137.989         calculate D2E/DX2 analytically  !
 ! D17   D(14,12,15,16)      -39.8008         calculate D2E/DX2 analytically  !
 ! D18   D(11,13,14,12)      -36.8236         calculate D2E/DX2 analytically  !
 ! D19   D(11,13,14,16)       146.1196        calculate D2E/DX2 analytically  !
 ! D20   D(12,14,16,15)      -39.8006         calculate D2E/DX2 analytically  !
 ! D21   D(13,14,16,15)       138.0026        calculate D2E/DX2 analytically  !
 ! D22   D(12,15,16,14)       38.343          calculate D2E/DX2 analytically  !
 ---------------------------------------------------------------------------
  Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07 EigMax=2.50D+02 EigMin=1.00D-
04
 Number of steps in this run=      2 maximum allowed number of steps=      2.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

  Leave Link  103 at Fri Aug 21 20:45:03 2026, MaxMem=    805306368 cpu:                0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l202.exe)
                     Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        3.622838   -0.673225    0.011716
     2          6           0        3.007490   -1.726810    0.053562
     3          6           0        3.621999    0.675252   -0.011480
     4          6           0        1.854973   -2.426482    0.055949
     5          6           0        3.006776    1.728897   -0.053436
     6          6           0        0.645010   -2.572333    0.063750
     7          6           0        1.853460    2.427305   -0.055958
     8          6           0       -0.665950   -2.254040    0.022016
     9          6           0        0.643485    2.572960   -0.063840
    10          6           0       -1.731260   -1.671693   -0.021876
    11          6           0       -0.667229    2.253563   -0.022166
    12          6           0       -2.686802   -0.680760   -0.166639
    13          6           0       -1.732278    1.670718    0.021456
    14          6           0       -2.687114    0.679138    0.166459
    15          6           0       -4.042735   -0.405345   -0.600841
    16          6           0       -4.042663    0.402855    0.601329
 ---------------------------------------------------------------------
               Distance matrix (angstroms):
                    1          2          3          4          5
    1  C    0.000000
    2  C    1.220838   0.000000
    3  C    1.348676   2.480273   0.000000
    4  C    2.490224   1.348274   3.570390   0.000000
```

```
   5  C    2.480719   3.457363   1.220831   4.313443   0.000000
   6  C    3.532248   2.509248   4.406237   1.218746   4.908385
   7  C    3.570513   4.312825   2.489860   4.855077   1.348302
   8  C    4.570862   3.711216   5.193108   2.527041   5.418338
   9  C    4.406809   4.908190   3.532079   5.145530   2.509521
  10  C    5.446506   4.739671   5.845138   3.665628   5.832151
  11  C    5.193449   5.417810   4.570411   5.316994   3.711410
  12  C    6.312164   5.793762   6.454751   4.870812   6.183534
  13  C    5.845633   5.831778   5.446129   5.445788   4.740002
  14  C    6.455101   6.183030   6.311624   5.503421   5.794026
  15  C    7.694673   7.202791   7.762937   6.268917   7.385814
  16  C    7.763085   7.385133   7.693945   6.563893   7.202895
                6          7          8          9         10
   6  C    0.000000
   7  C    5.145003   0.000000
   8  C    1.349692   5.316812   0.000000
   9  C    5.146875   1.218736   5.002191   0.000000
  10  C    2.542665   5.445472   1.214883   4.863975   0.000000
  11  C    5.001861   2.526896   4.507819   1.349713   4.066914
  12  C    3.838241   5.503299   2.568003   4.657046   1.384184
  13  C    4.863822   3.665506   4.067035   2.542748   3.342692
  14  C    4.656787   4.870562   3.565039   3.838293   2.544707
  15  C    5.206964   6.563987   3.899782   5.578471   2.698473
  16  C    5.578083   6.268548   4.335537   5.206899   3.167762
               11         12         13         14         15
  11  C    0.000000
  12  C    3.565080   0.000000
  13  C    1.214882   2.544788   0.000000
  14  C    2.567942   1.400099   1.384185   0.000000
  15  C    4.335746   1.450152   3.167886   1.898041   0.000000
  16  C    3.899669   1.897987   2.698446   1.450157   1.448586
               16
  16  C    0.000000
Stoichiometry    C16
Framework group  C1[X(C16)]
Deg. of freedom    42
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 4.71D-16
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        3.622628   -0.674380    0.010077
    2          6           0        3.006952   -1.727871    0.049402
    3          6           0        3.622209    0.674148   -0.009889
```

```
     4        6        0        1.854217   -2.427187    0.050122
     5        6        0        3.007314    1.728083   -0.049316
     6        6        0        0.644209   -2.572679    0.057583
     7        6        0        1.854216    2.426854   -0.050156
     8        6        0       -0.666652   -2.253878    0.016621
     9        6        0        0.644287    2.572905   -0.057680
    10        6        0       -1.731781   -1.671096   -0.025869
    11        6        0       -0.666527    2.253817   -0.016762
    12        6        0       -2.687015   -0.679522   -0.168250
    13        6        0       -1.731757    1.671202    0.025471
    14        6        0       -2.686902    0.679575    0.168105
    15        6        0       -4.042865   -0.402644   -0.601781
    16        6        0       -4.042533    0.402673    0.602322
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8474928           0.3941534           0.2718102
 Leave Link  202 at Fri Aug 21 20:45:03 2026, MaxMem=    805306368 cpu:                 0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   576 symmetry adapted cartesian basis functions of A   symmetry.
 There are   496 symmetry adapted basis functions of A   symmetry.
   496 basis functions,   816 primitive gaussians,   576 cartesian basis functions
    48 alpha electrons       48 beta electrons
       nuclear repulsion energy       717.6511336511 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   16 NActive=   16 NUniq=   16 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0074926751 Hartrees.
 Nuclear repulsion after empirical dispersion term =       717.6436409760 Hartrees.
 Leave Link  301 at Fri Aug 21 20:45:03 2026, MaxMem=    805306368 cpu:                 0.3 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   15576 NPrTT=   51712 LenC2=   14212 LenP2D=   33580.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
```

Supporting Information file

NBasis= 496 RedAO= T EigKep= 4.36D-06 NBF= 496
NBsUse= 496 1.00D-06 EigRej= -1.00D+00 NBFU= 496
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 564 564 564 564 564 MxSgAt= 16 MxSgA2= 16.
Leave Link 302 at Fri Aug 21 20:45:04 2026, MaxMem= 805306368 cpu: 3.9 elap: 0.7
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Aug 21 20:45:04 2026, MaxMem= 805306368 cpu: 0.6 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000000 0.000000 -0.000000 Ang= 0.00 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Fri Aug 21 20:45:04 2026, MaxMem= 805306368 cpu: 3.2 elap: 0.5
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804634234 LenY= 804301882
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -608.981540194378
DIIS: error= 1.54D-08 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -608.981540194378 IErMin= 1 ErrMin= 1.54D-08
ErrMax= 1.54D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-14 BMatP= 4.16D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.100D+01
Coeff: 0.100D+01
Gap= 0.247 Goal= None Shift= 0.000
RMSDP=2.74D-09 MaxDP=9.39D-08 OVMax= 2.55D-07

Supporting Information file

SCF Done: E(RwB97XD) = -608.981540194 A.U. after 1 cycles
NFock= 1 Conv=0.27D-08 -V/T= 2.0045
KE= 6.062420692550D+02 PE=-2.846286593461D+03 EE= 9.134193430358D+02
Leave Link 502 at Fri Aug 21 20:46:20 2026, MaxMem= 805306368 cpu: 454.4 elap: 75.8
(Enter /home/user/gauss16/g16/l801.exe)
DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000
Range of M.O.s used for correlation: 1 496
NBasis= 496 NAE= 48 NBE= 48 NFC= 0 NFV= 0
NROrb= 496 NOA= 48 NOB= 48 NVA= 448 NVB= 448

**** Warning!!: The largest alpha MO coefficient is 0.62069364D+02

Leave Link 801 at Fri Aug 21 20:46:20 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l1101.exe)
Using compressed storage, NAtomX= 16.
Will process 17 centers per pass.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 7 Len= 274
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
Leave Link 1101 at Fri Aug 21 20:46:22 2026, MaxMem= 805306368 cpu: 12.4 elap: 2.1
(Enter /home/user/gauss16/g16/l1102.exe)
Symmetrizing basis deriv contribution to polar:
IMax=3 JMax=2 DiffMx= 0.00D+00
Leave Link 1102 at Fri Aug 21 20:46:23 2026, MaxMem= 805306368 cpu: 0.8 elap: 0.2
(Enter /home/user/gauss16/g16/l1110.exe)
Forming Gx(P) for the SCF density, NAtomX= 16.
Integral derivatives from FoFJK, PRISM(SPDF).
Do as many integral derivatives as possible in FoFJK.
G2DrvN: MDV= 805304616.
G2DrvN: will do 17 centers at a time, making 1 passes.
Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.
FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 3507 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
End of G2Drv F.D. properties file 721 does not exist.
End of G2Drv F.D. properties file 722 does not exist.
End of G2Drv F.D. properties file 788 does not exist.

Supporting Information file

```
 Leave Link 1110 at Fri Aug 21 21:01:07 2026, MaxMem=    805306368 cpu:             5305.4 elap:
884.4
 (Enter /home/user/gauss16/g16/l1002.exe)
 Minotr:  Closed shell wavefunction.
        IDoAtm=1111111111111111
        Direct CPHF calculation.
        Differentiating once with respect to electric field.
             with respect to dipole field.
        Differentiating once with respect to nuclear coordinates.
        Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.
        Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.
        NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.
       4769 words used for storage of precomputed grid.
Two-electron integrals replicated using symmetry.
        MDV=     805306368 using IRadAn=       1.
        Solving linear equations simultaneously, MaxMat=     384.
FoF2E skips out because all densities are zero.
CalDSu exits because no D1Ps are significant.
FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
IRaf=         1 NMat=      48 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2 IDoP0=3 IntGTp=3.
FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
       NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=          0 NGrid=          0
       NMat0=   48 NMatS0=     48 NMatT0=    0 NMatD0=   48 NMtDS0=    0 NMtDT0=    0
Integrals replicated using symmetry in FoFCou.
        There are    51 degrees of freedom in the 1st order CPHF.  IDoFFX=6 NUNeed=     3.
   48 vectors produced by pass  0 Test12= 4.22D-14 1.96D-09 XBig12= 4.14D+02 1.03D+01.
AX will form    48 AO Fock derivatives at one time.
   48 vectors produced by pass  1 Test12= 4.22D-14 1.96D-09 XBig12= 7.35D+01 1.52D+00.
   48 vectors produced by pass  2 Test12= 4.22D-14 1.96D-09 XBig12= 5.91D+00 5.19D-01.
   48 vectors produced by pass  3 Test12= 4.22D-14 1.96D-09 XBig12= 2.41D-01 9.54D-02.
   48 vectors produced by pass  4 Test12= 4.22D-14 1.96D-09 XBig12= 4.53D-03 1.33D-02.
   48 vectors produced by pass  5 Test12= 4.22D-14 1.96D-09 XBig12= 5.55D-05 8.86D-04.
   48 vectors produced by pass  6 Test12= 4.22D-14 1.96D-09 XBig12= 5.43D-07 8.46D-05.
   48 vectors produced by pass  7 Test12= 4.22D-14 1.96D-09 XBig12= 4.09D-09 9.80D-06.
   21 vectors produced by pass  8 Test12= 4.22D-14 1.96D-09 XBig12= 3.74D-11 1.05D-06.
    3 vectors produced by pass  9 Test12= 4.22D-14 1.96D-09 XBig12= 3.42D-13 8.25D-08.
    3 vectors produced by pass 10 Test12= 4.22D-14 1.96D-09 XBig12= 7.80D-15 1.17D-08.
    3 vectors produced by pass 11 Test12= 4.22D-14 1.96D-09 XBig12= 2.77D-14 3.04D-08.
    2 vectors produced by pass 12 Test12= 4.22D-14 1.96D-09 XBig12= 6.72D-15 1.31D-08.
InvSVY:  IOpt=1 It=  1 EMax= 8.88D-15
Solved reduced A of dimension   416 with    51 vectors.
FullF1:  Do perturbations      1 to       3.
Isotropic polarizability for W=    0.000000      217.59 Bohr**3.
End of Minotr F.D. properties file   721 does not exist.
End of Minotr F.D. properties file   722 does not exist.
End of Minotr F.D. properties file   788 does not exist.
```

Supporting Information file

Leave Link 1002 at Fri Aug 21 21:42:01 2026, MaxMem= 805306368 cpu: 14720.2 elap: 2453.7
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

****

Population analysis using the SCF Density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -10.40290 -10.40234 -10.36614 -10.36566 -10.36544
Alpha occ. eigenvalues -- -10.36529 -10.36405 -10.36403 -10.36298 -10.36284
Alpha occ. eigenvalues -- -10.36095 -10.36086 -10.36059 -10.36016 -10.35396
Alpha occ. eigenvalues -- -10.35389 -1.09543 -0.98450 -0.96923 -0.95287
Alpha occ. eigenvalues -- -0.93288 -0.90789 -0.88055 -0.83369 -0.81518
Alpha occ. eigenvalues -- -0.78453 -0.75191 -0.72291 -0.69613 -0.67340
Alpha occ. eigenvalues -- -0.65377 -0.64116 -0.53785 -0.53390 -0.52300
Alpha occ. eigenvalues -- -0.52137 -0.50854 -0.50302 -0.46892 -0.46765
Alpha occ. eigenvalues -- -0.44455 -0.43078 -0.39179 -0.38998 -0.35360
Alpha occ. eigenvalues -- -0.33202 -0.32643 -0.32137
Alpha virt. eigenvalues -- -0.07459 -0.07451 -0.05079 -0.02464 0.01006
Alpha virt. eigenvalues -- 0.03001 0.04417 0.05669 0.07664 0.10061
Alpha virt. eigenvalues -- 0.10853 0.11107 0.12094 0.12326 0.12804
Alpha virt. eigenvalues -- 0.15818 0.17145 0.19752 0.21010 0.21648
Alpha virt. eigenvalues -- 0.22475 0.23038 0.23232 0.24300 0.25409
Alpha virt. eigenvalues -- 0.26086 0.26988 0.27033 0.28599 0.28782
Alpha virt. eigenvalues -- 0.29464 0.30645 0.31347 0.31443 0.31854
Alpha virt. eigenvalues -- 0.31986 0.32968 0.33624 0.35286 0.35445
Alpha virt. eigenvalues -- 0.35703 0.36916 0.37285 0.38176 0.38189
Alpha virt. eigenvalues -- 0.39249 0.39377 0.39588 0.40449 0.41584
Alpha virt. eigenvalues -- 0.42331 0.43001 0.43642 0.44709 0.46023
Alpha virt. eigenvalues -- 0.46495 0.46639 0.47553 0.47694 0.48811
Alpha virt. eigenvalues -- 0.49117 0.50284 0.50725 0.50921 0.52249
Alpha virt. eigenvalues -- 0.52732 0.52984 0.53200 0.54297 0.54536
Alpha virt. eigenvalues -- 0.54926 0.55685 0.56069 0.56549 0.58161
Alpha virt. eigenvalues -- 0.58302 0.59013 0.59185 0.59368 0.60396
Alpha virt. eigenvalues -- 0.61116 0.63299 0.63574 0.63723 0.64293
Alpha virt. eigenvalues -- 0.65210 0.67191 0.67561 0.67944 0.68624
Alpha virt. eigenvalues -- 0.70914 0.71012 0.72044 0.72422 0.74301
Alpha virt. eigenvalues -- 0.75848 0.76815 0.77208 0.78800 0.79808
Alpha virt. eigenvalues -- 0.80557 0.84401 0.84818 0.85440 0.85915
Alpha virt. eigenvalues -- 0.86699 0.90213 0.91512 0.92663 0.92870
Alpha virt. eigenvalues -- 0.93592 0.95722 0.96684 0.98165 0.99140
Alpha virt. eigenvalues -- 1.01137 1.01981 1.02368 1.05797 1.07381
Alpha virt. eigenvalues -- 1.09301 1.09335 1.09879 1.12188 1.12432
Alpha virt. eigenvalues -- 1.13358 1.15262 1.15994 1.16387 1.18464
Alpha virt. eigenvalues -- 1.19675 1.22055 1.23127 1.23523 1.23875
Alpha virt. eigenvalues -- 1.26222 1.27253 1.27711 1.27775 1.30100
Alpha virt. eigenvalues -- 1.31458 1.33407 1.34466 1.35849 1.36137
Alpha virt. eigenvalues -- 1.37502 1.38475 1.39202 1.39243 1.40757
Alpha virt. eigenvalues -- 1.41670 1.42611 1.43166 1.43339 1.43747

Alpha virt. eigenvalues --	1.45417	1.46011	1.47089	1.48236	1.48834
Alpha virt. eigenvalues --	1.49155	1.49688	1.49957	1.50561	1.50861
Alpha virt. eigenvalues --	1.51264	1.53178	1.54048	1.54566	1.57963
Alpha virt. eigenvalues --	1.59431	1.61318	1.61735	1.62193	1.62991
Alpha virt. eigenvalues --	1.63954	1.64765	1.65752	1.67667	1.69594
Alpha virt. eigenvalues --	1.69727	1.71038	1.71633	1.72894	1.72985
Alpha virt. eigenvalues --	1.74463	1.76303	1.77824	1.77871	1.78794
Alpha virt. eigenvalues --	1.79143	1.81311	1.82715	1.84830	1.85724
Alpha virt. eigenvalues --	1.85892	1.86104	1.90730	1.92761	1.97301
Alpha virt. eigenvalues --	1.97394	1.98529	2.00087	2.00338	2.03215
Alpha virt. eigenvalues --	2.06572	2.10393	2.10749	2.11554	2.15349
Alpha virt. eigenvalues --	2.16006	2.16253	2.20506	2.22128	2.22994
Alpha virt. eigenvalues --	2.25084	2.26037	2.34826	2.36193	2.39105
Alpha virt. eigenvalues --	2.39541	2.40646	2.43305	2.43825	2.45271
Alpha virt. eigenvalues --	2.45641	2.46458	2.48206	2.48369	2.48652
Alpha virt. eigenvalues --	2.49877	2.49972	2.50630	2.52333	2.52909
Alpha virt. eigenvalues --	2.54337	2.55896	2.57415	2.59904	2.60059
Alpha virt. eigenvalues --	2.61447	2.62912	2.63001	2.63543	2.63877
Alpha virt. eigenvalues --	2.65023	2.65556	2.66665	2.69415	2.72825
Alpha virt. eigenvalues --	2.72966	2.73587	2.73969	2.74220	2.75500
Alpha virt. eigenvalues --	2.76290	2.78373	2.79430	2.80787	2.81160
Alpha virt. eigenvalues --	2.81927	2.82119	2.82687	2.83545	2.84161
Alpha virt. eigenvalues --	2.84257	2.85323	2.85747	2.86362	2.86737
Alpha virt. eigenvalues --	2.87626	2.87915	2.88434	2.89145	2.89823
Alpha virt. eigenvalues --	2.90026	2.90920	2.91331	2.92171	2.93036
Alpha virt. eigenvalues --	2.93049	2.96180	2.97117	2.97353	2.98234
Alpha virt. eigenvalues --	2.99198	2.99330	3.00503	3.01157	3.02464
Alpha virt. eigenvalues --	3.03691	3.04173	3.05115	3.05290	3.06112
Alpha virt. eigenvalues --	3.06968	3.09380	3.10536	3.11850	3.12890
Alpha virt. eigenvalues --	3.13088	3.14267	3.15253	3.15528	3.16162
Alpha virt. eigenvalues --	3.17364	3.19726	3.20239	3.20541	3.22443
Alpha virt. eigenvalues --	3.22585	3.25884	3.26203	3.26424	3.26889
Alpha virt. eigenvalues --	3.27539	3.28972	3.30006	3.31788	3.31805
Alpha virt. eigenvalues --	3.32125	3.34004	3.34047	3.35084	3.36171
Alpha virt. eigenvalues --	3.36488	3.36557	3.37888	3.40448	3.40497
Alpha virt. eigenvalues --	3.41377	3.42553	3.43457	3.43521	3.44323
Alpha virt. eigenvalues --	3.48510	3.48779	3.49564	3.49721	3.52594
Alpha virt. eigenvalues --	3.54345	3.54886	3.55158	3.55931	3.57777
Alpha virt. eigenvalues --	3.58282	3.63219	3.63308	3.64243	3.66162
Alpha virt. eigenvalues --	3.66642	3.70949	3.71954	3.75863	3.76958
Alpha virt. eigenvalues --	3.79693	3.82502	3.83022	3.86054	3.87574
Alpha virt. eigenvalues --	3.88441	3.89760	3.91625	3.94769	3.96338
Alpha virt. eigenvalues --	3.98359	4.04724	4.04935	4.06137	4.08851
Alpha virt. eigenvalues --	4.09491	4.10420	4.10655	4.16563	4.16906
Alpha virt. eigenvalues --	4.19249	4.21263	4.22009	4.25228	4.30376
Alpha virt. eigenvalues --	4.31725	4.38658	4.40094	4.41147	4.48289
Alpha virt. eigenvalues --	4.49793	4.51308	4.53702	4.57236	4.58556
Alpha virt. eigenvalues --	4.61495	4.67897	4.73076	4.75597	4.76838

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Alpha virt. eigenvalues -- 4.77724 4.78139 4.79230 4.89536 4.90163
Alpha virt. eigenvalues -- 4.92645 4.96840 4.99803 5.03008 5.04347
Alpha virt. eigenvalues -- 5.05594 5.06108 5.08303 5.12228 5.14609
Alpha virt. eigenvalues -- 5.17477 5.18973 5.20311 5.21334 5.23774
Alpha virt. eigenvalues -- 5.23822 5.25105 5.28525 5.30983 5.32793
Alpha virt. eigenvalues -- 5.40418 5.40523 5.48109 5.55173 5.60214
Alpha virt. eigenvalues -- 5.62385 5.76190 5.82830 5.99685 6.02968
Alpha virt. eigenvalues -- 6.14446 6.22586 22.16659 22.23400 22.50352
Alpha virt. eigenvalues -- 22.84888 23.09533 23.23080 23.31108 23.42168
Alpha virt. eigenvalues -- 23.61197 23.69701 23.79969 23.83195 23.91931
Alpha virt. eigenvalues -- 23.94694 24.23848 24.29259

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.875929	0.884298	0.505163	-0.090050	-0.085682	-0.057731
2	C	0.884298	4.869912	-0.085968	0.525382	-0.051217	-0.093478
3	C	0.505163	-0.085968	4.877048	-0.013447	0.884280	-0.006946
4	C	-0.090050	0.525382	-0.013447	4.882921	-0.006879	0.919487
5	C	-0.085682	-0.051217	0.884280	-0.006879	4.868805	-0.002156
6	C	-0.057731	-0.093478	-0.006946	0.919487	-0.002156	4.996634
7	C	-0.013420	-0.006884	-0.090250	-0.001223	0.525000	-0.000513
8	C	-0.009837	-0.021991	-0.001051	-0.105374	-0.000494	0.513962
9	C	-0.006917	-0.002149	-0.057644	-0.000508	-0.093179	-0.000030
10	C	-0.002426	-0.009679	-0.000358	-0.077807	-0.000132	-0.206969
11	C	-0.001051	-0.000489	-0.009797	0.000209	-0.021911	0.001967
12	C	-0.000215	-0.000776	-0.000056	-0.007249	-0.000121	-0.031763
13	C	-0.000359	-0.000129	-0.002410	-0.000124	-0.009624	0.000372
14	C	-0.000057	-0.000121	-0.000213	-0.001250	-0.000770	-0.009122
15	C	-0.000002	-0.000016	0.000002	-0.000271	0.000006	-0.002747
16	C	0.000002	0.000006	-0.000002	0.000111	-0.000016	0.001037

		7	8	9	10	11	12
1	C	-0.013420	-0.009837	-0.006917	-0.002426	-0.001051	-0.000215
2	C	-0.006884	-0.021991	-0.002149	-0.009679	-0.000489	-0.000776
3	C	-0.090250	-0.001051	-0.057644	-0.000358	-0.009797	-0.000056
4	C	-0.001223	-0.105374	-0.000508	-0.077807	0.000209	-0.007249
5	C	0.525000	-0.000494	-0.093179	-0.000132	-0.021911	-0.000121
6	C	-0.000513	0.513962	-0.000030	-0.206969	0.001967	-0.031763
7	C	4.883748	0.000209	0.919368	-0.000122	-0.105232	-0.001243
8	C	0.000209	5.069291	0.001968	0.610821	0.013746	-0.159530
9	C	0.919368	0.001968	4.995279	0.000365	0.513482	-0.009099
10	C	-0.000122	0.610821	0.000365	5.493673	0.000349	0.491076
11	C	-0.105232	0.013746	0.513482	0.000349	5.068779	-0.075527
12	C	-0.001243	-0.159530	-0.009099	0.491076	-0.075527	5.217465
13	C	-0.077520	0.000351	-0.206536	0.003978	0.611039	-0.046164
14	C	-0.007204	-0.075562	-0.031555	-0.046324	-0.158943	0.364928
15	C	0.000111	-0.020940	0.001033	-0.093337	0.011950	0.036601
16	C	-0.000271	0.011952	-0.002738	0.010300	-0.020896	0.104612

		13	14	15	16
1	C	-0.000359	-0.000057	-0.000002	0.000002

2	C	-0.000129	-0.000121	-0.000016	0.000006
3	C	-0.002410	-0.000213	0.000002	-0.000002
4	C	-0.000124	-0.001250	-0.000271	0.000111
5	C	-0.009624	-0.000770	0.000006	-0.000016
6	C	0.000372	-0.009122	-0.002747	0.001037
7	C	-0.077520	-0.007204	0.000111	-0.000271
8	C	0.000351	-0.075562	-0.020940	0.011952
9	C	-0.206536	-0.031555	0.001033	-0.002738
10	C	0.003978	-0.046324	-0.093337	0.010300
11	C	0.611039	-0.158943	0.011950	-0.020896
12	C	-0.046164	0.364928	0.036601	0.104612
13	C	5.492106	0.490539	0.010203	-0.093142
14	C	0.490539	5.217036	0.104731	0.036670
15	C	0.010203	0.104731	5.913528	0.105640
16	C	-0.093142	0.036670	0.105640	5.913104

Mulliken charges:

		1
1	C	0.002356
2	C	-0.006702
3	C	0.001650
4	C	-0.023928
5	C	-0.005909
6	C	-0.022005
7	C	-0.024554
8	C	0.172479
9	C	-0.021142
10	C	-0.173407
11	C	0.172325
12	C	0.117063
13	C	-0.172581
14	C	0.117217
15	C	-0.066492
16	C	-0.066369

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.002356
2	C	-0.006702
3	C	0.001650
4	C	-0.023928
5	C	-0.005909
6	C	-0.022005
7	C	-0.024554
8	C	0.172479
9	C	-0.021142
10	C	-0.173407
11	C	0.172325
12	C	0.117063

13 C -0.172581
14 C 0.117217
15 C -0.066492
16 C -0.066369
APT charges:
1
1 C 0.013827
2 C -0.045402
3 C 0.015993
4 C 0.084501
5 C -0.047409
6 C -0.081372
7 C 0.086202
8 C 0.137229
9 C -0.082796
10 C -0.185599
11 C 0.138393
12 C 0.207257
13 C -0.186590
14 C 0.208124
15 C -0.131092
16 C -0.131265
Sum of APT charges = 0.00000
APT charges with hydrogens summed into heavy atoms:
1
1 C 0.013827
2 C -0.045402
3 C 0.015993
4 C 0.084501
5 C -0.047409
6 C -0.081372
7 C 0.086202
8 C 0.137229
9 C -0.082796
10 C -0.185599
11 C 0.138393
12 C 0.207257
13 C -0.186590
14 C 0.208124
15 C -0.131092
16 C -0.131265
Electronic spatial extent (au): <R**2>= 3544.7415
Charge= 0.0000 electrons
Dipole moment (field-independent basis, Debye):
X= 3.8545 Y= -0.0035 Z= -0.0003 Tot= 3.8545
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -103.3333 YY= -85.1444 ZZ= -90.9433
XY= -0.0031 XZ= 0.0018 YZ= -1.6871

Supporting Information file

Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= -10.1930 YY= 7.9960 ZZ= 2.1971
XY= -0.0031 XZ= 0.0018 YZ= -1.6871
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= 121.5883 YYY= -0.0319 ZZZ= -0.0049 XYY= 4.1229
XXY= -0.0097 XXZ= -0.0023 XZZ= 17.3257 YZZ= -0.0021
YYZ= 0.0005 XYZ= 6.8734
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -4135.0360 YYYY= -1695.6463 ZZZZ= -137.2008 XXXY= -0.0652
XXXZ= -0.0016 YYYX= -0.0240 YYYZ= -3.3929 ZZZX= 0.0197
ZZZY= -4.0586 XXYY= -878.9386 XXZZ= -703.0480 YYZZ= -309.2486
XXYZ= -32.3114 YYXZ= 0.0000 ZZXY= 0.0032
N-N= 7.176436409760D+02 E-N=-2.846286594380D+03 KE= 6.062420692550D+02
Exact polarizability: 354.639 0.004 213.576 -0.001 3.808 84.567
Approx polarizability: 510.448 0.003 312.109 0.005 6.877 106.046
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Fri Aug 21 21:42:02 2026, MaxMem= 805306368 cpu: 4.3 elap: 0.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral second derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 2nd derivatives to the Hessian.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 15576 NPrTT= 51712 LenC2= 14212 LenP2D= 33580.
LDataN: DoStor=T MaxTD1= 8 Len= 415
Leave Link 701 at Fri Aug 21 21:42:03 2026, MaxMem= 805306368 cpu: 6.8 elap: 1.1
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Aug 21 21:42:03 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral second derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 100527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Aug 21 22:47:47 2026, MaxMem= 805306368 cpu: 23660.1 elap: 3943.7
(Enter /home/user/gauss16/g16/l716.exe)

Supporting Information file

Dipole = 1.51648676D+00-1.36431139D-03-1.33960126D-04
Polarizability= 3.54638790D+02 4.05366868D-03 2.13575586D+02
-6.35958186D-04 3.80770050D+00 8.45666968D+01
Full mass-weighted force constant matrix:
Low frequencies --- -4.6599 -3.5184 -0.0007 0.0004 0.0008 1.3316
Low frequencies --- 61.9248 92.9960 93.5658
Diagonal vibrational polarizability:
19.8734280 54.8697081 15.6163733
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1			2			3		
	A			A			A		
Frequencies --	61.9196			92.9959			93.5656		
Red. masses --	12.0000			12.0000			12.0000		
Frc consts --	0.0271			0.0611			0.0619		
IR Inten --	1.9521			0.0757			0.1042		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	0.01	0.27	0.29	-0.00	-0.02	0.11	-0.16	0.04
2 6	-0.03	0.03	0.14	0.15	0.08	-0.05	0.22	-0.23	0.02
3 6	-0.01	0.01	0.27	0.29	0.00	0.02	-0.11	-0.16	0.04
4 6	-0.01	0.00	-0.06	0.04	0.26	-0.04	0.18	-0.18	-0.02
5 6	0.03	0.03	0.14	0.15	-0.08	0.05	-0.22	-0.23	0.02
6 6	-0.02	0.02	-0.22	0.03	0.37	-0.02	0.16	0.02	-0.04
7 6	0.01	0.00	-0.06	0.04	-0.26	0.04	-0.19	-0.18	-0.02
8 6	-0.02	-0.01	-0.28	0.00	0.28	0.03	0.20	0.20	-0.04
9 6	0.02	0.02	-0.22	0.02	-0.37	0.02	-0.16	0.02	-0.04
10 6	-0.02	-0.01	-0.23	-0.10	0.09	0.05	0.24	0.27	-0.01
11 6	0.02	-0.01	-0.28	0.00	-0.27	-0.03	-0.20	0.20	-0.04
12 6	-0.06	-0.01	-0.04	-0.20	-0.01	0.03	0.12	0.15	0.02
13 6	0.02	-0.01	-0.23	-0.11	-0.08	-0.05	-0.24	0.27	-0.01
14 6	0.06	-0.01	-0.04	-0.20	0.01	-0.03	-0.12	0.15	0.02
15 6	-0.21	-0.03	0.42	-0.20	-0.04	0.02	0.06	-0.08	0.04
16 6	0.22	-0.03	0.42	-0.20	0.04	-0.02	-0.06	-0.08	0.04

	4			5			6		
	A			A			A		
Frequencies --	111.5699			152.8709			226.1202		
Red. masses --	12.0000			12.0000			12.0000		
Frc consts --	0.0880			0.1652			0.3615		
IR Inten --	0.0004			1.4329			0.1768		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.04	0.00	0.15	0.03	-0.04	-0.29	0.13	-0.12	0.00
2 6	0.02	0.02	0.34	-0.01	-0.01	-0.01	0.28	-0.20	0.01
3 6	0.04	-0.00	-0.15	-0.03	-0.04	-0.29	-0.13	-0.12	0.00
4 6	-0.01	0.06	0.28	-0.01	-0.01	0.27	0.08	0.11	-0.01
5 6	0.02	-0.02	-0.34	0.01	-0.01	-0.01	-0.28	-0.20	0.01
6 6	-0.01	0.07	0.03	-0.01	0.05	0.31	0.06	0.33	-0.01

7	6	-0.01	-0.06	-0.28	0.01	-0.01	0.27	-0.08	0.11	-0.01
8	6	-0.00	0.05	-0.23	-0.00	0.05	0.08	0.01	0.15	0.02
9	6	-0.01	-0.07	-0.03	0.01	0.05	0.31	-0.06	0.33	-0.01
10	6	-0.01	0.03	-0.37	0.01	0.06	-0.23	-0.22	-0.26	0.01
11	6	-0.00	-0.05	0.23	0.00	0.05	0.08	-0.01	0.15	0.02
12	6	-0.02	0.04	-0.19	-0.03	0.01	-0.29	-0.15	-0.18	0.00
13	6	-0.01	-0.02	0.37	-0.01	0.06	-0.23	0.22	-0.26	0.01
14	6	-0.02	-0.04	0.19	0.03	0.01	-0.29	0.15	-0.18	0.00
15	6	-0.00	0.17	-0.12	-0.22	-0.12	0.16	-0.07	0.16	-0.03
16	6	-0.00	-0.17	0.12	0.22	-0.12	0.16	0.07	0.16	-0.03

	7	8	9
	A	A	A
Frequencies --	233.2281	259.1251	270.4374
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.3846	0.4747	0.5171
IR Inten --	0.0095	0.0483	9.9603

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	0.00	0.18	-0.29	0.01	-0.04	-0.15	0.08	-0.24
2	6	0.03	-0.04	0.32	0.06	-0.20	-0.07	0.13	-0.07	0.16
3	6	-0.06	-0.00	-0.18	-0.29	-0.01	0.04	0.15	0.08	-0.24
4	6	0.05	-0.09	0.00	0.12	-0.32	-0.00	0.02	0.08	0.28
5	6	0.03	0.04	-0.32	0.06	0.20	0.07	-0.13	-0.07	0.16
6	6	0.04	-0.03	-0.34	0.08	0.05	0.09	0.05	-0.17	-0.02
7	6	0.05	0.09	-0.00	0.12	0.32	0.00	-0.02	0.08	0.28
8	6	0.05	0.02	-0.22	0.16	0.35	0.05	0.07	-0.05	-0.27
9	6	0.04	0.03	0.34	0.08	-0.05	-0.09	-0.05	-0.17	-0.02
10	6	0.03	0.03	0.18	0.09	0.21	-0.09	0.05	-0.07	-0.16
11	6	0.05	-0.02	0.22	0.16	-0.35	-0.05	-0.07	-0.06	-0.27
12	6	-0.04	-0.04	0.22	-0.11	0.02	-0.04	0.02	-0.03	0.22
13	6	0.03	-0.03	-0.18	0.09	-0.21	0.09	-0.05	-0.07	-0.16
14	6	-0.04	0.04	-0.22	-0.11	-0.02	0.04	-0.02	-0.03	0.22
15	6	-0.11	-0.23	0.17	-0.12	0.02	-0.02	0.17	0.24	0.02
16	6	-0.11	0.23	-0.17	-0.12	-0.02	0.02	-0.17	0.24	0.02

	10	11	12
	A	A	A
Frequencies --	298.5004	351.0421	359.5839
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.6300	0.8713	0.9142
IR Inten --	140.6285	18.8782	0.0994

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.42	0.14	0.12	0.04	0.07	0.18	0.14	-0.01	-0.17
2	6	0.22	-0.23	-0.09	-0.03	0.09	-0.21	-0.04	0.09	-0.17
3	6	0.42	0.14	0.12	-0.04	0.07	0.18	0.14	0.01	0.18
4	6	-0.08	0.21	-0.13	0.13	-0.19	-0.14	0.00	0.02	0.19
5	6	-0.21	-0.23	-0.09	0.03	0.09	-0.22	-0.04	-0.09	0.17
6	6	-0.02	-0.21	0.06	0.11	-0.11	0.24	0.02	-0.21	0.18
7	6	0.08	0.21	-0.13	-0.13	-0.19	-0.14	0.00	-0.02	-0.19
8	6	0.04	0.13	0.12	0.10	-0.04	0.13	0.04	-0.10	-0.19

9	6	0.02	-0.21	0.06	-0.11	-0.11	0.24	0.02	0.21	-0.18
10	6	-0.02	-0.00	-0.01	0.08	-0.07	-0.25	0.14	0.11	-0.22
11	6	-0.04	0.13	0.12	-0.10	-0.04	0.12	0.04	0.09	0.19
12	6	0.02	0.02	-0.12	-0.05	-0.10	0.01	-0.06	-0.01	0.12
13	6	0.02	-0.00	-0.01	-0.08	-0.07	-0.26	0.14	-0.11	0.22
14	6	-0.02	0.02	-0.12	0.05	-0.10	0.02	-0.06	0.01	-0.12
15	6	-0.07	-0.05	0.05	0.03	0.36	0.05	-0.23	-0.24	0.20
16	6	0.07	-0.05	0.05	-0.02	0.36	0.05	-0.23	0.24	-0.20

	13	14	15
	A	A	A
Frequencies --	402.3573	411.0813	434.8547
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.1446	1.1948	1.3370
IR Inten --	0.1682	2.7035	1.5677

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.25	-0.12	0.11	-0.18	0.01	-0.16	0.05	-0.01	0.54
2	6	0.16	-0.08	-0.14	0.22	-0.23	-0.11	0.06	-0.04	-0.32
3	6	-0.25	-0.12	0.11	-0.18	-0.01	0.16	0.05	0.01	-0.54
4	6	-0.10	0.37	-0.04	0.07	-0.02	0.20	0.04	-0.07	0.12
5	6	-0.16	-0.08	-0.15	0.22	0.23	0.11	0.06	0.04	0.32
6	6	-0.05	0.01	0.15	0.03	0.28	0.04	0.03	-0.00	-0.09
7	6	0.10	0.37	-0.04	0.07	0.02	-0.20	0.04	0.07	-0.12
8	6	-0.13	-0.31	-0.02	-0.07	-0.14	-0.17	-0.04	-0.09	0.14
9	6	0.05	0.01	0.15	0.03	-0.28	-0.04	0.03	0.00	0.09
10	6	0.09	0.08	-0.14	-0.18	-0.30	-0.02	-0.02	-0.06	-0.13
11	6	0.14	-0.31	-0.02	-0.07	0.14	0.17	-0.04	0.09	-0.14
12	6	0.10	0.10	0.06	0.05	-0.04	0.06	-0.06	-0.02	-0.02
13	6	-0.09	0.08	-0.14	-0.18	0.30	0.02	-0.02	0.06	0.13
14	6	-0.10	0.10	0.06	0.05	0.04	-0.06	-0.06	0.02	0.02
15	6	0.12	-0.04	0.03	0.05	-0.09	0.07	-0.06	-0.06	0.02
16	6	-0.12	-0.04	0.04	0.05	0.09	-0.07	-0.06	0.06	-0.02

	16	17	18
	A	A	A
Frequencies --	451.6357	455.3021	482.6042
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.4421	1.4657	1.6467
IR Inten --	0.8725	1.5609	67.0569

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.17	0.00	-0.13	0.02	-0.00	-0.08	0.20	-0.03	-0.02
2	6	0.12	0.03	0.25	-0.16	0.11	-0.24	-0.27	0.25	0.04
3	6	-0.17	0.00	-0.13	0.02	0.00	0.08	0.20	0.03	0.02
4	6	0.05	0.10	-0.08	-0.04	-0.03	0.43	0.13	-0.44	-0.06
5	6	-0.12	0.03	0.25	-0.16	-0.11	0.24	-0.27	-0.25	-0.04
6	6	0.08	-0.23	-0.21	-0.04	0.00	-0.22	0.04	0.22	0.07
7	6	-0.05	0.10	-0.08	-0.04	0.03	-0.42	0.14	0.44	0.06
8	6	0.01	-0.17	0.23	0.04	0.17	-0.14	-0.01	-0.02	-0.03
9	6	-0.08	-0.23	-0.21	-0.04	-0.00	0.22	0.04	-0.22	-0.07
10	6	0.09	0.04	0.14	0.01	0.10	0.24	-0.11	-0.17	-0.04

11	6	-0.01	-0.17	0.23	0.04	-0.17	0.14	-0.01	0.02	0.03
12	6	-0.02	-0.01	-0.23	0.02	-0.00	0.01	-0.00	-0.03	-0.00
13	6	-0.09	0.04	0.14	0.01	-0.10	-0.24	-0.11	0.17	0.04
14	6	0.02	-0.01	-0.23	0.02	0.00	-0.01	-0.00	0.03	0.00
15	6	-0.18	0.24	0.03	0.16	0.09	-0.11	0.01	-0.05	0.02
16	6	0.18	0.24	0.03	0.16	-0.09	0.11	0.01	0.05	-0.02

	19	20	21
	A	A	A
Frequencies --	496.3280	498.9982	502.6511
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.7417	1.7605	1.7863
IR Inten --	9.1949	1.2747	0.8005

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.28	0.11	-0.07	-0.05	0.07	0.15	0.17	-0.04	-0.21
2	6	0.08	-0.08	0.15	0.09	-0.02	-0.37	0.18	-0.07	0.07
3	6	0.28	0.11	-0.07	0.05	0.07	0.15	0.17	0.04	0.21
4	6	0.10	-0.18	-0.12	0.08	-0.07	0.38	0.11	-0.15	0.13
5	6	-0.09	-0.09	0.15	-0.09	-0.02	-0.37	0.18	0.07	-0.07
6	6	0.03	0.36	0.00	0.05	0.03	-0.14	0.08	-0.24	-0.24
7	6	-0.10	-0.18	-0.12	-0.08	-0.07	0.38	0.11	0.15	-0.13
8	6	-0.16	-0.35	0.10	-0.04	-0.17	-0.11	-0.03	-0.10	0.21
9	6	-0.03	0.36	-0.00	-0.05	0.03	-0.14	0.08	0.24	0.24
10	6	0.07	0.06	-0.07	0.03	0.05	0.23	-0.10	-0.13	0.02
11	6	0.16	-0.35	0.10	0.05	-0.17	-0.11	-0.03	0.10	-0.21
12	6	0.06	0.06	-0.02	-0.02	0.02	-0.12	-0.18	-0.01	-0.08
13	6	-0.07	0.06	-0.07	-0.04	0.05	0.23	-0.10	0.13	-0.02
14	6	-0.06	0.06	-0.02	0.02	0.02	-0.12	-0.18	0.01	0.09
15	6	0.04	0.02	0.03	-0.14	0.10	-0.02	-0.23	0.17	-0.09
16	6	-0.03	0.02	0.03	0.14	0.10	-0.02	-0.24	-0.17	0.09

	22	23	24
	A	A	A
Frequencies --	511.1834	531.6258	532.9193
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.8475	1.9982	2.0080
IR Inten --	94.3506	0.4710	0.5998

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	0.01	0.06	-0.01	-0.02	0.02	0.09	-0.02	0.16
2	6	-0.02	0.03	-0.01	-0.04	-0.00	-0.09	0.11	-0.06	-0.06
3	6	0.03	-0.01	-0.06	0.00	-0.02	0.03	0.09	0.02	-0.16
4	6	-0.03	0.09	-0.04	-0.04	0.02	0.22	0.05	-0.07	-0.10
5	6	-0.02	-0.03	0.02	0.03	-0.00	-0.09	0.11	0.06	0.06
6	6	0.01	-0.31	0.07	-0.02	0.03	-0.38	0.03	-0.11	0.28
7	6	-0.03	-0.09	0.04	0.03	0.01	0.22	0.05	0.08	0.11
8	6	0.18	0.38	-0.05	-0.02	0.06	0.42	-0.02	-0.08	-0.35
9	6	0.01	0.31	-0.07	0.02	0.02	-0.36	0.03	0.11	-0.30
10	6	-0.24	-0.37	-0.05	-0.01	-0.02	-0.32	-0.04	0.01	0.30
11	6	0.18	-0.38	0.05	0.02	0.06	0.40	-0.02	0.08	0.37
12	6	0.03	-0.03	0.02	0.01	0.01	0.10	-0.09	0.01	0.02

13	6	-0.24	0.37	0.05	0.01	-0.02	-0.30	-0.04	-0.01	-0.31
14	6	0.04	0.03	-0.02	-0.00	0.01	0.10	-0.09	-0.01	-0.02
15	6	0.05	-0.06	0.05	0.12	-0.07	0.01	-0.12	0.25	-0.11
16	6	0.05	0.06	-0.05	-0.11	-0.06	0.01	-0.13	-0.25	0.11

	25	26	27
	A	A	A
Frequencies --	619.8844	678.7639	702.9138
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.7168	3.2574	3.4933
IR Inten --	4.9908	0.4912	2.1400

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.09	-0.05	-0.02	0.09	0.07	-0.00	-0.00	-0.00	0.01
2	6	0.10	-0.07	0.03	0.09	0.05	-0.00	0.00	-0.00	-0.01
3	6	0.09	0.05	0.02	-0.09	0.07	-0.00	-0.00	0.00	-0.01
4	6	-0.02	-0.06	-0.04	0.10	-0.11	0.01	-0.00	0.00	0.01
5	6	0.10	0.07	-0.03	-0.09	0.05	-0.00	0.00	0.00	0.01
6	6	-0.02	-0.09	0.05	0.05	-0.09	0.00	-0.00	-0.00	-0.00
7	6	-0.02	0.06	0.04	-0.10	-0.11	0.01	-0.00	-0.00	-0.01
8	6	-0.09	-0.01	-0.05	-0.04	0.01	0.00	0.00	0.00	-0.05
9	6	-0.02	0.09	-0.05	-0.05	-0.09	0.00	-0.00	0.00	0.00
10	6	-0.03	0.08	0.01	-0.28	-0.30	0.02	-0.01	0.01	0.19
11	6	-0.09	0.01	0.05	0.04	0.01	0.00	0.00	-0.00	0.05
12	6	-0.31	-0.14	-0.13	0.28	0.38	-0.14	0.16	0.09	-0.58
13	6	-0.03	-0.08	-0.01	0.28	-0.30	0.01	-0.01	-0.01	-0.19
14	6	-0.31	0.14	0.13	-0.28	0.38	-0.14	0.16	-0.09	0.58
15	6	0.29	-0.38	-0.28	0.15	-0.02	0.12	-0.15	-0.20	0.17
16	6	0.29	0.38	0.28	-0.15	-0.02	0.12	-0.15	0.20	-0.17

	28	29	30
	A	A	A
Frequencies --	749.9623	774.6939	977.9677
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.9766	4.2432	6.7621
IR Inten --	53.5471	4.4243	5.8715

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.08	-0.14	0.01	0.26	-0.17	-0.01	0.12	0.17	-0.01
2	6	-0.21	-0.03	-0.02	0.14	-0.23	0.02	0.21	0.03	0.00
3	6	0.08	-0.14	0.01	0.26	0.17	0.01	-0.12	0.17	-0.01
4	6	-0.10	0.12	0.02	-0.17	-0.20	0.00	-0.03	-0.16	0.00
5	6	0.21	-0.03	-0.02	0.14	0.23	-0.02	-0.21	0.03	0.00
6	6	-0.02	0.16	-0.04	-0.24	-0.04	-0.00	-0.15	-0.08	-0.00
7	6	0.10	0.12	0.02	-0.17	0.20	-0.00	0.03	-0.16	0.00
8	6	0.17	0.03	-0.01	-0.20	0.13	0.00	-0.23	0.08	-0.01
9	6	0.02	0.17	-0.04	-0.24	0.04	0.00	0.15	-0.08	-0.00
10	6	0.16	-0.09	0.11	-0.12	0.16	-0.05	-0.10	0.22	0.04
11	6	-0.17	0.03	-0.01	-0.20	-0.13	-0.00	0.23	0.08	-0.01
12	6	0.28	-0.19	-0.26	0.20	0.14	0.08	-0.11	-0.24	-0.17
13	6	-0.16	-0.09	0.11	-0.12	-0.16	0.05	0.10	0.22	0.04
14	6	-0.28	-0.19	-0.26	0.20	-0.14	-0.08	0.11	-0.24	-0.17

15	6	0.25	0.14	0.18	0.12	0.02	0.17	0.35	-0.02	0.14
16	6	-0.25	0.14	0.18	0.11	-0.02	-0.17	-0.35	-0.02	0.14

	31	32	33
	A	A	A
Frequencies --	1110.1688	1211.8512	1227.8555
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	8.7138	10.3832	10.6592
IR Inten --	1.9878	1.4432	2.4680

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.12	-0.25	0.00	-0.02	0.02	0.00	0.12	0.18	-0.01
2	6	-0.14	-0.25	0.01	0.03	0.04	-0.00	0.18	-0.01	0.00
3	6	0.12	0.25	-0.00	-0.02	-0.02	-0.00	-0.12	0.18	-0.01
4	6	-0.25	-0.01	0.00	0.01	-0.01	0.00	-0.23	-0.16	0.00
5	6	-0.14	0.25	-0.01	0.03	-0.04	0.00	-0.18	-0.01	0.00
6	6	-0.13	0.12	-0.01	0.01	-0.00	-0.00	-0.30	0.04	-0.01
7	6	-0.25	0.01	-0.00	0.01	0.01	-0.00	0.23	-0.16	0.00
8	6	0.28	-0.03	0.01	-0.05	0.02	0.00	0.04	0.06	0.00
9	6	-0.13	-0.12	0.01	0.01	0.00	0.00	0.30	0.04	-0.01
10	6	0.26	-0.19	0.02	-0.04	-0.02	0.00	0.12	-0.06	-0.03
11	6	0.28	0.03	-0.01	-0.05	-0.02	-0.00	-0.04	0.06	0.00
12	6	0.01	-0.16	-0.02	0.27	0.33	0.13	0.37	-0.11	0.11
13	6	0.26	0.19	-0.02	-0.04	0.02	-0.00	-0.12	-0.06	-0.03
14	6	0.01	0.16	0.02	0.27	-0.33	-0.13	-0.37	-0.11	0.11
15	6	-0.14	-0.02	-0.14	-0.21	-0.23	-0.44	-0.24	0.06	-0.08
16	6	-0.14	0.02	0.14	-0.22	0.23	0.44	0.23	0.06	-0.08

	34	35	36
	A	A	A
Frequencies --	1442.2673	1452.5346	1608.5413
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	14.7070	14.9171	18.2935
IR Inten --	0.2587	14.0776	7.2492

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.37	-0.01	-0.07	-0.11	0.00	0.01	-0.08	0.00
2	6	0.29	0.21	-0.00	-0.08	0.03	-0.00	-0.11	-0.09	-0.00
3	6	-0.01	-0.37	0.01	0.07	-0.11	0.00	0.01	0.08	-0.00
4	6	-0.15	-0.15	0.00	0.24	0.09	0.00	0.18	0.07	0.00
5	6	0.29	-0.21	0.00	0.08	0.03	-0.00	-0.11	0.09	0.00
6	6	-0.30	0.01	-0.00	0.17	-0.07	0.01	0.07	-0.04	0.00
7	6	-0.15	0.15	-0.00	-0.24	0.09	0.00	0.18	-0.07	-0.00
8	6	0.03	0.04	-0.00	-0.27	0.08	-0.01	-0.17	0.05	-0.01
9	6	-0.30	-0.01	0.00	-0.17	-0.07	0.01	0.07	0.04	-0.00
10	6	0.11	-0.05	0.00	-0.20	0.19	-0.04	-0.13	0.14	-0.03
11	6	0.03	-0.04	0.00	0.27	0.08	-0.01	-0.17	-0.05	0.01
12	6	0.10	-0.24	-0.01	0.37	-0.24	0.08	0.29	-0.50	0.00
13	6	0.11	0.05	-0.00	0.20	0.19	-0.04	-0.13	-0.14	0.03
14	6	0.10	0.24	0.01	-0.37	-0.24	0.08	0.29	0.50	-0.00
15	6	-0.08	0.00	-0.05	-0.12	0.03	-0.04	-0.13	-0.01	-0.11
16	6	-0.08	-0.00	0.05	0.12	0.03	-0.04	-0.13	0.01	0.11

Supporting Information file

	37			38			39		
	A			A			A		
Frequencies --	2060.0743			2145.9350			2216.3405		
Red. masses --	12.0000			12.0000			12.0000		
Frc consts --	30.0052			32.5585			34.7300		
IR Inten --	0.0033			0.1842			6.7119		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.15	0.36	-0.00	-0.18	-0.32	0.01	-0.05	-0.16	0.00
2 6	-0.21	-0.29	0.00	0.22	0.34	-0.01	-0.01	0.03	-0.00
3 6	0.15	-0.36	0.00	0.18	-0.32	0.01	-0.05	0.16	-0.00
4 6	0.22	0.05	0.00	0.21	0.01	-0.00	0.42	0.09	-0.00
5 6	-0.21	0.29	-0.00	-0.22	0.34	-0.01	-0.01	-0.03	0.00
6 6	-0.23	0.00	-0.00	-0.29	-0.02	-0.00	-0.38	-0.03	-0.00
7 6	0.22	-0.05	-0.00	-0.21	0.01	-0.00	0.42	-0.09	0.00
8 6	0.25	-0.12	0.01	-0.10	0.07	-0.00	-0.18	0.10	-0.01
9 6	-0.23	-0.00	0.00	0.29	-0.02	-0.00	-0.38	0.03	0.00
10 6	-0.17	0.10	-0.01	0.18	-0.11	0.01	0.26	-0.16	0.02
11 6	0.25	0.12	-0.01	0.10	0.07	-0.00	-0.18	-0.10	0.01
12 6	-0.02	0.06	0.00	-0.03	0.03	-0.01	-0.05	0.06	-0.01
13 6	-0.17	-0.10	0.01	-0.18	-0.11	0.01	0.26	0.16	-0.02
14 6	-0.02	-0.06	-0.00	0.03	0.03	-0.01	-0.05	-0.06	0.01
15 6	0.02	-0.02	-0.01	0.00	0.00	0.00	0.01	0.00	0.01
16 6	0.02	0.02	0.01	-0.00	0.00	0.00	0.01	-0.00	-0.01

	40			41			42		
	A			A			A		
Frequencies --	2261.1337			2277.1383			2278.7681		
Red. masses --	12.0000			12.0000			12.0000		
Frc consts --	36.1480			36.6615			36.7140		
IR Inten --	25.0541			53.7806			3.3255		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.10	-0.20	0.01	-0.13	-0.33	0.01	0.04	0.06	-0.00
2 6	0.22	0.27	-0.01	0.16	0.22	-0.01	-0.05	-0.07	0.00
3 6	0.10	-0.20	0.01	-0.13	0.33	-0.01	-0.04	0.07	-0.00
4 6	-0.42	-0.11	-0.00	0.08	0.01	0.00	-0.10	-0.01	-0.00
5 6	-0.22	0.27	-0.01	0.16	-0.22	0.01	0.05	-0.07	0.00
6 6	0.35	0.02	0.00	-0.22	0.00	-0.00	0.23	-0.01	0.01
7 6	0.42	-0.11	-0.00	0.08	-0.01	0.00	0.10	-0.01	-0.00
8 6	0.04	-0.03	0.00	0.35	-0.16	0.01	-0.44	0.20	-0.02
9 6	-0.35	0.02	0.00	-0.21	-0.00	0.00	-0.23	-0.01	0.01
10 6	-0.10	0.06	-0.01	-0.27	0.17	-0.02	0.37	-0.23	0.02
11 6	-0.04	-0.03	0.00	0.34	0.16	-0.01	0.44	0.21	-0.02
12 6	0.03	-0.02	0.00	0.03	-0.02	0.01	-0.03	0.04	-0.01
13 6	0.10	0.06	-0.01	-0.27	-0.17	0.02	-0.37	-0.23	0.02
14 6	-0.03	-0.02	0.00	0.03	0.02	-0.01	0.03	0.04	-0.01
15 6	-0.00	0.00	-0.00	0.00	-0.01	-0.01	0.00	0.01	0.00
16 6	0.00	0.00	-0.00	0.00	0.01	0.01	0.00	0.01	0.00

Supporting Information file

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 6 and mass 12.00000
Atom 2 has atomic number 6 and mass 12.00000
Atom 3 has atomic number 6 and mass 12.00000
Atom 4 has atomic number 6 and mass 12.00000
Atom 5 has atomic number 6 and mass 12.00000
Atom 6 has atomic number 6 and mass 12.00000
Atom 7 has atomic number 6 and mass 12.00000
Atom 8 has atomic number 6 and mass 12.00000
Atom 9 has atomic number 6 and mass 12.00000
Atom 10 has atomic number 6 and mass 12.00000
Atom 11 has atomic number 6 and mass 12.00000
Atom 12 has atomic number 6 and mass 12.00000
Atom 13 has atomic number 6 and mass 12.00000
Atom 14 has atomic number 6 and mass 12.00000
Atom 15 has atomic number 6 and mass 12.00000
Atom 16 has atomic number 6 and mass 12.00000
Molecular mass: 192.00000 amu.
Principal axes and moments of inertia in atomic units:

	1	2	3
Eigenvalues --	2129.50630	4578.77873	6639.71053
X	1.00000	0.00000	0.00000
Y	-0.00000	1.00000	0.00000
Z	0.00000	-0.00000	1.00000

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.04067 0.01892 0.01304
Rotational constants (GHZ): 0.84749 0.39415 0.27181
Zero-point vibrational energy 203480.6 (Joules/Mol)
48.63302 (Kcal/Mol)
Warning -- explicit consideration of 25 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 89.09 133.80 134.62 160.52 219.95
(Kelvin) 325.34 335.56 372.82 389.10 429.48
505.07 517.36 578.90 591.45 625.66
649.80 655.08 694.36 714.11 717.95
723.20 735.48 764.89 766.75 891.88
976.59 1011.34 1079.03 1114.61 1407.08
1597.29 1743.58 1766.61 2075.10 2089.87
2314.33 2963.99 3087.52 3188.82 3253.27
3276.29 3278.64

Zero-point correction= 0.077502 (Hartree/Particle)
Thermal correction to Energy= 0.090696

Supporting Information file

Thermal correction to Enthalpy= 0.091640
Thermal correction to Gibbs Free Energy= 0.037966
Sum of electronic and zero-point Energies= -608.904039
Sum of electronic and thermal Energies= -608.890844
Sum of electronic and thermal Enthalpies= -608.889900
Sum of electronic and thermal Free Energies= -608.943575

		E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total		56.912	48.627	112.967
Electronic		0.000	0.000	0.000
Translational		0.889	2.981	41.662
Rotational		0.889	2.981	32.537
Vibrational		55.135	42.665	38.767
Vibration	1	0.597	1.972	4.395
Vibration	2	0.602	1.954	3.596
Vibration	3	0.603	1.954	3.584
Vibration	4	0.607	1.940	3.241
Vibration	5	0.619	1.899	2.636
Vibration	6	0.650	1.801	1.910
Vibration	7	0.654	1.790	1.854
Vibration	8	0.668	1.747	1.668
Vibration	9	0.674	1.728	1.593
Vibration	10	0.692	1.677	1.425
Vibration	11	0.728	1.573	1.162
Vibration	12	0.734	1.556	1.124
Vibration	13	0.768	1.465	0.954
Vibration	14	0.775	1.446	0.923
Vibration	15	0.795	1.394	0.843
Vibration	16	0.810	1.357	0.791
Vibration	17	0.814	1.349	0.780
Vibration	18	0.839	1.289	0.703
Vibration	19	0.852	1.258	0.667
Vibration	20	0.854	1.252	0.661
Vibration	21	0.858	1.244	0.652
Vibration	22	0.866	1.225	0.631
Vibration	23	0.887	1.180	0.584
Vibration	24	0.888	1.177	0.581
Vibration	25	0.980	0.990	0.417

		Q	Log10(Q)	Ln(Q)
Total Bot		0.344399D-17	-17.462938	-40.209900
Total V=0		0.153221D+19	18.185318	41.873242
Vib (Bot)		0.114346D-31	-31.941778	-73.548662
Vib (Bot)	1	0.333425D+01	0.522998	1.204248
Vib (Bot)	2	0.220973D+01	0.344339	0.792870
Vib (Bot)	3	0.219605D+01	0.341642	0.786660
Vib (Bot)	4	0.183511D+01	0.263661	0.607103
Vib (Bot)	5	0.132530D+01	0.122313	0.281636

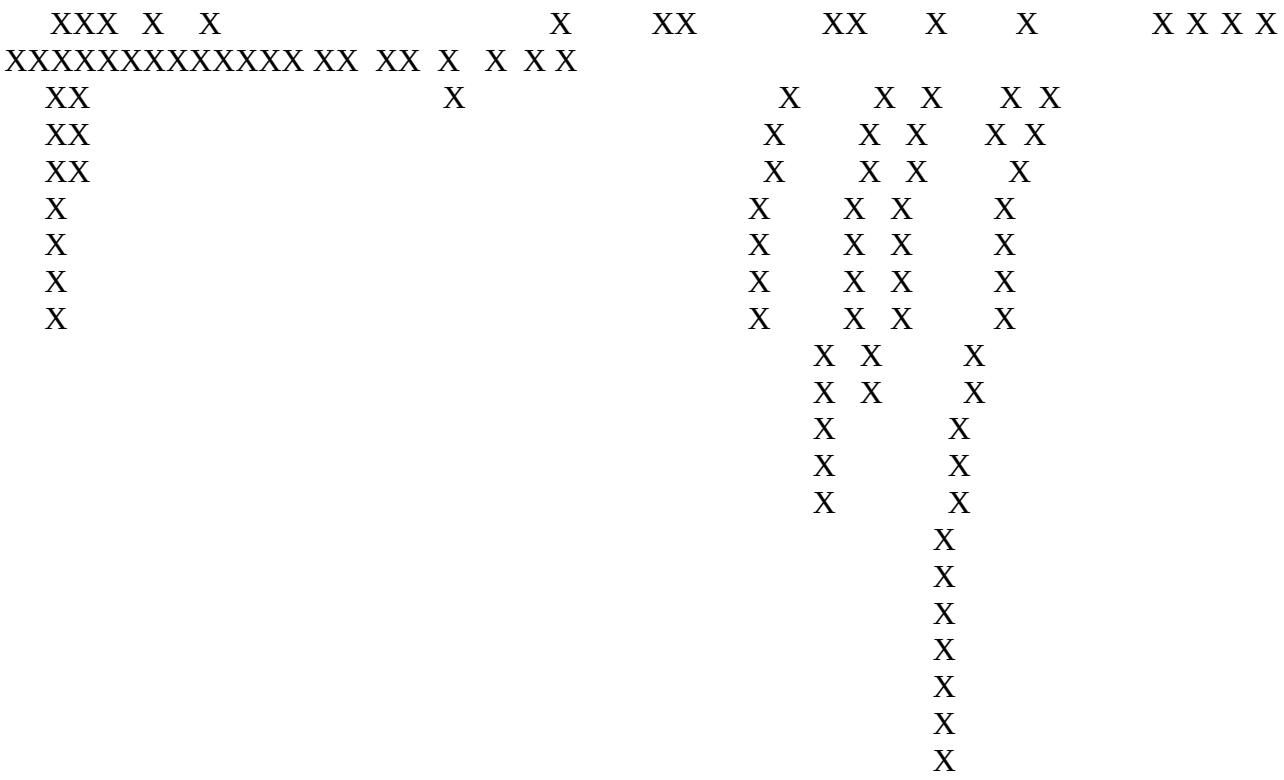
Vib (Bot)	6	0.872501D+00	-0.059234	-0.136392
Vib (Bot)	7	0.843288D+00	-0.074024	-0.170447
Vib (Bot)	8	0.749888D+00	-0.125003	-0.287831
Vib (Bot)	9	0.714465D+00	-0.146019	-0.336221
Vib (Bot)	10	0.637643D+00	-0.195422	-0.449977
Vib (Bot)	11	0.525220D+00	-0.279659	-0.643938
Vib (Bot)	12	0.509870D+00	-0.292540	-0.673599
Vib (Bot)	13	0.442214D+00	-0.354368	-0.815961
Vib (Bot)	14	0.430033D+00	-0.366498	-0.843892
Vib (Bot)	15	0.399160D+00	-0.398853	-0.918393
Vib (Bot)	16	0.379198D+00	-0.421134	-0.969698
Vib (Bot)	17	0.375019D+00	-0.425947	-0.980778
Vib (Bot)	18	0.345775D+00	-0.461207	-1.061968
Vib (Bot)	19	0.332215D+00	-0.478581	-1.101972
Vib (Bot)	20	0.329658D+00	-0.481936	-1.109699
Vib (Bot)	21	0.326202D+00	-0.486514	-1.120239
Vib (Bot)	22	0.318310D+00	-0.497150	-1.144731
Vib (Bot)	23	0.300374D+00	-0.522338	-1.202728
Vib (Bot)	24	0.299283D+00	-0.523919	-1.206367
Vib (Bot)	25	0.235945D+00	-0.627190	-1.444159
Vib (V=0)		0.508719D+04	3.706478	8.534481
Vib (V=0)	1	0.387153D+01	0.587883	1.353651
Vib (V=0)	2	0.276559D+01	0.441788	1.017255
Vib (V=0)	3	0.275225D+01	0.439688	1.012419
Vib (V=0)	4	0.240200D+01	0.380574	0.876303
Vib (V=0)	5	0.191648D+01	0.282504	0.650489
Vib (V=0)	6	0.150561D+01	0.177713	0.409200
Vib (V=0)	7	0.148037D+01	0.170372	0.392295
Vib (V=0)	8	0.140129D+01	0.146530	0.337397
Vib (V=0)	9	0.137204D+01	0.137368	0.316302
Vib (V=0)	10	0.131030D+01	0.117371	0.270257
Vib (V=0)	11	0.122516D+01	0.088193	0.203071
Vib (V=0)	12	0.121412D+01	0.084262	0.194020
Vib (V=0)	13	0.116750D+01	0.067256	0.154863
Vib (V=0)	14	0.115949D+01	0.064267	0.147981
Vib (V=0)	15	0.113979D+01	0.056824	0.130842
Vib (V=0)	16	0.112753D+01	0.052127	0.120027
Vib (V=0)	17	0.112501D+01	0.051157	0.117793
Vib (V=0)	18	0.110791D+01	0.044506	0.102480
Vib (V=0)	19	0.110031D+01	0.041513	0.095588
Vib (V=0)	20	0.109889D+01	0.040956	0.094305
Vib (V=0)	21	0.109700D+01	0.040206	0.092578
Vib (V=0)	22	0.109272D+01	0.038510	0.088673
Vib (V=0)	23	0.108329D+01	0.034744	0.080000
Vib (V=0)	24	0.108273D+01	0.034519	0.079482
Vib (V=0)	25	0.105287D+01	0.022376	0.051524
Electronic		0.100000D+01	0.000000	0.000000
Translational		0.104570D+09	8.019406	18.465364

Supporting Information file

Rotational 0.288028D+07 6.459434 14.873398

title card
IR Spectrum

222 2 2 2 1 11 11 1
222 2 1 0 6 44 22 1 9 7 7 7 6 6555544444444 33 22222 1 1
776 1 4 6 0 54 21 1 7 7 5 0 7 2331099855310 65 97532 5 19 6
971 6 6 0 9 32 82 0 8 5 0 3 9 0321396352512 01 90936 3 23 2



***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000026742	-0.000040611	-0.000199520
2	6	0.000064859	0.000017183	0.000201419
3	6	0.000005187	0.000048474	0.000198639
4	6	-0.000028936	-0.000005904	-0.000184805
5	6	0.000041066	-0.000035119	-0.000201666
6	6	0.000000976	-0.000053270	0.000163739
7	6	-0.000017691	0.000026573	0.000189349
8	6	0.000014151	0.000044729	-0.000031424

```
     9        6        -0.000002066    0.000037143   -0.000162688
    10        6        -0.000075355   -0.000105387   -0.000118614
    11        6         0.000014127   -0.000038154    0.000013721
    12        6         0.000110762    0.000188922    0.000193861
    13        6        -0.000074882    0.000102586    0.000136524
    14        6         0.000105298   -0.000185016   -0.000193031
    15        6        -0.000070752   -0.000082656   -0.000131268
    16        6        -0.000060001    0.000080507    0.000125764
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000201666 RMS     0.000111412
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Leave Link  716 at Fri Aug 21 22:47:47 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.1
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Red2BG is reusing G-inverse.
 Internal  Forces:  Max     0.000108474 RMS     0.000041763
 Search for a local minimum.
 Step number   1 out of a maximum of    2
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Second derivative matrix not updated -- analytic derivatives used.
 ITU=  0
    Eigenvalues ---    0.00193   0.00207   0.00288   0.00298   0.00470
    Eigenvalues ---    0.00684   0.00989   0.01227   0.01569   0.01612
    Eigenvalues ---    0.02528   0.04620   0.05086   0.05343   0.06241
    Eigenvalues ---    0.06663   0.06989   0.07334   0.08641   0.08700
    Eigenvalues ---    0.09441   0.09790   0.09900   0.10735   0.11714
    Eigenvalues ---    0.15191   0.21168   0.26179   0.33581   0.40931
    Eigenvalues ---    0.44213   0.45351   0.48684   0.51551   0.53549
    Eigenvalues ---    0.55101   0.94020   0.94665   0.99374   1.01760
    Eigenvalues ---    1.03111   1.03334
 Angle between quadratic step and forces=  70.18 degrees.
 Linear search not attempted -- first point.
 Iteration  1 RMS(Cart)=  0.00133676 RMS(Int)=  0.00000737
 Iteration  2 RMS(Cart)=  0.00000391 RMS(Int)=  0.00000449
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000449
  ITry=  1 IFail=0 DXMaxC=  3.58D-03 DCOld=  1.00D+10 DXMaxT=  3.00D-01 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
    R1        2.30705   0.00001   0.00000   0.00004   0.00004   2.30709
    R2        2.54863   0.00005   0.00000   0.00000   0.00000   2.54863
    R3        2.54787   0.00006   0.00000   0.00008   0.00008   2.54795
    R4        2.30704   0.00001   0.00000   0.00006   0.00005   2.30709
    R5        2.30310   0.00002   0.00000   0.00006   0.00006   2.30316
    R6        2.54792   0.00005   0.00000   0.00003   0.00003   2.54795
```

R7	2.55055	0.00003	0.00000	0.00005	0.00005	2.55060
R8	2.30308	0.00002	0.00000	0.00008	0.00008	2.30316
R9	2.29580	0.00002	0.00000	0.00004	0.00004	2.29583
R10	2.55059	0.00002	0.00000	0.00001	0.00001	2.55060
R11	2.61573	0.00002	0.00000	0.00006	0.00006	2.61579
R12	2.29579	0.00002	0.00000	0.00004	0.00004	2.29583
R13	2.64580	-0.00007	0.00000	-0.00078	-0.00078	2.64502
R14	2.74039	0.00007	0.00000	0.00068	0.00068	2.74107
R15	2.61573	0.00002	0.00000	0.00006	0.00006	2.61579
R16	2.74040	0.00006	0.00000	0.00067	0.00067	2.74107
R17	2.73743	0.00009	0.00000	-0.00011	-0.00011	2.73732
A1	2.61227	0.00005	0.00000	0.00105	0.00104	2.61331
A2	2.64406	-0.00001	0.00000	-0.00095	-0.00096	2.64310
A3	2.61362	0.00003	0.00000	-0.00030	-0.00031	2.61331
A4	2.71592	-0.00001	0.00000	0.00055	0.00054	2.71646
A5	2.64284	0.00001	0.00000	0.00027	0.00026	2.64310
A6	2.78155	-0.00007	0.00000	-0.00158	-0.00158	2.77997
A7	2.71687	-0.00002	0.00000	-0.00040	-0.00041	2.71646
A8	2.78088	-0.00006	0.00000	-0.00090	-0.00091	2.77997
A9	2.83141	-0.00004	0.00000	-0.00060	-0.00060	2.83080
A10	2.30583	0.00008	0.00000	0.00117	0.00117	2.30700
A11	2.51966	-0.00011	0.00000	-0.00118	-0.00118	2.51848
A12	1.45711	0.00002	0.00000	0.00003	0.00003	1.45714
A13	2.83109	-0.00004	0.00000	-0.00029	-0.00030	2.83080
A14	2.30597	0.00008	0.00000	0.00103	0.00103	2.30700
A15	1.45705	0.00002	0.00000	0.00009	0.00009	1.45714
A16	2.51958	-0.00010	0.00000	-0.00110	-0.00110	2.51848
A17	1.42774	-0.00003	0.00000	-0.00012	-0.00012	1.42762
A18	1.42779	-0.00002	0.00000	-0.00017	-0.00017	1.42762
A19	2.87961	0.00000	0.00000	0.00063	0.00063	2.88024
A20	2.87999	-0.00000	0.00000	0.00026	0.00025	2.88024
A21	3.14134	0.00005	0.00000	0.00081	0.00081	3.14216
A22	3.14152	0.00004	0.00000	0.00064	0.00064	3.14216
D1	0.08402	0.00004	0.00000	0.01461	0.01460	0.09862
D2	-0.07724	-0.00002	0.00000	-0.01438	-0.01438	-0.09162
D3	-0.08021	-0.00003	0.00000	-0.01433	-0.01433	-0.09454
D4	0.08406	0.00004	0.00000	0.01456	0.01456	0.09862
D5	0.11480	0.00002	0.00000	0.01372	0.01372	0.12851
D6	-0.08003	-0.00003	0.00000	-0.01450	-0.01451	-0.09453
D7	0.09506	-0.00003	0.00000	-0.00902	-0.00902	0.08604
D8	0.11458	0.00002	0.00000	0.01393	0.01393	0.12851
D9	0.09592	-0.00003	0.00000	-0.00987	-0.00987	0.08605
D10	-0.64137	0.00002	0.00000	0.00529	0.00529	-0.63608
D11	2.55190	0.00000	0.00000	0.00424	0.00424	2.55614
D12	0.75102	-0.00000	0.00000	-0.00094	-0.00094	0.75008
D13	-2.42069	0.00001	0.00000	-0.00055	-0.00055	-2.42124
D14	-2.42086	0.00001	0.00000	-0.00038	-0.00038	-2.42124
D15	0.69061	0.00002	0.00000	0.00001	0.00001	0.69063

```
  D16        2.40836   0.00001   0.00000   0.00055   0.00055   2.40891
  D17       -0.69466  -0.00001   0.00000  -0.00027  -0.00027  -0.69493
  D18       -0.64269   0.00003   0.00000   0.00660   0.00660  -0.63609
  D19        2.55027   0.00000   0.00000   0.00586   0.00586   2.55613
  D20       -0.69465  -0.00002   0.00000  -0.00028  -0.00028  -0.69493
  D21        2.40860   0.00000   0.00000   0.00031   0.00031   2.40891
  D22        0.66921  -0.00002   0.00000  -0.00014  -0.00014   0.66907
       Item               Value     Threshold  Converged?
Maximum Force            0.000108     0.000450     YES
RMS     Force            0.000042     0.000300     YES
Maximum Displacement     0.003576     0.001800     NO
RMS     Displacement     0.001337     0.001200     NO
Predicted change in Energy=-2.312353D-06
                         ---------------------------
                         ! Non-Optimized Parameters !
                         ! (Angstroms and Degrees)  !
--------------------------                         --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.2209         -DE/DX =    0.0                 !
! R2    R(1,3)                  1.3487         -DE/DX =    0.0001              !
! R3    R(2,4)                  1.3483         -DE/DX =    0.0001              !
! R4    R(3,5)                  1.2209         -DE/DX =    0.0                 !
! R5    R(4,6)                  1.2188         -DE/DX =    0.0                 !
! R6    R(5,7)                  1.3483         -DE/DX =    0.0001              !
! R7    R(6,8)                  1.3497         -DE/DX =    0.0                 !
! R8    R(7,9)                  1.2188         -DE/DX =    0.0                 !
! R9    R(8,10)                 1.2149         -DE/DX =    0.0                 !
! R10   R(9,11)                 1.3497         -DE/DX =    0.0                 !
! R11   R(10,12)                1.3842         -DE/DX =    0.0                 !
! R12   R(11,13)                1.2149         -DE/DX =    0.0                 !
! R13   R(12,14)                1.3997         -DE/DX =   -0.0001              !
! R14   R(12,15)                1.4505         -DE/DX =    0.0001              !
! R15   R(13,14)                1.3842         -DE/DX =    0.0                 !
! R16   R(14,16)                1.4505         -DE/DX =    0.0001              !
! R17   R(15,16)                1.4485         -DE/DX =    0.0001              !
! A1    A(2,1,3)              149.7316         -DE/DX =    0.0001              !
! A2    A(1,2,4)              151.4383         -DE/DX =    0.0                 !
! A3    A(1,3,5)              149.7316         -DE/DX =    0.0                 !
! A4    A(2,4,6)              155.6416         -DE/DX =    0.0                 !
! A5    A(3,5,7)              151.4384         -DE/DX =    0.0                 !
! A6    A(4,6,8)              159.2805         -DE/DX =   -0.0001              !
! A7    A(5,7,9)              155.6417         -DE/DX =    0.0                 !
! A8    A(7,9,11)             159.2805         -DE/DX =   -0.0001              !
! A9    A(8,10,12)            162.1931         -DE/DX =    0.0                 !
! A10   A(10,12,14)           132.1816         -DE/DX =    0.0001              !
! A11   A(10,12,15)           144.2984         -DE/DX =   -0.0001              !
! A12   A(14,12,15)            83.4881         -DE/DX =    0.0                 !
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Supporting Information file

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 ! A13   A(11,13,14)          162.1928        -DE/DX =    0.0              !
 ! A14   A(12,14,13)          132.1816        -DE/DX =    0.0001           !
 ! A15   A(12,14,16)          83.4881         -DE/DX =    0.0              !
 ! A16   A(13,14,16)          144.2984        -DE/DX =   -0.0001           !
 ! A17   A(12,15,16)          81.7965         -DE/DX =    0.0              !
 ! A18   A(14,16,15)          81.7965         -DE/DX =    0.0              !
 ! A19   L(6,8,10,7,-1)       165.0255        -DE/DX =    0.0              !
 ! A20   L(9,11,13,4,-1)      165.0256        -DE/DX =    0.0              !
 ! A21   L(6,8,10,7,-2)       180.0323        -DE/DX =    0.0001           !
 ! A22   L(9,11,13,4,-2)      180.0323        -DE/DX =    0.0              !
 ! D1    D(3,1,2,4)           5.6505          -DE/DX =    0.0              !
 ! D2    D(2,1,3,5)           -5.2492         -DE/DX =    0.0              !
 ! D3    D(1,2,4,6)           -5.4165         -DE/DX =    0.0              !
 ! D4    D(1,3,5,7)           5.6503          -DE/DX =    0.0              !
 ! D5    D(2,4,6,8)           7.3633          -DE/DX =    0.0              !
 ! D6    D(3,5,7,9)           -5.4163         -DE/DX =    0.0              !
 ! D7    D(4,6,10,12)         4.9298          -DE/DX =    0.0              !
 ! D8    D(5,7,9,11)          7.3631          -DE/DX =    0.0              !
 ! D9    D(7,9,13,14)         4.9302          -DE/DX =    0.0              !
 ! D10   D(8,10,12,14)        -36.4448        -DE/DX =    0.0              !
 ! D11   D(8,10,12,15)        146.4559        -DE/DX =    0.0              !
 ! D12   D(10,12,14,13)       42.9765         -DE/DX =    0.0              !
 ! D13   D(10,12,14,16)       -138.7266       -DE/DX =    0.0              !
 ! D14   D(15,12,14,13)       -138.7267       -DE/DX =    0.0              !
 ! D15   D(15,12,14,16)       39.5701         -DE/DX =    0.0              !
 ! D16   D(10,12,15,16)       138.0205        -DE/DX =    0.0              !
 ! D17   D(14,12,15,16)       -39.8165        -DE/DX =    0.0              !
 ! D18   D(11,13,14,12)       -36.4454        -DE/DX =    0.0              !
 ! D19   D(11,13,14,16)       146.4552        -DE/DX =    0.0              !
 ! D20   D(12,14,16,15)       -39.8165        -DE/DX =    0.0              !
 ! D21   D(13,14,16,15)       138.0205        -DE/DX =    0.0              !
 ! D22   D(12,15,16,14)       38.3348         -DE/DX =    0.0              !
 ---------------------------------------------------------------------------
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

  Leave Link  103 at Fri Aug 21 22:47:47 2026, MaxMem=    805306368 cpu:                0.1 elap:
 0.0
 (Enter /home/user/gauss16/g16/l9999.exe)

 ----------------------------------------------------------------------

 Electric dipole moment (input orientation):
 (Debye = 10**-18 statcoulomb cm , SI units = C m)
                 (au)           (Debye)        (10**-30 SI)
   Tot       0.151649D+01      0.385453D+01      0.128573D+02
   x         0.151649D+01      0.385453D+01      0.128573D+02
   y        -0.891933D-03     -0.226707D-02     -0.756213D-02
   z        -0.120768D-03     -0.306961D-03     -0.102391D-02
```

Supporting Information file

Dipole polarizability, Alpha (input orientation).
(esu units = cm**3 , SI units = C**2 m**2 J**-1)
Alpha(0;0):

	(au)	(10**-24 esu)	(10**-40 SI)
iso	0.217594D+03	0.322441D+02	0.358764D+02
aniso	0.234060D+03	0.346841D+02	0.385913D+02
xx	0.354639D+03	0.525520D+02	0.584720D+02
yx	0.479937D-01	0.711194D-02	0.791310D-02
yy	0.213593D+03	0.316512D+02	0.352167D+02
zx	0.312236D-04	0.462686D-05	0.514807D-05
zy	0.349858D+01	0.518437D+00	0.576839D+00
zz	0.845492D+02	0.125289D+02	0.139403D+02

Dipole orientation:

6	-0.02343150	-1.26817043	6.84691624
6	-0.10358678	-3.25979494	5.68524330
6	0.02190278	1.28005365	6.84383621
6	-0.10870319	-4.58326100	3.50807837
6	0.10245058	3.27042323	5.68006817
6	-0.12342659	-4.86021446	1.22174192
6	0.10816503	4.58893825	3.49984129
6	-0.04401045	-4.26023164	-1.25596022
6	0.12340312	4.86283290	1.21316017
6	0.03974177	-3.16098960	-3.26974532
6	0.04449213	4.25784831	-1.26338215
6	0.31454788	-1.28962190	-5.07653704
6	-0.03842917	3.15529643	-3.27539029
6	-0.31340481	1.28058279	-5.07868946
6	1.13558051	-0.77115269	-7.63911986
6	-1.13529320	0.75745923	-7.64006323

Electric dipole moment (dipole orientation):
(Debye = 10**-18 statcoulomb cm , SI units = C m)

	(au)	(Debye)	(10**-30 SI)
Tot	0.151649D+01	0.385453D+01	0.128573D+02
x	0.000000D+00	0.000000D+00	0.000000D+00
y	0.000000D+00	0.000000D+00	0.000000D+00
z	0.151649D+01	0.385453D+01	0.128573D+02

Dipole polarizability, Alpha (dipole orientation).
(esu units = cm**3 , SI units = C**2 m**2 J**-1)
Alpha(0;0):

	(au)	(10**-24 esu)	(10**-40 SI)
iso	0.217594D+03	0.322441D+02	0.358764D+02
aniso	0.234060D+03	0.346841D+02	0.385913D+02

xx	0.845451D+02	0.125283D+02	0.139396D+02
yx	-0.342269D+01	-0.507191D+00	-0.564326D+00
yy	0.213597D+03	0.316519D+02	0.352174D+02
zx	-0.194056D-01	-0.287561D-02	-0.319955D-02
zy	0.130684D+00	0.193653D-01	0.215468D-01
zz	0.354639D+03	0.525520D+02	0.584720D+02

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Supporting Information file

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339,0.01150982,0.15564203,0.00270904,0.00374048,-0.00076836,-0.0042323
7,-0.00206523,0.00053020,-0.00069669,-0.00466134,0.00112399,0.00561382
,0.00060644,0.00000931,-0.00224887,0.00449262,-0.00129336,-0.00687705,
0.00155399,-0.00091551,0.00453614,-0.00334087,0.00169471,0.01003863,-0
.00684800,-0.00122113,-0.00674889,0.00068157,-0.00274063,-0.02235669,0
.01403315,0.00616757,0.00840918,0.00199789,0.00137761,-0.18948495,0.06
672953,-0.06668775,-0.00780525,-0.00740296,0.01625618,-0.00716340,-0.0
4512337,-0.06300634,0.24398238,-0.00039565,-0.00652842,0.00079839,0.00
428301,0.00598751,-0.00088391,-0.00244071,0.00547533,-0.00053209,-0.00
787156,-0.00413677,0.00111198,0.00455752,-0.00338539,0.00029077,0.0113
0141,-0.00035712,-0.00139801,-0.00546070,0.00145184,-0.00008281,-0.014
27462,0.00509679,0.00070625,0.00548190,0.00058376,0.00005445,0.0382196
6,-0.01447993,0.01062938,-0.00517253,-0.00184777,-0.00002743,-0.003118
61,-0.05737341,0.00529490,0.00512595,0.00131638,-0.00272449,-0.0685189
6,0.01676168,-0.01628805,0.00695662,0.11456242,-0.00076314,-0.00616845
,0.00034356,0.00418243,0.00518113,-0.00042179,-0.00209390,0.00568927,-
0.00015033,-0.00677333,-0.00323675,0.00046530,0.00462424,-0.00398389,0
.00005252,0.00882126,-0.00010589,-0.00067892,-0.00638475,0.00205743,0.
00032632,-0.01091685,0.00276945,0.00075042,0.00720326,0.00081183,-0.00
144906,0.01387339,-0.00728406,0.00588899,-0.00843151,-0.00312988,0.000
52569,-0.11140302,0.00780324,-0.08143414,0.01632961,0.00215774,0.01209
393,-0.06872541,-0.00564536,0.00911126,0.13498292,0.07320590,0.2226058
2,-0.00069606,0.00466432,-0.00112452,-0.00225040,-0.00449624,0.0012939
7,0.00271306,-0.00374537,0.00076915,0.00453635,0.00334157,-0.00169464,
-0.00423755,0.00206823,-0.00052951,-0.00674987,-0.00068387,0.00274115,
0.00562175,-0.00060484,-0.00001046,0.00840533,-0.00199158,-0.00137762,
-0.00688276,-0.00155889,0.00091490,-0.00780995,0.00739293,-0.01625000,
0.01003823,0.00685448,0.00122076,-0.00718171,0.04512590,0.06303386,-0.
02234036,-0.01404098,-0.00615351,-0.18933345,-0.06682239,0.06671041,-0
.02767504,0.03132727,0.02547480,0.24384242,0.00243527,0.00547636,-0.00
053223,-0.00455431,-0.00338783,0.00029207,0.00039998,-0.00653113,0.000
79835,0.00545643,0.00145648,-0.00008467,-0.00428900,0.00598677,-0.0008
8340,-0.00548035,0.00057934,0.00005619,0.00788099,-0.00413572,0.001111
43,0.00517464,-0.00184326,-0.00002898,-0.01130897,-0.00036387,-0.00139
725,-0.00512983,0.00131872,-0.00273099,0.01428203,0.00511158,0.0007072
9,0.06849882,0.01682881,-0.01628815,-0.03822544,-0.01451101,0.01063738
,0.00304077,-0.05742544,0.00534297,-0.03135051,-0.06312689,-0.07012171
,-0.00683053,0.11456708,0.00208831,0.00568287,-0.00014942,-0.00461670,
-0.00398073,0.00005192,0.00076429,-0.00616371,0.00034300,0.00637382,0.
00205847,0.00032692,-0.00418075,0.00517499,-0.00042168,-0.00719386,0.0
0080667,-0.00145157,0.00677140,-0.00323264,0.00046575,0.00842959,-0.00
312159,0.00052638,-0.00881613,-0.00010999,-0.00067927,-0.01632402,0.00
214481,0.01211313,0.01091044,0.00277310,0.00074993,0.06872972,-0.00562
867,0.00903876,-0.01385832,-0.00728614,0.00589667,0.11145038,0.0079161

Supporting Information file

0,-0.08151932,-0.02550941,-0.07015524,-0.16802957,-0.13501874,0.073121
71,0.22273839\\0.00002674,0.00004061,0.00019952,-0.00006486,-0.0000171
8,-0.00020142,-0.00000519,-0.00004847,-0.00019864,0.00002894,0.0000059
0,0.00018481,-0.00004107,0.00003512,0.00020167,-0.00000098,0.00005327,
-0.00016374,0.00001769,-0.00002657,-0.00018935,-0.00001415,-0.00004473
,0.00003142,0.00000207,-0.00003714,0.00016269,0.00007536,0.00010539,0.
00011861,-0.00001413,0.00003815,-0.00001372,-0.00011076,-0.00018892,-0
.00019386,0.00007488,-0.00010259,-0.00013652,-0.00010530,0.00018502,0.
00019303,0.00007075,0.00008266,0.00013127,0.00006000,-0.00008051,-0.00
012576\\\@
The archive entry for this job was punched.

Statistics are no substitute for judgment.
-- Henry Clay
Job cpu time: 0 days 12 hours 16 minutes 17.2 seconds.
Elapsed time: 0 days 2 hours 2 minutes 43.8 seconds.
File lengths (MBytes): RWF= 340 Int= 0 D2E= 0 Chk= 21 Scr= 1
Normal termination of Gaussian 16 at Fri Aug 21 22:47:47 2026.

Supporting Information file

S2.3 CDCA - $(NH_3)_2$

```
 Entering Gaussian System, Link 0=g16
 Input=cdca-n2-b-4h2.gjf
 Output=cdca-n2-b-4h2.log
 Initial command:
                /home/user/gauss16/g16/l1.exe                "/home/user/paper/rahul/grun/Gau-135690.inp"
-scrdir="/home/user/paper/rahul/grun/"
 Entering Link 1 = /home/user/gauss16/g16/l1.exe PID=    135692.

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 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
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Gaussian 16, Revision C.01,
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M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone,
G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich,
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G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda,
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J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas,
J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

****
Gaussian 16: ES64L-G16RevC.01 3-Jul-2019
25-Sep-2026
****
%chk=cdca-n2-b-4h2.chk
%nprocshared=6
Will use up to 6 processors via shared memory.
%mem=6GB

#p opt freq wb97xd def2tzvp

1/18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=44,7=101,11=2,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;

7//1,2,3,16;
1/18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=44,7=101,11=2,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
Leave Link 1 at Fri Sep 25 17:39:46 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l101.exe)
---
title card

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	4.41321	0.67387	-0.00063
C	3.74239	1.69532	-0.00207
C	4.41329	-0.67389	0.00083
C	2.53503	2.2916	-0.00304
C	3.74235	-1.69526	0.00218
C	1.31688	2.34061	-0.00326
C	2.53504	-2.29164	0.00302
C	0.01565	1.98966	-0.00248
C	1.31688	-2.3406	0.0031
C	-1.0687	1.44414	-0.00125
C	0.01565	-1.98969	0.00222
C	-2.24548	0.69117	-0.00033
C	-1.0687	-1.44415	0.00113
C	-2.24549	-0.69119	0.0003
C	-3.48786	1.40415	0.00013
C	-3.48786	-1.40417	-0.0001
N	-4.47522	1.98955	0.01085
N	-4.47531	-1.98949	-0.01063
H	-4.43761	2.71912	-0.67202
H	-5.23158	1.37138	-0.20312
H	-4.43723	-2.71973	0.67149
H	-5.23145	-1.37146	0.20453
H	-4.6166	2.38812	0.91702
H	-3.9452	0.62566	-0.57407
H	-3.94613	-0.62385	0.57085
H	-4.61744	-2.38715	-0.91708

Supporting Information file

```
 ITRead=  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 ITRead=  0  0  0  0  0  0
 MicOpt= -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 MicOpt= -1 -1 -1 -1 -1 -1
 NAtoms=     26 NQM=       26 NQMF=       0 NMMI=      0 NMMIF=      0
              NMic=       0 NMicF=      0.
                  Isotopes and Nuclear Properties:
 (Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic moments (NMagM)
  in nuclear magnetons)

  Atom        1         2         3         4         5         6         7         8         9        10
 IAtWgt=        12        12        12        12        12        12        12        12        12        12
  AtmWgt=    12.0000000  12.0000000  12.0000000  12.0000000  12.0000000  12.0000000
12.0000000  12.0000000  12.0000000  12.0000000
 NucSpn=         0         0         0         0         0         0         0         0         0         0
 AtZEff=  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -
0.0000000  -0.0000000  -0.0000000
 NQMom=    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
0.0000000   0.0000000   0.0000000
 NMagM=    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
0.0000000   0.0000000   0.0000000
 AtZNuc=   6.0000000   6.0000000   6.0000000   6.0000000   6.0000000   6.0000000   6.0000000
6.0000000   6.0000000   6.0000000

  Atom       11        12        13        14        15        16        17        18        19        20
 IAtWgt=        12        12        12        12        12        12        14        14         1         1
  AtmWgt=    12.0000000  12.0000000  12.0000000  12.0000000  12.0000000  12.0000000
14.0030740  14.0030740   1.0078250   1.0078250
 NucSpn=         0         0         0         0         0         0         2         2         1         1
 AtZEff=  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -
0.0000000  -0.0000000  -0.0000000
 NQMom=    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   2.0440000
2.0440000   0.0000000   0.0000000
 NMagM=    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.4037610
0.4037610   2.7928460   2.7928460
 AtZNuc=   6.0000000   6.0000000   6.0000000   6.0000000   6.0000000   6.0000000   7.0000000
7.0000000   1.0000000   1.0000000

  Atom       21        22        23        24        25        26
 IAtWgt=         1         1         1         1         1         1
 AtmWgt=   1.0078250   1.0078250   1.0078250   1.0078250   1.0078250   1.0078250
 NucSpn=         1         1         1         1         1         1
 AtZEff=  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000  -0.0000000
 NQMom=    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
 NMagM=    2.7928460   2.7928460   2.7928460   2.7928460   2.7928460   2.7928460
 AtZNuc=   1.0000000   1.0000000   1.0000000   1.0000000   1.0000000   1.0000000
 Leave Link  101 at Fri Sep 25 17:39:46 2026, MaxMem=    805306368 cpu:                2.1 elap:
0.4
```

Supporting Information file

(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

```
                     --------------------------
                     !    Initial Parameters    !
                     ! (Angstroms and Degrees)  !
--------------------------                     --------------------------
! Name  Definition              Value          Derivative Info.            !
-------------------------------------------------------------------------------
! R1    R(1,2)                  1.222          estimate D2E/DX2            !
! R2    R(1,3)                  1.3478         estimate D2E/DX2            !
! R3    R(2,4)                  1.3466         estimate D2E/DX2            !
! R4    R(3,5)                  1.222          estimate D2E/DX2            !
! R5    R(4,6)                  1.2191         estimate D2E/DX2            !
! R6    R(5,7)                  1.3466         estimate D2E/DX2            !
! R7    R(6,8)                  1.3477         estimate D2E/DX2            !
! R8    R(7,9)                  1.2191         estimate D2E/DX2            !
! R9    R(8,10)                 1.2138         estimate D2E/DX2            !
! R10   R(9,11)                 1.3477         estimate D2E/DX2            !
! R11   R(10,12)                1.3971         estimate D2E/DX2            !
! R12   R(11,13)                1.2138         estimate D2E/DX2            !
! R13   R(12,14)                1.3824         estimate D2E/DX2            !
! R14   R(12,15)                1.4324         estimate D2E/DX2            !
! R15   R(13,14)                1.3971         estimate D2E/DX2            !
! R16   R(14,16)                1.4324         estimate D2E/DX2            !
! R17   R(15,17)                1.1479         estimate D2E/DX2            !
! R18   R(15,24)                1.07           estimate D2E/DX2            !
! R19   R(16,18)                1.1479         estimate D2E/DX2            !
! R20   R(16,25)                1.07           estimate D2E/DX2            !
! R21   R(17,19)                1.0            estimate D2E/DX2            !
! R22   R(17,20)                1.0            estimate D2E/DX2            !
! R23   R(17,23)                1.0            estimate D2E/DX2            !
! R24   R(18,21)                1.0            estimate D2E/DX2            !
! R25   R(18,22)                1.0            estimate D2E/DX2            !
! R26   R(18,26)                1.0            estimate D2E/DX2            !
! A1    A(2,1,3)                146.7089       estimate D2E/DX2            !
! A2    A(1,2,4)                149.578        estimate D2E/DX2            !
! A3    A(1,3,5)                146.6958       estimate D2E/DX2            !
! A4    A(2,4,6)                156.0201       estimate D2E/DX2            !
! A5    A(3,5,7)                149.5893       estimate D2E/DX2            !
! A6    A(4,6,8)                162.6021       estimate D2E/DX2            !
! A7    A(5,7,9)                156.013        estimate D2E/DX2            !
! A8    A(7,9,11)               162.6064       estimate D2E/DX2            !
! A9    A(10,12,14)             122.6139       estimate D2E/DX2            !
! A10   A(10,12,15)             117.5353       estimate D2E/DX2            !
! A11   A(14,12,15)             119.8508       estimate D2E/DX2            !
```

```
! A12   A(12,14,13)          122.613        estimate D2E/DX2             !
! A13   A(12,14,16)          119.8511        estimate D2E/DX2             !
! A14   A(13,14,16)          117.5359        estimate D2E/DX2             !
! A15   A(12,15,24)           90.4814       estimate D2E/DX2             !
! A16   A(17,15,24)           90.4814       estimate D2E/DX2             !
! A17   A(14,16,25)           90.477        estimate D2E/DX2             !
! A18   A(18,16,25)           90.477        estimate D2E/DX2             !
! A19   A(15,17,19)          109.4712        estimate D2E/DX2             !
! A20   A(15,17,20)          109.4712        estimate D2E/DX2             !
! A21   A(15,17,23)          109.4712        estimate D2E/DX2             !
! A22   A(19,17,20)          109.4712        estimate D2E/DX2             !
! A23   A(19,17,23)          109.4712        estimate D2E/DX2             !
! A24   A(20,17,23)          109.4712        estimate D2E/DX2             !
! A25   A(16,18,21)          109.4712        estimate D2E/DX2             !
! A26   A(16,18,22)          109.4712        estimate D2E/DX2             !
! A27   A(16,18,26)          109.4712        estimate D2E/DX2             !
! A28   A(21,18,22)          109.4712        estimate D2E/DX2             !
! A29   A(21,18,26)          109.4712        estimate D2E/DX2             !
! A30   A(22,18,26)          109.4712        estimate D2E/DX2             !
! A31   L(6,8,10,7,-1)       168.3878        estimate D2E/DX2             !
! A32   L(8,10,12,7,-1)       174.0924        estimate D2E/DX2             !
! A33   L(9,11,13,4,-1)       168.3855        estimate D2E/DX2             !
! A34   L(11,13,14,4,-1)      174.0936        estimate D2E/DX2             !
! A35   L(12,15,17,24,-1)     180.9627        estimate D2E/DX2             !
! A36   L(14,16,18,25,-1)     180.954         estimate D2E/DX2             !
! A37   L(6,8,10,7,-2)        179.99         estimate D2E/DX2             !
! A38   L(8,10,12,7,-2)       180.0275        estimate D2E/DX2             !
! A39   L(9,11,13,4,-2)       180.0          estimate D2E/DX2             !
! A40   L(11,13,14,4,-2)      180.0244        estimate D2E/DX2             !
! A41   L(12,15,17,24,-2)     180.0          estimate D2E/DX2             !
! A42   L(14,16,18,25,-2)     180.0          estimate D2E/DX2             !
! D1    D(3,1,2,4)            0.0233        estimate D2E/DX2             !
! D2    D(2,1,3,5)           -0.0483        estimate D2E/DX2             !
! D3    D(1,2,4,6)            0.0029        estimate D2E/DX2             !
! D4    D(1,3,5,7)            0.0196        estimate D2E/DX2             !
! D5    D(2,4,6,8)            0.0681        estimate D2E/DX2             !
! D6    D(3,5,7,9)            0.0076        estimate D2E/DX2             !
! D7    D(4,6,12,14)          -0.0972        estimate D2E/DX2             !
! D8    D(4,6,12,15)         179.9012        estimate D2E/DX2             !
! D9    D(5,7,9,11)           0.0571        estimate D2E/DX2             !
! D10   D(7,9,14,12)          -0.0773        estimate D2E/DX2             !
! D11   D(7,9,14,16)         179.9214        estimate D2E/DX2             !
! D12   D(10,12,14,13)         0.051         estimate D2E/DX2             !
! D13   D(10,12,14,16)      -179.9384        estimate D2E/DX2             !
! D14   D(15,12,14,13)      -179.9403        estimate D2E/DX2             !
! D15   D(15,12,14,16)         0.0703        estimate D2E/DX2             !
! D16   D(10,12,15,24)       147.5112        estimate D2E/DX2             !
! D17   D(14,12,15,24)       -32.497         estimate D2E/DX2             !
```

Supporting Information file

```
 ! D18   D(12,14,16,25)       -32.2902         estimate D2E/DX2              !
 ! D19   D(13,14,16,25)       147.7199         estimate D2E/DX2              !
 ! D20   D(24,15,17,19)      -100.86           estimate D2E/DX2              !
 ! D21   D(24,15,17,20)        19.14           estimate D2E/DX2              !
 ! D22   D(24,15,17,23)       139.14           estimate D2E/DX2              !
 ! D23   D(25,16,18,21)      -101.1367         estimate D2E/DX2              !
 ! D24   D(25,16,18,22)        18.8633         estimate D2E/DX2              !
 ! D25   D(25,16,18,26)       138.8633         estimate D2E/DX2              !
 ---------------------------------------------------------------------------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06 EigMax=2.50D+02 EigMin=1.00D-
04
 Number of steps in this run=    103 maximum allowed number of steps=    156.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link  103 at Fri Sep 25 17:39:46 2026, MaxMem=    805306368 cpu:                  0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l202.exe)
                      Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        4.413214    0.673868   -0.000632
      2          6           0        3.742394    1.695315   -0.002073
      3          6           0        4.413289   -0.673893    0.000834
      4          6           0        2.535032    2.291604   -0.003038
      5          6           0        3.742349   -1.695263    0.002181
      6          6           0        1.316878    2.340613   -0.003262
      7          6           0        2.535039   -2.291645    0.003021
      8          6           0        0.015653    1.989663   -0.002475
      9          6           0        1.316881   -2.340598    0.003098
     10          6           0       -1.068704    1.444144   -0.001249
     11          6           0        0.015649   -1.989687    0.002217
     12          6           0       -2.245485    0.691165   -0.000333
     13          6           0       -1.068702   -1.444154    0.001128
     14          6           0       -2.245489   -0.691186    0.000303
     15          6           0       -3.487860    1.404150    0.000128
     16          6           0       -3.487857   -1.404165   -0.000104
     17          7           0       -4.475218    1.989548    0.010848
     18          7           0       -4.475308   -1.989487   -0.010629
     19          1           0       -4.437609    2.719118   -0.672024
     20          1           0       -5.231583    1.371380   -0.203116
     21          1           0       -4.437229   -2.719731    0.671495
     22          1           0       -5.231451   -1.371464    0.204534
     23          1           0       -4.616603    2.388118    0.917022
     24          1           0       -3.945202    0.625665   -0.574067
     25          1           0       -3.946130   -0.623845    0.570849
     26          1           0       -4.617436   -2.387153   -0.917084
```

Supporting Information file

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.222029	0.000000			
3	C	1.347762	2.462368	0.000000		
4	C	2.478839	1.346583	3.510276	0.000000	
5	C	2.462285	3.390581	1.222031	4.165663	0.000000
6	C	3.516439	2.509888	4.321461	1.219139	4.708634
7	C	3.510245	4.165763	2.478901	4.583253	1.346577
8	C	4.590192	3.738347	5.141376	2.537408	5.240893
9	C	4.321377	4.708687	3.516483	4.789700	2.509851
10	C	5.535770	4.817650	5.876932	3.702041	5.744747
11	C	5.141314	5.240981	4.590267	4.967572	3.738312
12	C	6.658721	6.071492	6.797254	5.041305	6.445867
13	C	5.876855	5.744817	5.535840	5.190646	4.817600
14	C	6.797183	6.445939	6.658800	5.634752	6.071440
15	C	7.934752	7.236115	8.169848	6.087924	7.866530
16	C	8.169770	7.866595	7.934822	7.066393	7.236064
17	N	8.985286	8.222888	9.278986	7.016768	9.005904
18	N	9.278975	9.006024	8.985437	8.214175	8.222932
19	H	9.108835	8.271000	9.502823	7.017694	9.319497
20	H	9.672105	8.982071	9.861454	7.823500	9.485668
21	H	9.502558	9.319472	9.108617	8.612833	8.270611
22	H	9.861290	9.485659	9.672079	8.589495	8.981920
23	H	9.236793	8.437864	9.578845	7.211221	9.347889
24	H	8.378202	7.782702	8.478427	6.715270	8.050913
25	H	8.478755	8.051096	8.378980	7.129842	7.783574
26	H	9.579268	9.348291	9.237523	8.595583	8.438588

		6	7	8	9	10
6	C	0.000000				
7	C	4.789757	0.000000			
8	C	1.347721	4.967588	0.000000		
9	C	4.681215	1.219141	4.521547	0.000000	
10	C	2.548463	5.190674	1.213846	4.473847	0.000000
11	C	4.521584	2.537421	3.979353	1.347718	3.600976
12	C	3.925700	5.634765	2.607460	4.677825	1.397065
13	C	4.473865	3.702053	3.600963	2.548455	2.888299
14	C	4.677850	5.041322	3.507096	3.925691	2.438126
15	C	4.895149	7.066415	3.552103	6.091690	2.419487
16	C	6.091703	6.087931	4.877772	4.895143	3.737000
17	N	5.802743	8.214157	4.490891	7.231780	3.449920
18	N	7.231821	7.016869	6.000203	5.802837	4.836823
19	H	5.805568	8.612853	4.562010	7.692247	3.664016
20	H	6.622816	8.589566	5.287344	7.530184	4.168405
21	H	7.692342	7.017310	6.516194	5.805194	5.397907
22	H	7.530160	7.823408	6.234752	6.622722	5.029758
23	H	6.004613	8.595439	4.739414	7.642137	3.784429

24	H	5.563843	7.130024	4.227952	6.068060	3.045040
25	H	6.067690	6.716363	4.780675	5.564968	3.589353
26	H	7.642181	7.212046	6.438831	6.005416	5.301989

		11	12	13	14	15
11	C	0.000000				
12	C	3.507093	0.000000			
13	C	1.213847	2.438116	0.000000		
14	C	2.607461	1.382351	1.397064	0.000000	
15	C	4.877777	1.432426	3.736999	2.435964	0.000000
16	C	3.552097	2.435959	2.419486	1.432417	2.808315
17	N	6.000189	2.580239	4.836813	3.486852	1.147903
18	N	4.490975	3.486848	3.449999	2.580271	3.534394
19	H	6.516053	3.060909	5.397731	4.109450	1.755833
20	H	6.234771	3.069298	5.029763	3.634874	1.755833
21	H	4.561690	4.109660	3.663804	3.060918	4.284674
22	H	5.287267	3.634887	4.168350	3.069277	3.284193
23	H	6.438929	3.056696	5.302148	3.993078	1.755833
24	H	4.781266	1.795132	3.590160	2.225538	1.070000
25	H	4.229014	2.224341	3.045830	1.795059	2.156038
26	H	4.740102	3.992822	3.784954	3.056802	4.060936

		16	17	18	19	20
16	C	0.000000				
17	N	3.534443	0.000000			
18	N	1.147943	3.979093	0.000000		
19	H	4.284269	1.000000	4.754979	0.000000	
20	H	3.284119	1.000000	3.450279	1.632993	0.000000
21	H	1.755866	4.755545	1.000000	5.602332	4.258302
22	H	1.755866	3.450479	1.000000	4.258098	2.772971
23	H	4.061601	1.000000	4.477045	1.632993	1.632993
24	H	2.158427	1.575824	2.727177	2.152813	1.532472
25	H	1.070000	2.724584	1.575793	3.600234	2.496464
26	H	1.755866	4.476248	1.000000	5.115310	3.874725

		21	22	23	24	25
21	H	0.000000				
22	H	1.632993	0.000000			
23	H	5.116892	3.875582	0.000000		
24	H	3.603497	2.499836	2.404240	0.000000	
25	H	2.155005	1.531395	3.105043	1.694729	0.000000
26	H	1.632993	1.632993	5.115385	3.105903	2.402884

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Supporting Information file

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.722219	-0.673888	-0.000403
2	6	0	4.051391	-1.695331	-0.000553
3	6	0	4.722305	0.673873	0.000224
4	6	0	2.844024	-2.291611	-0.000521
5	6	0	4.051373	1.695250	0.000458
6	6	0	1.625870	-2.340611	-0.000382
7	6	0	2.844068	2.291642	0.000536
8	6	0	0.324647	-1.989649	-0.000632
9	6	0	1.625910	2.340605	0.000527
10	6	0	-0.759705	-1.444120	-0.001019
11	6	0	0.324675	1.989703	0.000854
12	6	0	-1.936480	-0.691131	-0.000773
13	6	0	-0.759680	1.444178	0.001089
14	6	0	-1.936473	0.691219	0.000737
15	6	0	-3.178861	-1.404105	-0.002350
16	6	0	-3.178835	1.404207	0.002243
17	7	0	-4.166223	-1.989477	-0.013985
18	7	0	-4.166282	1.989519	0.013670
19	1	0	-4.128624	-2.720107	0.667753
20	1	0	-4.922584	-1.371636	0.200933
21	1	0	-4.128192	2.720822	-0.667319
22	1	0	-4.922428	1.371838	-0.202457
23	1	0	-4.307606	-2.386639	-0.920778
24	1	0	-3.636200	-0.626508	0.573050
25	1	0	-3.637111	0.624778	-0.569924
26	1	0	-4.308412	2.385779	0.920741

Rotational constants (GHZ): 0.7362472 0.2331782 0.1775084
Leave Link 202 at Fri Sep 25 17:39:47 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1016.0099611591 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0153383473 Hartrees.
Nuclear repulsion after empirical dispersion term = 1015.9946228118 Hartrees.
Leave Link 301 at Fri Sep 25 17:39:47 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 22986 LenP2D= 51608.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.77D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 682 682 682 682 682 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Fri Sep 25 17:39:48 2026, MaxMem= 805306368 cpu: 5.8 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 17:39:48 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.440936932903
JPrj=0 DoOrth=F DoCkMO=F.
Leave Link 401 at Fri Sep 25 17:39:55 2026, MaxMem= 805306368 cpu: 45.3 elap: 7.6
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:

Supporting Information file

```
Using DIIS extrapolation, IDIIS=  1040.
NGot=   805306368 LenX=   804326778 LenY=   803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on            energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for  20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle   1  Pass 0  IDiag  1:
FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
      NFxFlg=          0 DoJE=T BraDBF=F KetDBF=F FulRan=T
      wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=          0 NGrid=          0
      NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
Symmetry not used in FoFCou.
E= -722.520845790514
DIIS: error= 4.38D-02 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -722.520845790514     IErMin= 1 ErrMin= 4.38D-02
ErrMax= 4.38D-02  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D+00 BMatP= 1.65D+00
IDIUse=3 WtCom= 5.62D-01 WtEn= 4.38D-01
Coeff-Com:  0.100D+01
Coeff-En:   0.100D+01
Coeff:      0.100D+01
Gap=     0.256 Goal=   None    Shift=    0.000
GapD=    0.256 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.
Damping current iteration by 5.00D-01
RMSDP=7.18D-02 MaxDP=2.90D+00             OVMax= 3.11D-01

Cycle   2  Pass 0  IDiag  1:
RMSU=  3.39D-02    CP:  2.14D+00
E= -722.706948570220     Delta-E=       -0.186102779706 Rises=F Damp=T
DIIS: error= 2.15D-02 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -722.706948570220     IErMin= 2 ErrMin= 2.15D-02
ErrMax= 2.15D-02  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.63D-01 BMatP= 1.65D+00
IDIUse=3 WtCom= 7.85D-01 WtEn= 2.15D-01
Coeff-Com: -0.758D+00 0.176D+01
Coeff-En:   0.000D+00 0.100D+01
Coeff:     -0.595D+00 0.159D+01
Gap=     0.306 Goal=   None    Shift=    0.000
RMSDP=5.21D+02 MaxDP=1.77D+04 DE=-1.86D-01 OVMax= 9.92D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle   3  Pass 1  IDiag  1:
E= -722.834001470583     Delta-E=       -0.127052900363 Rises=F Damp=F
DIIS: error= 2.26D-02 at cycle   1 NSaved=   1.
```

NSaved= 1 IEnMin= 1 EnMin= -722.834001470583 IErMin= 1 ErrMin= 2.26D-02
ErrMax= 2.26D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-01 BMatP= 3.98D-01
IDIUse=3 WtCom= 7.74D-01 WtEn= 2.26D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.189 Goal= None Shift= 0.000
GapD= 0.189 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.
Damping current iteration by 5.00D-01
RMSDP=3.61D-02 MaxDP=1.52D+00 DE=-1.27D-01 OVMax= 1.28D-01

Cycle 4 Pass 1 IDiag 1:
RMSU= 4.45D-03 CP: 5.69D-01
E= -722.797417999892 Delta-E= 0.036583470692 Rises=F Damp=T
DIIS: error= 9.33D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -722.834001470583 IErMin= 2 ErrMin= 9.33D-03
ErrMax= 9.33D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.35D-02 BMatP= 3.98D-01
IDIUse=3 WtCom= 9.07D-01 WtEn= 9.33D-02
Coeff-Com: -0.696D+00 0.170D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.631D+00 0.163D+01
Gap= 0.176 Goal= None Shift= 0.000
GapD= 0.176 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=1.93D-02 MaxDP=8.06D-01 DE= 3.66D-02 OVMax= 7.24D-02

Cycle 5 Pass 1 IDiag 1:
RMSU= 1.59D-03 CP: 1.04D-01 1.78D+00
E= -722.888347027748 Delta-E= -0.090929027856 Rises=F Damp=F
DIIS: error= 4.31D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -722.888347027748 IErMin= 3 ErrMin= 4.31D-03
ErrMax= 4.31D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.10D-03 BMatP= 7.35D-02
IDIUse=3 WtCom= 9.57D-01 WtEn= 4.31D-02
Coeff-Com: -0.369D+00 0.836D+00 0.533D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.353D+00 0.800D+00 0.553D+00
Gap= 0.170 Goal= None Shift= 0.000
RMSDP=6.09D-04 MaxDP=3.63D-02 DE=-9.09D-02 OVMax= 2.60D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 5.41D-04 CP: 1.01D-01 1.83D+00 9.21D-01
E= -722.895210916300 Delta-E= -0.006863888553 Rises=F Damp=F
DIIS: error= 2.82D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -722.895210916300 IErMin= 4 ErrMin= 2.82D-03
ErrMax= 2.82D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-03 BMatP= 7.10D-03
IDIUse=3 WtCom= 9.72D-01 WtEn= 2.82D-02
Coeff-Com: -0.175D+00 0.374D+00 0.332D+00 0.469D+00
Coeff-En: 0.000D+00 0.000D+00 0.387D-01 0.961D+00
Coeff: -0.170D+00 0.363D+00 0.323D+00 0.483D+00

Gap= 0.171 Goal= None Shift= 0.000
RMSDP=1.82D-04 MaxDP=1.67D-02 DE=-6.86D-03 OVMax= 2.52D-02

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.17D-04 CP: 9.95D-02 1.81D+00 9.86D-01 9.88D-01
E= -722.896889001107 Delta-E= -0.001678084806 Rises=F Damp=F
DIIS: error= 8.59D-04 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -722.896889001107 IErMin= 5 ErrMin= 8.59D-04
ErrMax= 8.59D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-04 BMatP= 1.30D-03
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.59D-03
Coeff-Com: 0.165D-01-0.590D-01-0.711D-01 0.763D-01 0.104D+01
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.163D-01-0.585D-01-0.705D-01 0.756D-01 0.104D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=2.38D-04 MaxDP=1.70D-02 DE=-1.68D-03 OVMax= 2.16D-02

Cycle 8 Pass 1 IDiag 1:
RMSU= 7.27D-05 CP: 9.71D-02 1.79D+00 1.06D+00 1.21D+00 1.75D+00
E= -722.897382768354 Delta-E= -0.000493767247 Rises=F Damp=F
DIIS: error= 3.62D-04 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -722.897382768354 IErMin= 6 ErrMin= 3.62D-04
ErrMax= 3.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.99D-05 BMatP= 1.15D-04
IDIUse=3 WtCom= 9.96D-01 WtEn= 3.62D-03
Coeff-Com: 0.341D-01-0.763D-01-0.770D-01-0.613D-01 0.188D+00 0.993D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.340D-01-0.761D-01-0.767D-01-0.611D-01 0.187D+00 0.993D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=9.67D-05 MaxDP=5.90D-03 DE=-4.94D-04 OVMax= 1.29D-02

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.30D-05 CP: 9.66D-02 1.79D+00 1.08D+00 1.31D+00 2.07D+00
CP: 1.51D+00
E= -722.897526485770 Delta-E= -0.000143717416 Rises=F Damp=F
DIIS: error= 2.07D-04 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -722.897526485770 IErMin= 7 ErrMin= 2.07D-04
ErrMax= 2.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.84D-06 BMatP= 1.99D-05
IDIUse=3 WtCom= 9.98D-01 WtEn= 2.07D-03
Coeff-Com: 0.145D-01-0.265D-01-0.156D-01-0.186D-01-0.105D+00 0.325D+00
Coeff-Com: 0.827D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
Coeff-En: 0.100D+01
Coeff: 0.145D-01-0.265D-01-0.156D-01-0.186D-01-0.105D+00 0.324D+00
Coeff: 0.827D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=3.43D-05 MaxDP=1.18D-03 DE=-1.44D-04 OVMax= 6.24D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.89D-05 CP: 9.68D-02 1.78D+00 1.09D+00 1.31D+00 2.14D+00

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               CP:  1.71D+00  1.63D+00
E= -722.897561854926     Delta-E=       -0.000035369156 Rises=F Damp=F
DIIS: error= 1.61D-04 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -722.897561854926     IErMin= 8 ErrMin= 1.61D-04
ErrMax= 1.61D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-06 BMatP= 6.84D-06
IDIUse=3 WtCom= 9.98D-01 WtEn= 1.61D-03
Coeff-Com:  0.876D-04 0.238D-02 0.108D-01 0.175D-01-0.665D-01-0.199D+00
Coeff-Com:  0.313D+00 0.921D+00
Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
Coeff-En:   0.000D+00 0.100D+01
Coeff:      0.874D-04 0.238D-02 0.107D-01 0.175D-01-0.664D-01-0.198D+00
Coeff:      0.313D+00 0.921D+00
Gap=     0.176 Goal=   None    Shift=    0.000
RMSDP=2.64D-05 MaxDP=7.77D-04 DE=-3.54D-05 OVMax= 3.83D-03

Cycle  11  Pass 1  IDiag  1:
RMSU=  1.07D-05    CP:  9.69D-02  1.78D+00  1.09D+00  1.31D+00  2.16D+00
               CP:  1.82D+00  2.15D+00  1.67D+00
E= -722.897574645961     Delta-E=       -0.000012791035 Rises=F Damp=F
DIIS: error= 7.07D-05 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -722.897574645961     IErMin= 9 ErrMin= 7.07D-05
ErrMax= 7.07D-05  0.00D+00 EMaxC= 1.00D-01 BMatC= 7.78D-07 BMatP= 2.31D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.381D-02 0.802D-02 0.957D-02 0.165D-01-0.334D-02-0.224D+00
Coeff-Com: -0.925D-01 0.540D+00 0.749D+00
Coeff:     -0.381D-02 0.802D-02 0.957D-02 0.165D-01-0.334D-02-0.224D+00
Coeff:     -0.925D-01 0.540D+00 0.749D+00
Gap=     0.176 Goal=   None    Shift=    0.000
RMSDP=2.01D-05 MaxDP=6.63D-04 DE=-1.28D-05 OVMax= 1.96D-03

Cycle  12  Pass 1  IDiag  1:
RMSU=  4.98D-06    CP:  9.70D-02  1.78D+00  1.09D+00  1.30D+00  2.17D+00
               CP:  1.89D+00  2.44D+00  2.30D+00  1.93D+00
E= -722.897577868513     Delta-E=       -0.000003222552 Rises=F Damp=F
DIIS: error= 1.78D-05 at cycle  10 NSaved=  10.
NSaved=10 IEnMin=10 EnMin= -722.897577868513     IErMin=10 ErrMin= 1.78D-05
ErrMax= 1.78D-05  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-07 BMatP= 7.78D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.204D-02 0.375D-02 0.212D-02 0.299D-02 0.907D-02-0.520D-01
Coeff-Com: -0.958D-01 0.821D-01 0.309D+00 0.741D+00
Coeff:     -0.204D-02 0.375D-02 0.212D-02 0.299D-02 0.907D-02-0.520D-01
Coeff:     -0.958D-01 0.821D-01 0.309D+00 0.741D+00
Gap=     0.176 Goal=   None    Shift=    0.000
RMSDP=1.27D-05 MaxDP=4.97D-04 DE=-3.22D-06 OVMax= 4.84D-04

Cycle  13  Pass 1  IDiag  1:
RMSU=  2.25D-06    CP:  9.70D-02  1.78D+00  1.09D+00  1.29D+00  2.18D+00
               CP:  1.90D+00  2.50D+00  2.67D+00  2.59D+00  1.76D+00
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Supporting Information file

E= -722.897578210877 Delta-E= -0.000000342363 Rises=F Damp=F
DIIS: error= 6.74D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -722.897578210877 IErMin=11 ErrMin= 6.74D-06
ErrMax= 6.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-08 BMatP= 1.12D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.384D-03 0.753D-03-0.696D-03-0.346D-02-0.177D-02 0.376D-01
Coeff-Com: -0.263D-02-0.785D-01-0.870D-01 0.104D+00 0.103D+01
Coeff: -0.384D-03 0.753D-03-0.696D-03-0.346D-02-0.177D-02 0.376D-01
Coeff: -0.263D-02-0.785D-01-0.870D-01 0.104D+00 0.103D+01
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.11D-05 MaxDP=4.72D-04 DE=-3.42D-07 OVMax= 2.56D-04

Cycle 14 Pass 1 IDiag 1:
RMSU= 2.37D-06 CP: 9.71D-02 1.78D+00 1.09D+00 1.28D+00 2.18D+00
CP: 1.92D+00 2.53D+00 2.95D+00 3.00D+00 2.50D+00
CP: 1.94D+00
E= -722.897578307946 Delta-E= -0.000000097070 Rises=F Damp=F
DIIS: error= 2.91D-06 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -722.897578307946 IErMin=12 ErrMin= 2.91D-06
ErrMax= 2.91D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.26D-09 BMatP= 1.97D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.222D-03-0.384D-03-0.603D-03-0.187D-02-0.306D-02 0.223D-01
Coeff-Com: 0.158D-01-0.406D-01-0.904D-01-0.122D+00 0.352D+00 0.869D+00
Coeff: 0.222D-03-0.384D-03-0.603D-03-0.187D-02-0.306D-02 0.223D-01
Coeff: 0.158D-01-0.406D-01-0.904D-01-0.122D+00 0.352D+00 0.869D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=6.66D-06 MaxDP=2.82D-04 DE=-9.71D-08 OVMax= 1.62D-04

Cycle 15 Pass 1 IDiag 1:
RMSU= 2.46D-06 CP: 9.71D-02 1.78D+00 1.09D+00 1.27D+00 2.19D+00
CP: 1.93D+00 2.55D+00 3.00D+00 3.00D+00 2.94D+00
CP: 2.62D+00 2.56D+00
E= -722.897578332495 Delta-E= -0.000000024549 Rises=F Damp=F
DIIS: error= 2.57D-06 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -722.897578332495 IErMin=13 ErrMin= 2.57D-06
ErrMax= 2.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-09 BMatP= 4.26D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.187D-03-0.350D-03-0.132D-03-0.107D-03-0.791D-03 0.306D-02
Coeff-Com: 0.678D-02-0.504D-02-0.225D-01-0.637D-01-0.351D-01 0.382D+00
Coeff-Com: 0.736D+00
Coeff: 0.187D-03-0.350D-03-0.132D-03-0.107D-03-0.791D-03 0.306D-02
Coeff: 0.678D-02-0.504D-02-0.225D-01-0.637D-01-0.351D-01 0.382D+00
Coeff: 0.736D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=2.95D-06 MaxDP=1.17D-04 DE=-2.45D-08 OVMax= 6.27D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 9.36D-07 CP: 9.71D-02 1.78D+00 1.09D+00 1.27D+00 2.19D+00

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              CP:  1.94D+00  2.56D+00  3.00D+00  3.00D+00  3.00D+00
              CP:  2.96D+00  3.00D+00  1.56D+00
E= -722.897578338092     Delta-E=       -0.000000005597 Rises=F Damp=F
DIIS: error= 1.65D-06 at cycle  14 NSaved=  14.
NSaved=14 IEnMin=14 EnMin= -722.897578338092     IErMin=14 ErrMin= 1.65D-06
ErrMax= 1.65D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 5.62D-10 BMatP= 1.24D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.569D-04-0.130D-03 0.165D-03 0.805D-03 0.102D-02-0.798D-02
Coeff-Com: -0.254D-02 0.140D-01 0.259D-01 0.169D-01-0.177D+00-0.125D+00
Coeff-Com:  0.453D+00 0.801D+00
Coeff:      0.569D-04-0.130D-03 0.165D-03 0.805D-03 0.102D-02-0.798D-02
Coeff:     -0.254D-02 0.140D-01 0.259D-01 0.169D-01-0.177D+00-0.125D+00
Coeff:      0.453D+00 0.801D+00
Gap=     0.176 Goal=   None    Shift=    0.000
RMSDP=2.31D-06 MaxDP=9.51D-05 DE=-5.60D-09 OVMax= 4.93D-05

Cycle  17  Pass 1  IDiag  1:
RMSU=  7.92D-07    CP:  9.71D-02  1.78D+00  1.09D+00  1.27D+00  2.19D+00
              CP:  1.94D+00  2.57D+00  3.00D+00  3.00D+00  3.00D+00
              CP:  3.00D+00  3.00D+00  1.97D+00  2.49D+00
E= -722.897578340909     Delta-E=       -0.000000002817 Rises=F Damp=F
DIIS: error= 5.90D-07 at cycle  15 NSaved=  15.
NSaved=15 IEnMin=15 EnMin= -722.897578340909     IErMin=15 ErrMin= 5.90D-07
ErrMax= 5.90D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 7.70D-11 BMatP= 5.62D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.536D-05-0.570D-06 0.500D-04 0.204D-03 0.479D-03-0.225D-02
Coeff-Com: -0.190D-02 0.330D-02 0.105D-01 0.190D-01-0.370D-01-0.116D+00
Coeff-Com: -0.821D-01 0.157D+00 0.105D+01
Coeff:     -0.536D-05-0.570D-06 0.500D-04 0.204D-03 0.479D-03-0.225D-02
Coeff:     -0.190D-02 0.330D-02 0.105D-01 0.190D-01-0.370D-01-0.116D+00
Coeff:     -0.821D-01 0.157D+00 0.105D+01
Gap=     0.176 Goal=   None    Shift=    0.000
RMSDP=1.28D-06 MaxDP=5.40D-05 DE=-2.82D-09 OVMax= 2.89D-05

Cycle  18  Pass 1  IDiag  1:
RMSU=  3.06D-07    CP:  9.71D-02  1.78D+00  1.09D+00  1.27D+00  2.19D+00
              CP:  1.94D+00  2.58D+00  3.00D+00  3.00D+00  3.00D+00
              CP:  3.00D+00  3.00D+00  2.20D+00  3.00D+00  1.61D+00
E= -722.897578341679     Delta-E=       -0.000000000770 Rises=F Damp=F
DIIS: error= 2.65D-07 at cycle  16 NSaved=  16.
NSaved=16 IEnMin=16 EnMin= -722.897578341679     IErMin=16 ErrMin= 2.65D-07
ErrMax= 2.65D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-11 BMatP= 7.70D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.240D-04 0.500D-04-0.161D-04-0.148D-03-0.131D-03 0.129D-02
Coeff-Com:  0.171D-04-0.234D-02-0.301D-02 0.220D-02 0.355D-01-0.456D-02
Coeff-Com: -0.161D+00-0.174D+00 0.383D+00 0.924D+00
Coeff:     -0.240D-04 0.500D-04-0.161D-04-0.148D-03-0.131D-03 0.129D-02
Coeff:      0.171D-04-0.234D-02-0.301D-02 0.220D-02 0.355D-01-0.456D-02
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Coeff: -0.161D+00-0.174D+00 0.383D+00 0.924D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=5.17D-07 MaxDP=2.09D-05 DE=-7.70D-10 OVMax= 1.19D-05

Cycle 19 Pass 1 IDiag 1:
RMSU= 5.74D-08 CP: 9.71D-02 1.78D+00 1.09D+00 1.27D+00 2.19D+00
CP: 1.95D+00 2.58D+00 3.00D+00 3.00D+00 3.00D+00
CP: 3.00D+00 3.00D+00 2.30D+00 3.00D+00 1.84D+00
CP: 2.00D+00
E= -722.897578341819 Delta-E= -0.000000000141 Rises=F Damp=F
DIIS: error= 1.05D-07 at cycle 17 NSaved= 17.
NSaved=17 IEnMin=17 EnMin= -722.897578341819 IErMin=17 ErrMin= 1.05D-07
ErrMax= 1.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.81D-12 BMatP= 1.97D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.702D-05 0.160D-04-0.105D-04-0.698D-04-0.111D-03 0.573D-03
Coeff-Com: 0.301D-03-0.881D-03-0.218D-02-0.280D-02 0.125D-01 0.158D-01
Coeff-Com: -0.231D-01-0.578D-01-0.453D-01 0.192D+00 0.911D+00
Coeff: -0.702D-05 0.160D-04-0.105D-04-0.698D-04-0.111D-03 0.573D-03
Coeff: 0.301D-03-0.881D-03-0.218D-02-0.280D-02 0.125D-01 0.158D-01
Coeff: -0.231D-01-0.578D-01-0.453D-01 0.192D+00 0.911D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=7.99D-08 MaxDP=3.39D-06 DE=-1.41D-10 OVMax= 3.23D-06

Cycle 20 Pass 1 IDiag 1:
RMSU= 2.80D-08 CP: 9.71D-02 1.78D+00 1.09D+00 1.27D+00 2.19D+00
CP: 1.95D+00 2.58D+00 3.00D+00 3.00D+00 3.00D+00
CP: 3.00D+00 3.00D+00 2.32D+00 3.00D+00 1.86D+00
CP: 2.12D+00 1.34D+00
E= -722.897578341829 Delta-E= -0.000000000010 Rises=F Damp=F
DIIS: error= 4.68D-08 at cycle 18 NSaved= 18.
NSaved=18 IEnMin=18 EnMin= -722.897578341829 IErMin=18 ErrMin= 4.68D-08
ErrMax= 4.68D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.50D-13 BMatP= 2.81D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.748D-07 0.339D-06 0.170D-05 0.993D-05-0.103D-04-0.126D-03
Coeff-Com: 0.551D-04 0.334D-03 0.102D-03-0.111D-02-0.360D-02 0.567D-02
Coeff-Com: 0.235D-01 0.180D-01-0.885D-01-0.140D+00 0.284D+00 0.902D+00
Coeff: -0.748D-07 0.339D-06 0.170D-05 0.993D-05-0.103D-04-0.126D-03
Coeff: 0.551D-04 0.334D-03 0.102D-03-0.111D-02-0.360D-02 0.567D-02
Coeff: 0.235D-01 0.180D-01-0.885D-01-0.140D+00 0.284D+00 0.902D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=3.21D-08 MaxDP=3.09D-06 DE=-9.55D-12 OVMax= 1.55D-06

Cycle 21 Pass 1 IDiag 1:
RMSU= 6.79D-09 CP: 9.71D-02 1.78D+00 1.09D+00 1.27D+00 2.19D+00
CP: 1.95D+00 2.58D+00 3.00D+00 3.00D+00 3.00D+00
CP: 3.00D+00 3.00D+00 2.32D+00 3.00D+00 1.86D+00
CP: 2.13D+00 1.55D+00 1.76D+00
E= -722.897578341836 Delta-E= -0.000000000007 Rises=F Damp=F

DIIS: error= 2.21D-08 at cycle 19 NSaved= 19.
NSaved=19 IEnMin=19 EnMin= -722.897578341836 IErMin=19 ErrMin= 2.21D-08
ErrMax= 2.21D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-13 BMatP= 6.50D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.923D-06-0.207D-05 0.183D-05 0.137D-04 0.137D-04-0.124D-03
Coeff-Com: -0.374D-04 0.237D-03 0.369D-03 0.964D-04-0.311D-02-0.277D-03
Coeff-Com: 0.951D-02 0.140D-01-0.172D-01-0.721D-01-0.514D-01 0.279D+00
Coeff-Com: 0.841D+00
Coeff: 0.923D-06-0.207D-05 0.183D-05 0.137D-04 0.137D-04-0.124D-03
Coeff: -0.374D-04 0.237D-03 0.369D-03 0.964D-04-0.311D-02-0.277D-03
Coeff: 0.951D-02 0.140D-01-0.172D-01-0.721D-01-0.514D-01 0.279D+00
Coeff: 0.841D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.52D-08 MaxDP=1.31D-06 DE=-6.82D-12 OVMax= 6.32D-07

Cycle 22 Pass 1 IDiag 1:
RMSU= 3.81D-09 CP: 9.71D-02 1.78D+00 1.09D+00 1.27D+00 2.19D+00
CP: 1.95D+00 2.58D+00 3.00D+00 3.00D+00 3.00D+00
CP: 3.00D+00 3.00D+00 2.32D+00 3.00D+00 1.85D+00
CP: 2.11D+00 1.63D+00 2.10D+00 1.55D+00
E= -722.897578341835 Delta-E= 0.000000000001 Rises=F Damp=F
DIIS: error= 9.43D-09 at cycle 20 NSaved= 20.
NSaved=20 IEnMin=19 EnMin= -722.897578341836 IErMin=20 ErrMin= 9.43D-09
ErrMax= 9.43D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.05D-14 BMatP= 1.05D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.592D-06-0.133D-05 0.232D-06 0.385D-05 0.985D-05-0.227D-04
Coeff-Com: -0.322D-04 0.156D-04 0.143D-03 0.325D-03-0.511D-03-0.138D-02
Coeff-Com: -0.196D-02 0.109D-02 0.164D-01 0.302D-02-0.941D-01-0.118D+00
Coeff-Com: 0.371D+00 0.824D+00
Coeff: 0.592D-06-0.133D-05 0.232D-06 0.385D-05 0.985D-05-0.227D-04
Coeff: -0.322D-04 0.156D-04 0.143D-03 0.325D-03-0.511D-03-0.138D-02
Coeff: -0.196D-02 0.109D-02 0.164D-01 0.302D-02-0.941D-01-0.118D+00
Coeff: 0.371D+00 0.824D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.04D-08 MaxDP=7.92D-07 DE= 1.14D-12 OVMax= 5.19D-07

Cycle 23 Pass 1 IDiag 1:
Restarting incremental Fock formation.
E= -722.897578341827 Delta-E= 0.000000000007 Rises=F Damp=F
DIIS: error= 5.31D-09 at cycle 21 NSaved= 20.
NSaved=20 IEnMin=18 EnMin= -722.897578341836 IErMin=20 ErrMin= 5.31D-09
ErrMax= 5.31D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-14 BMatP= 4.05D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.927D-09-0.340D-06-0.191D-05 0.886D-06 0.226D-04-0.435D-05
Coeff-Com: -0.580D-04-0.354D-04 0.123D-03 0.626D-03-0.419D-03-0.343D-02
Coeff-Com: -0.357D-02 0.117D-01 0.194D-01-0.223D-01-0.128D+00-0.517D-01
Coeff-Com: 0.308D+00 0.870D+00
Coeff: 0.927D-09-0.340D-06-0.191D-05 0.886D-06 0.226D-04-0.435D-05

Supporting Information file

Coeff: -0.580D-04-0.354D-04 0.123D-03 0.626D-03-0.419D-03-0.343D-02
Coeff: -0.357D-02 0.117D-01 0.194D-01-0.223D-01-0.128D+00-0.517D-01
Coeff: 0.308D+00 0.870D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=7.89D-09 MaxDP=3.49D-07 DE= 7.28D-12 OVMax= 4.48D-07

SCF Done: E(RwB97XD) = -722.897578342 A.U. after 23 cycles
NFock= 23 Conv=0.79D-08 -V/T= 2.0002
KE= 7.227431672232D+02 PE=-3.714345824043D+03 EE= 1.252710455666D+03
Leave Link 502 at Fri Sep 25 18:08:30 2026, MaxMem= 805306368 cpu: 10283.1 elap: 1714.4
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

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Population analysis using the SCF Density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Alpha virt. eigenvalues --	0.44472	0.44868	0.44892	0.45603	0.45736
Alpha virt. eigenvalues --	0.46905	0.47228	0.48097	0.48714	0.48780
Alpha virt. eigenvalues --	0.49348	0.50334	0.50718	0.51497	0.52019
Alpha virt. eigenvalues --	0.52335	0.53349	0.54239	0.54984	0.55385
Alpha virt. eigenvalues --	0.55603	0.55887	0.56882	0.57886	0.58147
Alpha virt. eigenvalues --	0.58689	0.59175	0.59590	0.59954	0.60181
Alpha virt. eigenvalues --	0.60585	0.61106	0.61710	0.62320	0.63369
Alpha virt. eigenvalues --	0.63665	0.64469	0.64588	0.65246	0.65635
Alpha virt. eigenvalues --	0.66363	0.67701	0.68062	0.68789	0.69713
Alpha virt. eigenvalues --	0.69794	0.70207	0.72396	0.72859	0.73148
Alpha virt. eigenvalues --	0.73596	0.74505	0.75699	0.76285	0.77471
Alpha virt. eigenvalues --	0.78390	0.80093	0.80265	0.80885	0.81471
Alpha virt. eigenvalues --	0.82953	0.83258	0.85033	0.85801	0.85805
Alpha virt. eigenvalues --	0.86357	0.89309	0.89942	0.90461	0.90561
Alpha virt. eigenvalues --	0.91513	0.93163	0.94759	0.95391	0.98299
Alpha virt. eigenvalues --	0.98673	0.99336	1.00218	1.00301	1.01009
Alpha virt. eigenvalues --	1.01289	1.03294	1.03928	1.04697	1.06848
Alpha virt. eigenvalues --	1.07698	1.09468	1.10198	1.11627	1.12269
Alpha virt. eigenvalues --	1.13127	1.15720	1.15814	1.16778	1.18345
Alpha virt. eigenvalues --	1.19237	1.20875	1.21289	1.24281	1.25068
Alpha virt. eigenvalues --	1.26487	1.27528	1.28700	1.29516	1.29949
Alpha virt. eigenvalues --	1.30613	1.31195	1.31618	1.33515	1.34468
Alpha virt. eigenvalues --	1.36165	1.38262	1.39311	1.39672	1.40098
Alpha virt. eigenvalues --	1.40998	1.41445	1.42749	1.44084	1.44603
Alpha virt. eigenvalues --	1.45006	1.47056	1.47525	1.49275	1.49664
Alpha virt. eigenvalues --	1.49979	1.50515	1.51563	1.52181	1.53119
Alpha virt. eigenvalues --	1.53894	1.54861	1.55349	1.55744	1.56137
Alpha virt. eigenvalues --	1.56722	1.56918	1.56963	1.57869	1.58748
Alpha virt. eigenvalues --	1.59407	1.59662	1.62285	1.63318	1.64453
Alpha virt. eigenvalues --	1.65158	1.65327	1.66818	1.67553	1.68994
Alpha virt. eigenvalues --	1.69021	1.70970	1.71607	1.71986	1.72284
Alpha virt. eigenvalues --	1.72889	1.73189	1.74221	1.74516	1.75543
Alpha virt. eigenvalues --	1.76470	1.77583	1.77653	1.78344	1.79156
Alpha virt. eigenvalues --	1.81308	1.81814	1.83509	1.84036	1.84818
Alpha virt. eigenvalues --	1.85523	1.86513	1.86972	1.87308	1.87735
Alpha virt. eigenvalues --	1.90603	1.90852	1.93307	1.95319	1.96020
Alpha virt. eigenvalues --	1.96159	1.98471	1.99571	1.99890	2.00790
Alpha virt. eigenvalues --	2.00950	2.04257	2.05557	2.07356	2.08515
Alpha virt. eigenvalues --	2.08598	2.08967	2.09461	2.13314	2.14414
Alpha virt. eigenvalues --	2.15777	2.17168	2.19409	2.21523	2.21577
Alpha virt. eigenvalues --	2.23808	2.25343	2.26649	2.27723	2.28002
Alpha virt. eigenvalues --	2.31902	2.32318	2.33968	2.35909	2.40043
Alpha virt. eigenvalues --	2.40145	2.41853	2.44305	2.44878	2.45909
Alpha virt. eigenvalues --	2.47834	2.48035	2.50019	2.50342	2.50557
Alpha virt. eigenvalues --	2.50937	2.53043	2.53106	2.54851	2.54929
Alpha virt. eigenvalues --	2.56204	2.56353	2.57169	2.57998	2.58193
Alpha virt. eigenvalues --	2.59086	2.60070	2.60775	2.61426	2.61563
Alpha virt. eigenvalues --	2.63872	2.65413	2.66942	2.67688	2.68143

Alpha virt. eigenvalues --	2.69361	2.69906	2.70390	2.71346	2.72743
Alpha virt. eigenvalues --	2.73150	2.73297	2.74367	2.75515	2.77750
Alpha virt. eigenvalues --	2.77939	2.78939	2.79247	2.81719	2.81941
Alpha virt. eigenvalues --	2.82792	2.84534	2.84768	2.85826	2.86593
Alpha virt. eigenvalues --	2.86751	2.87616	2.88996	2.89293	2.89311
Alpha virt. eigenvalues --	2.89844	2.90293	2.90697	2.91536	2.91638
Alpha virt. eigenvalues --	2.91888	2.92148	2.92559	2.93385	2.94620
Alpha virt. eigenvalues --	2.94936	2.96380	2.96975	2.97635	2.97973
Alpha virt. eigenvalues --	2.98734	2.99562	3.00300	3.01547	3.01846
Alpha virt. eigenvalues --	3.02283	3.02633	3.03903	3.04864	3.04885
Alpha virt. eigenvalues --	3.06666	3.06821	3.07990	3.08245	3.09406
Alpha virt. eigenvalues --	3.09558	3.09699	3.10974	3.12020	3.13032
Alpha virt. eigenvalues --	3.13166	3.14064	3.14697	3.16885	3.17102
Alpha virt. eigenvalues --	3.17948	3.20651	3.20678	3.22311	3.23040
Alpha virt. eigenvalues --	3.23465	3.24055	3.24640	3.25110	3.25513
Alpha virt. eigenvalues --	3.26235	3.27618	3.28275	3.30571	3.31573
Alpha virt. eigenvalues --	3.31932	3.32877	3.33076	3.33394	3.35559
Alpha virt. eigenvalues --	3.35593	3.36423	3.36855	3.38199	3.39539
Alpha virt. eigenvalues --	3.40360	3.40394	3.42252	3.42805	3.44355
Alpha virt. eigenvalues --	3.45143	3.45981	3.46386	3.47854	3.48307
Alpha virt. eigenvalues --	3.49275	3.49601	3.50581	3.51766	3.51852
Alpha virt. eigenvalues --	3.52236	3.54130	3.54343	3.56113	3.57839
Alpha virt. eigenvalues --	3.58681	3.61920	3.62508	3.64873	3.65063
Alpha virt. eigenvalues --	3.66499	3.67352	3.67375	3.69728	3.70832
Alpha virt. eigenvalues --	3.71135	3.73176	3.73621	3.75116	3.76271
Alpha virt. eigenvalues --	3.76446	3.81043	3.82708	3.86213	3.87093
Alpha virt. eigenvalues --	3.92706	3.94619	3.95092	3.95681	4.00890
Alpha virt. eigenvalues --	4.03371	4.03886	4.04590	4.06524	4.07354
Alpha virt. eigenvalues --	4.09990	4.10185	4.14895	4.17037	4.18243
Alpha virt. eigenvalues --	4.20461	4.20743	4.21833	4.24408	4.28849
Alpha virt. eigenvalues --	4.32408	4.33489	4.35879	4.38562	4.39140
Alpha virt. eigenvalues --	4.39166	4.41997	4.43605	4.44993	4.47445
Alpha virt. eigenvalues --	4.47630	4.49048	4.52535	4.53890	4.54827
Alpha virt. eigenvalues --	4.57019	4.61109	4.66691	4.67334	4.67732
Alpha virt. eigenvalues --	4.73270	4.74751	4.79132	4.79207	4.81578
Alpha virt. eigenvalues --	4.81860	4.83192	4.85410	4.85672	4.90103
Alpha virt. eigenvalues --	4.91809	4.93129	4.94691	4.96630	4.98359
Alpha virt. eigenvalues --	5.00833	5.04282	5.06014	5.06350	5.06502
Alpha virt. eigenvalues --	5.09418	5.09905	5.11691	5.13803	5.15230
Alpha virt. eigenvalues --	5.18377	5.18750	5.20341	5.23138	5.25662
Alpha virt. eigenvalues --	5.29096	5.32240	5.32980	5.33139	5.35812
Alpha virt. eigenvalues --	5.36875	5.37962	5.38932	5.41030	5.42329
Alpha virt. eigenvalues --	5.45325	5.48707	5.52572	5.55338	5.59771
Alpha virt. eigenvalues --	5.64632	5.65542	5.71369	5.79422	5.81801
Alpha virt. eigenvalues --	5.82346	5.87199	5.91289	5.92125	5.93038
Alpha virt. eigenvalues --	6.01339	6.07286	6.10462	6.14180	6.23064
Alpha virt. eigenvalues --	6.25730	6.26337	6.32053	6.50857	22.60501
Alpha virt. eigenvalues --	22.98805	22.99279	23.24600	23.29219	23.50995

Supporting Information file

Alpha virt. eigenvalues -- 23.52010 23.66775 23.78837 23.87402 23.87911
Alpha virt. eigenvalues -- 24.16510 24.19635 24.40175 24.43279 24.75024
Alpha virt. eigenvalues -- 32.18955 32.24767

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	4.964986	0.854975	0.505716	-0.119282	-0.079259	-0.039519
2	C	0.854975	4.933143	-0.079177	0.458234	-0.052745	-0.094369
3	C	0.505716	-0.079177	4.964498	-0.013035	0.854973	-0.007936
4	C	-0.119282	0.458234	-0.013035	5.021195	-0.006176	0.817662
5	C	-0.079259	-0.052745	0.854973	-0.006176	4.933264	-0.004684
6	C	-0.039519	-0.094369	-0.007936	0.817662	-0.004684	5.353083
7	C	-0.013014	-0.006170	-0.119195	-0.004344	0.458146	0.000369
8	C	-0.005407	-0.024868	-0.001300	-0.069800	-0.000934	0.221308
9	C	-0.007932	-0.004670	-0.039391	0.000371	-0.094307	0.000899
10	C	-0.001731	-0.006073	-0.000139	-0.067822	-0.000278	-0.074993
11	C	-0.001294	-0.000928	-0.005382	-0.000554	-0.024746	0.001306
12	C	-0.000099	-0.001361	-0.000018	-0.012648	0.000070	-0.023901
13	C	-0.000139	-0.000279	-0.001724	0.002425	-0.006058	0.003149
14	C	-0.000017	0.000070	-0.000099	0.002405	-0.001356	-0.001154
15	C	-0.000001	-0.000052	-0.000002	-0.000487	0.000006	-0.004150
16	C	-0.000002	0.000006	-0.000001	-0.000034	-0.000052	0.000776
17	N	-0.000000	-0.000000	-0.000000	-0.000009	0.000000	-0.000559
18	N	-0.000000	0.000000	-0.000000	-0.000000	-0.000000	0.000002
19	H	0.000000	-0.000001	-0.000000	0.000005	0.000000	-0.000777
20	H	-0.000000	0.000000	0.000000	-0.000001	-0.000000	0.000096
21	H	-0.000000	0.000000	0.000000	-0.000000	-0.000001	-0.000002
22	H	0.000000	-0.000000	-0.000000	0.000000	0.000000	0.000000
23	H	-0.000000	0.000000	-0.000000	-0.000004	0.000000	-0.000080
24	H	-0.000000	-0.000002	0.000000	-0.000037	-0.000000	-0.001393
25	H	0.000000	-0.000000	-0.000000	-0.000007	-0.000002	-0.000158
26	H	-0.000000	0.000000	-0.000000	-0.000000	0.000000	0.000002

		7	8	9	10	11	12
1	C	-0.013014	-0.005407	-0.007932	-0.001731	-0.001294	-0.000099
2	C	-0.006170	-0.024868	-0.004670	-0.006073	-0.000928	-0.001361
3	C	-0.119195	-0.001300	-0.039391	-0.000139	-0.005382	-0.000018
4	C	-0.004344	-0.069800	0.000371	-0.067822	-0.000554	-0.012648
5	C	0.458146	-0.000934	-0.094307	-0.000278	-0.024746	0.000070
6	C	0.000369	0.221308	0.000899	-0.074993	0.001306	-0.023901
7	C	5.019682	-0.000550	0.818303	0.002427	-0.069521	0.002401
8	C	-0.000550	5.577967	0.001279	0.483067	-0.000114	-0.300045
9	C	0.818303	0.001279	5.351759	0.003142	0.222083	-0.001201
10	C	0.002427	0.483067	0.003142	5.701986	-0.003756	0.265281
11	C	-0.069521	-0.000114	0.222083	-0.003756	5.575687	0.009796
12	C	0.002401	-0.300045	-0.001201	0.265281	0.009796	5.954357
13	C	-0.067525	-0.003828	-0.075025	-0.082330	0.482972	0.048423
14	C	-0.012606	0.009677	-0.023783	0.047616	-0.299497	0.222717
15	C	-0.000034	0.010016	0.000771	-0.119465	-0.003495	-0.178085
16	C	-0.000482	-0.003425	-0.004098	-0.037512	0.010182	0.214929

17	N	-0.000000	-0.002846	0.000002	0.021110	0.000020	-0.036615
18	N	-0.000009	0.000020	-0.000557	-0.000121	-0.002818	0.015668
19	H	-0.000000	-0.003795	-0.000002	0.010893	-0.000043	-0.100374
20	H	0.000000	0.000840	0.000000	-0.008331	0.000064	0.105738
21	H	0.000005	-0.000043	-0.000784	-0.000569	-0.003821	0.018256
22	H	-0.000001	0.000065	0.000096	0.002345	0.000836	-0.030171
23	H	-0.000000	0.000064	0.000002	0.013266	-0.000037	-0.009049
24	H	-0.000007	-0.007086	-0.000159	0.068793	-0.003692	-0.311779
25	H	-0.000036	-0.003741	-0.001376	-0.049305	-0.007025	-0.118453
26	H	-0.000004	-0.000037	-0.000073	-0.001443	0.000102	-0.008667

		13	14	15	16	17	18
1	C	-0.000139	-0.000017	-0.000001	-0.000002	-0.000000	-0.000000
2	C	-0.000279	0.000070	-0.000052	0.000006	-0.000000	0.000000
3	C	-0.001724	-0.000099	-0.000002	-0.000001	-0.000000	-0.000000
4	C	0.002425	0.002405	-0.000487	-0.000034	-0.000009	-0.000000
5	C	-0.006058	-0.001356	0.000006	-0.000052	0.000000	-0.000000
6	C	0.003149	-0.001154	-0.004150	0.000776	-0.000559	0.000002
7	C	-0.067525	-0.012606	-0.000034	-0.000482	-0.000000	-0.000009
8	C	-0.003828	0.009677	0.010016	-0.003425	-0.002846	0.000020
9	C	-0.075025	-0.023783	0.000771	-0.004098	0.000002	-0.000557
10	C	-0.082330	0.047616	-0.119465	-0.037512	0.021110	-0.000121
11	C	0.482972	-0.299497	-0.003495	0.010182	0.000020	-0.002818
12	C	0.048423	0.222717	-0.178085	0.214929	-0.036615	0.015668
13	C	5.701006	0.265339	-0.038043	-0.119616	-0.000104	0.021307
14	C	0.265339	5.951291	0.216135	-0.175644	0.015530	-0.036967
15	C	-0.038043	0.216135	7.372831	-0.534855	0.160341	-0.026479
16	C	-0.119616	-0.175644	-0.534855	7.369694	-0.026320	0.160180
17	N	-0.000104	0.015530	0.160341	-0.026320	5.685577	0.000787
18	N	0.021307	-0.036967	-0.026479	0.160180	0.000787	5.685960
19	H	-0.000587	0.018310	-0.200883	-0.019458	0.477213	-0.000837
20	H	0.002350	-0.030565	-0.159558	0.070477	0.378948	0.002735
21	H	0.011019	-0.100458	-0.019417	-0.201122	-0.000835	0.476418
22	H	-0.008385	0.105106	0.070051	-0.156816	0.002681	0.379426
23	H	-0.001418	-0.008641	-0.271898	0.005787	0.399813	0.000783
24	H	-0.048579	-0.117967	0.317144	0.143903	-0.060696	0.004979
25	H	0.068798	-0.310624	0.143899	0.315626	0.005174	-0.060535
26	H	0.013204	-0.008632	0.005761	-0.273270	0.000794	0.400428

		19	20	21	22	23	24
1	C	0.000000	-0.000000	-0.000000	0.000000	-0.000000	-0.000000
2	C	-0.000001	0.000000	0.000000	-0.000000	0.000000	-0.000002
3	C	-0.000000	0.000000	0.000000	-0.000000	-0.000000	0.000000
4	C	0.000005	-0.000001	-0.000000	0.000000	-0.000004	-0.000037
5	C	0.000000	-0.000000	-0.000001	0.000000	0.000000	-0.000000
6	C	-0.000777	0.000096	-0.000002	0.000000	-0.000080	-0.001393
7	C	-0.000000	0.000000	0.000005	-0.000001	-0.000000	-0.000007
8	C	-0.003795	0.000840	-0.000043	0.000065	0.000064	-0.007086
9	C	-0.000002	0.000000	-0.000784	0.000096	0.000002	-0.000159
10	C	0.010893	-0.008331	-0.000569	0.002345	0.013266	0.068793

11	C	-0.000043	0.000064	-0.003821	0.000836	-0.000037	-0.003692
12	C	-0.100374	0.105738	0.018256	-0.030171	-0.009049	-0.311779
13	C	-0.000587	0.002350	0.011019	-0.008385	-0.001418	-0.048579
14	C	0.018310	-0.030565	-0.100458	0.105106	-0.008641	-0.117967
15	C	-0.200883	-0.159558	-0.019417	0.070051	-0.271898	0.317144
16	C	-0.019458	0.070477	-0.201122	-0.156816	0.005787	0.143903
17	N	0.477213	0.378948	-0.000835	0.002681	0.399813	-0.060696
18	N	-0.000837	0.002735	0.476418	0.379426	0.000783	0.004979
19	H	0.890490	-0.144555	-0.000246	0.003503	-0.141935	-0.043027
20	H	-0.144555	0.632778	0.003535	-0.024880	0.002644	-0.072034
21	H	-0.000246	0.003535	0.890280	-0.143139	0.000236	0.012828
22	H	0.003503	-0.024880	-0.143139	0.629856	-0.002326	-0.019413
23	H	-0.141935	0.002644	0.000236	-0.002326	0.692198	0.094604
24	H	-0.043027	-0.072034	0.012828	-0.019413	0.094604	1.226898
25	H	0.012892	-0.019785	-0.042505	-0.073603	-0.021020	-0.124448
26	H	0.000237	-0.002368	-0.142421	0.002030	-0.000209	-0.021043

		25	26
1	C	0.000000	-0.000000
2	C	-0.000000	0.000000
3	C	-0.000000	-0.000000
4	C	-0.000007	-0.000000
5	C	-0.000002	0.000000
6	C	-0.000158	0.000002
7	C	-0.000036	-0.000004
8	C	-0.003741	-0.000037
9	C	-0.001376	-0.000073
10	C	-0.049305	-0.001443
11	C	-0.007025	0.000102
12	C	-0.118453	-0.008667
13	C	0.068798	0.013204
14	C	-0.310624	-0.008632
15	C	0.143899	0.005761
16	C	0.315626	-0.273270
17	N	0.005174	0.000794
18	N	-0.060535	0.400428
19	H	0.012892	0.000237
20	H	-0.019785	-0.002368
21	H	-0.042505	-0.142421
22	H	-0.073603	0.002030
23	H	-0.021020	-0.000209
24	H	-0.124448	-0.021043
25	H	1.229208	0.094837
26	H	0.094837	0.693340

Mulliken charges:

		1
1	C	-0.057979
2	C	0.024269
3	C	-0.057790

```
   4  C   -0.008056
   5  C    0.024140
   6  C   -0.144978
   7  C   -0.007835
   8  C    0.123515
   9  C   -0.145348
  10  C   -0.166057
  11  C    0.123674
  12  C    0.274833
  13  C   -0.166352
  14  C    0.273813
  15  C   -0.740051
  16  C   -0.738854
  17  N   -0.020007
  18  N   -0.020370
  19  H    0.242977
  20  H    0.261872
  21  H    0.242788
  22  H    0.262738
  23  H    0.247220
  24  H   -0.037788
  25  H   -0.037809
  26  H    0.247433
Sum of Mulliken charges =  -0.00000
Mulliken charges with hydrogens summed into heavy atoms:
                1
   1  C   -0.057979
   2  C    0.024269
   3  C   -0.057790
   4  C   -0.008056
   5  C    0.024140
   6  C   -0.144978
   7  C   -0.007835
   8  C    0.123515
   9  C   -0.145348
  10  C   -0.166057
  11  C    0.123674
  12  C    0.274833
  13  C   -0.166352
  14  C    0.273813
  15  C   -0.777838
  16  C   -0.776663
  17  N    0.732062
  18  N    0.732589
Electronic spatial extent (au):  <R**2>=          5599.8355
Charge=           -0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=          -18.7328    Y=           0.0071    Z=          -0.0026  Tot=          18.7328
```

Supporting Information file

Quadrupole moment (field-independent basis, Debye-Ang):
XX= -45.4127 YY= -95.4811 ZZ= -104.5248
XY= -0.0164 XZ= 0.0124 YZ= 1.2404
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= 36.3935 YY= -13.6749 ZZ= -22.7186
XY= -0.0164 XZ= 0.0124 YZ= 1.2404
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= -509.5466 YYY= 0.0363 ZZZ= -0.0068 XYY= -126.7656
XXY= 0.1060 XXZ= -0.0647 XZZ= -32.7960 YZZ= -0.0022
YYZ= -0.0152 XYZ= -4.7546
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -4546.2106 YYYY= -1933.3406 ZZZZ= -133.7333 XXXY= -0.4558
XXXZ= 0.3328 YYYX= -0.0355 YYYZ= 6.0157 ZZZX= 0.0311
ZZZY= 4.9636 XXYY= -1022.3429 XXZZ= -998.9696 YYZZ= -343.2641
XXYZ= 17.4387 YYXZ= 0.0502 ZZXY= 0.0144
N-N= 1.015994622812D+03 E-N=-3.714345824386D+03 KE= 7.227431672232D+02
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Fri Sep 25 18:08:30 2026, MaxMem= 805306368 cpu: 2.8 elap: 0.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 22986 LenP2D= 51608.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 18:08:31 2026, MaxMem= 805306368 cpu: 2.9 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 18:08:31 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 18:22:03 2026, MaxMem= 805306368 cpu: 4874.7 elap: 812.5

Supporting Information file

(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-7.37004091D+00 2.80265719D-03-1.01326099D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.003431704	-0.001362709	0.000734551
2	6	-0.002163908	0.001353983	-0.000715021
3	6	0.003406917	0.001363708	-0.000735706
4	6	0.005275467	0.003726394	0.000469046
5	6	-0.002138558	-0.001359051	0.000718359
6	6	-0.005055648	-0.002108330	-0.000819765
7	6	0.005237796	-0.003716577	-0.000475494
8	6	0.007601979	0.008622865	-0.000719142
9	6	-0.005002752	0.002092014	0.000825620
10	6	0.004694409	-0.016293212	0.007340462
11	6	0.007522076	-0.008579305	0.000721892
12	6	0.014130807	0.082953744	0.030988049
13	6	0.004806633	0.016213452	-0.007356406
14	6	0.013988745	-0.083065586	-0.030780549
15	6	0.352817751	-0.347438918	-0.058910163
16	6	0.352757062	0.347825912	0.058615389
17	7	-0.303170009	0.255049192	0.048702841
18	7	-0.303278606	-0.255158079	-0.048320146
19	1	-0.036707220	0.052345366	-0.022803757
20	1	-0.040358820	0.018173204	0.002572176
21	1	-0.036666369	-0.052406571	0.022772734
22	1	-0.040192507	-0.018319821	-0.002576818
23	1	-0.030271936	0.039111992	0.025971185
24	1	0.029779261	-0.050586292	-0.028792075
25	1	0.029917279	0.050681419	0.028571244
26	1	-0.030361554	-0.039118793	-0.025998506

Cartesian Forces: Max 0.352817751 RMS 0.105090464
Leave Link 716 at Fri Sep 25 18:22:03 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.539714923 RMS 0.086104858
Search for a local minimum.
Step number 1 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .86105D-01 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search

Supporting Information file

Second derivative matrix not updated -- first step.
ITU= 0
Eigenvalues --- 0.00442 0.01059 0.01660 0.01660 0.01669
Eigenvalues --- 0.01763 0.02167 0.02405 0.02739 0.02830
Eigenvalues --- 0.03123 0.03320 0.03789 0.03848 0.04437
Eigenvalues --- 0.04460 0.04466 0.05026 0.05026 0.05027
Eigenvalues --- 0.05027 0.08684 0.08684 0.10044 0.11779
Eigenvalues --- 0.11779 0.11779 0.11779 0.14915 0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000
Eigenvalues --- 0.16000 0.16000 0.25000 0.25000 0.25000
Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000
Eigenvalues --- 0.25000 0.37230 0.37230 0.40643 0.40644
Eigenvalues --- 0.45853 0.46045 0.47688 0.47688 0.47688
Eigenvalues --- 0.47688 0.47688 0.47688 0.48558 0.54808
Eigenvalues --- 0.55314 0.55508 0.55659 0.55723 0.93705
Eigenvalues --- 0.94044 0.95021 0.95764 0.97667 0.98046
Eigenvalues --- 1.36020 1.36049
RFO step: Lambda=-4.85636584D-01 EMin= 4.42043410D-03
Linear search not attempted -- first point.
Maximum step size (0.300) exceeded in Quadratic search.
-- Step size scaled by 0.449
Iteration 1 RMS(Cart)= 0.12577969 RMS(Int)= 0.00409510
Iteration 2 RMS(Cart)= 0.01105868 RMS(Int)= 0.00013095
Iteration 3 RMS(Cart)= 0.00007933 RMS(Int)= 0.00012677
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00012677
ITry= 1 IFail=0 DXMaxC= 5.64D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.30930	0.00376	0.00000	0.00124	0.00124	2.31054
R2	2.54690	0.00088	0.00000	0.00048	0.00048	2.54738
R3	2.54467	0.00153	0.00000	0.00070	0.00070	2.54537
R4	2.30930	0.00375	0.00000	0.00124	0.00124	2.31054
R5	2.30384	0.00642	0.00000	0.00200	0.00200	2.30584
R6	2.54466	0.00154	0.00000	0.00071	0.00071	2.54537
R7	2.54682	0.00162	0.00000	0.00067	0.00067	2.54750
R8	2.30384	0.00639	0.00000	0.00199	0.00199	2.30584
R9	2.29384	0.01232	0.00000	0.00374	0.00374	2.29758
R10	2.54682	0.00165	0.00000	0.00069	0.00069	2.54750
R11	2.64007	0.00786	0.00000	0.00367	0.00367	2.64374
R12	2.29384	0.01226	0.00000	0.00372	0.00372	2.29756
R13	2.61227	0.04266	0.00000	0.01961	0.01961	2.63187
R14	2.70689	0.00760	0.00000	0.00383	0.00383	2.71072
R15	2.64007	0.00793	0.00000	0.00371	0.00371	2.64378
R16	2.70688	0.00745	0.00000	0.00375	0.00375	2.71063
R17	2.16922	0.53958	0.00000	0.13133	0.13133	2.30055
R18	2.02201	0.03953	0.00000	0.02070	0.02070	2.04271
R19	2.16930	0.53971	0.00000	0.13138	0.13138	2.30068

R20	2.02201	0.03939	0.00000	0.02063	0.02063	2.04264
R21	1.88973	0.05238	0.00000	0.02445	0.02445	1.91418
R22	1.88973	0.01874	0.00000	0.00875	0.00875	1.89848
R23	1.88973	0.04340	0.00000	0.02026	0.02026	1.90999
R24	1.88973	0.05241	0.00000	0.02447	0.02447	1.91419
R25	1.88973	0.01852	0.00000	0.00864	0.00864	1.89837
R26	1.88973	0.04344	0.00000	0.02028	0.02028	1.91000
A1	2.56055	-0.00448	0.00000	-0.00268	-0.00269	2.55786
A2	2.61063	-0.00072	0.00000	-0.00056	-0.00057	2.61006
A3	2.56033	-0.00447	0.00000	-0.00267	-0.00268	2.55764
A4	2.72307	-0.00134	0.00000	-0.00126	-0.00127	2.72180
A5	2.61082	-0.00073	0.00000	-0.00057	-0.00058	2.61025
A6	2.83794	0.00579	0.00000	0.00276	0.00276	2.84070
A7	2.72294	-0.00132	0.00000	-0.00126	-0.00126	2.72168
A8	2.83802	0.00578	0.00000	0.00276	0.00276	2.84077
A9	2.14002	-0.02223	0.00000	-0.01474	-0.01473	2.12529
A10	2.05138	-0.00356	0.00000	-0.00159	-0.00160	2.04978
A11	2.09179	0.02579	0.00000	0.01633	0.01633	2.10812
A12	2.14000	-0.02223	0.00000	-0.01473	-0.01473	2.12527
A13	2.09180	0.02579	0.00000	0.01633	0.01633	2.10812
A14	2.05139	-0.00356	0.00000	-0.00160	-0.00160	2.04979
A15	1.57920	0.01854	0.00000	0.01917	0.01917	1.59836
A16	1.57920	0.12237	0.00000	0.09143	0.09143	1.67062
A17	1.57912	0.01844	0.00000	0.01910	0.01910	1.59822
A18	1.57912	0.12259	0.00000	0.09159	0.09159	1.67071
A19	1.91063	0.04245	0.00000	0.02951	0.02915	1.93978
A20	1.91063	0.04170	0.00000	0.02917	0.02879	1.93942
A21	1.91063	0.02621	0.00000	0.01811	0.01783	1.92846
A22	1.91063	-0.03546	0.00000	-0.02442	-0.02486	1.88577
A23	1.91063	-0.04238	0.00000	-0.02981	-0.03005	1.88058
A24	1.91063	-0.03251	0.00000	-0.02257	-0.02287	1.88777
A25	1.91063	0.04240	0.00000	0.02948	0.02912	1.93975
A26	1.91063	0.04170	0.00000	0.02918	0.02879	1.93942
A27	1.91063	0.02631	0.00000	0.01818	0.01790	1.92853
A28	1.91063	-0.03546	0.00000	-0.02442	-0.02486	1.88577
A29	1.91063	-0.04242	0.00000	-0.02984	-0.03008	1.88055
A30	1.91063	-0.03253	0.00000	-0.02258	-0.02288	1.88775
A31	2.93892	0.00659	0.00000	0.00402	0.00402	2.94295
A32	3.03849	0.01639	0.00000	0.01247	0.01247	3.05096
A33	2.93888	0.00660	0.00000	0.00402	0.00402	2.94290
A34	3.03851	0.01637	0.00000	0.01246	0.01246	3.05097
A35	3.15840	0.14090	0.00000	0.11059	0.11059	3.26899
A36	3.15824	0.14103	0.00000	0.11069	0.11069	3.26894
A37	3.14142	-0.00109	0.00000	-0.00092	-0.00090	3.14052
A38	3.14207	0.00357	0.00000	0.00317	0.00319	3.14526
A39	3.14159	-0.00110	0.00000	-0.00092	-0.00090	3.14069
A40	3.14202	0.00358	0.00000	0.00319	0.00320	3.14522
A41	3.14159	0.01993	0.00000	0.01671	0.01671	3.15830

A42	3.14159	0.01990	0.00000	0.01669	0.01669	3.15828
D1	0.00041	0.00012	0.00000	0.00013	0.00014	0.00054
D2	-0.00084	-0.00041	0.00000	-0.00033	-0.00032	-0.00116
D3	0.00005	0.00050	0.00000	0.00046	0.00046	0.00051
D4	0.00034	0.00012	0.00000	0.00013	0.00014	0.00048
D5	0.00119	0.00139	0.00000	0.00118	0.00117	0.00236
D6	0.00013	0.00051	0.00000	0.00046	0.00046	0.00059
D7	-0.00170	-0.00076	0.00000	-0.00066	-0.00063	-0.00233
D8	3.13987	0.00381	0.00000	0.00344	0.00340	-3.13991
D9	0.00100	0.00139	0.00000	0.00118	0.00117	0.00217
D10	-0.00135	-0.00075	0.00000	-0.00065	-0.00062	-0.00197
D11	3.14022	0.00380	0.00000	0.00344	0.00340	-3.13957
D12	0.00089	-0.00350	0.00000	-0.00307	-0.00307	-0.00217
D13	-3.14052	-0.00563	0.00000	-0.00498	-0.00499	3.13768
D14	-3.14055	-0.00565	0.00000	-0.00500	-0.00501	3.13763
D15	0.00123	-0.00777	0.00000	-0.00691	-0.00693	-0.00570
D16	2.57456	-0.00053	0.00000	-0.00048	-0.00049	2.57406
D17	-0.56718	0.00151	0.00000	0.00135	0.00137	-0.56581
D18	-0.56357	0.00147	0.00000	0.00132	0.00134	-0.56223
D19	2.57820	-0.00054	0.00000	-0.00049	-0.00050	2.57769
D20	-1.76034	0.00008	0.00000	0.00063	0.00048	-1.75986
D21	0.33406	0.00818	0.00000	0.00666	0.00677	0.34083
D22	2.42845	0.00995	0.00000	0.00798	0.00802	2.43647
D23	-1.76517	0.00004	0.00000	0.00060	0.00044	-1.76473
D24	0.32923	0.00811	0.00000	0.00661	0.00672	0.33594
D25	2.42362	0.00992	0.00000	0.00795	0.00799	2.43161

Item	Value	Threshold	Converged?
Maximum Force	0.539715	0.000450	NO
RMS Force	0.086105	0.000300	NO
Maximum Displacement	0.563949	0.001800	NO
RMS Displacement	0.133602	0.001200	NO

Predicted change in Energy=-1.911209D-01
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 18:22:04 2026, MaxMem= 805306368 cpu: 0.6 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.417565	0.673891	-0.008911
2	6	0	3.743655	1.693991	-0.023096
3	6	0	4.417616	-0.674004	0.009236
4	6	0	2.534033	2.286466	-0.031512
5	6	0	3.743561	-1.694010	0.023299

6	6	0	1.314612	2.330013	-0.032122
7	6	0	2.533968	-2.286541	0.031540
8	6	0	0.013659	1.976742	-0.026146
9	6	0	1.314547	-2.330003	0.031951
10	6	0	-1.073704	1.432887	-0.016366
11	6	0	0.013591	-1.976733	0.025824
12	6	0	-2.263112	0.696360	-0.008618
13	6	0	-1.073741	-1.432835	0.016129
14	6	0	-2.263142	-0.696262	0.008430
15	6	0	-3.495403	1.430494	-0.021128
16	6	0	-3.495420	-1.430321	0.020924
17	7	0	-4.460416	2.170691	0.032888
18	7	0	-4.460436	-2.170661	-0.032592
19	1	0	-4.384929	2.919454	-0.645125
20	1	0	-5.311683	1.669617	-0.150280
21	1	0	-4.384048	-2.919937	0.644765
22	1	0	-5.311524	-1.669893	0.151933
23	1	0	-4.533165	2.590938	0.949217
24	1	0	-3.986227	0.655097	-0.592366
25	1	0	-3.987143	-0.653115	0.588851
26	1	0	-4.534201	-2.590248	-0.949151

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.222686	0.000000			
3	C	1.348016	2.462249	0.000000		
4	C	2.479638	1.346954	3.509120	0.000000	
5	C	2.462168	3.388319	1.222686	4.160547	0.000000
6	C	3.517329	2.510948	4.319081	1.220198	4.700599
7	C	3.509092	4.160645	2.479698	4.573442	1.346950
8	C	4.592614	3.740699	5.140286	2.539338	5.233453
9	C	4.319001	4.700652	3.517370	4.775245	2.510911
10	C	5.543479	4.824434	5.881686	3.707369	5.743265
11	C	5.140233	5.233544	4.592692	4.952855	3.740670
12	C	6.680714	6.089066	6.819849	5.053865	6.464906
13	C	5.881612	5.743335	5.543544	5.181843	4.824382
14	C	6.819785	6.464976	6.680795	5.648995	6.089023
15	C	7.949066	7.243852	8.188144	6.089900	7.884611
16	C	8.188035	7.884635	7.949106	7.083188	7.243782
17	N	9.003372	8.218100	9.322677	6.995703	9.068696
18	N	9.322604	9.068779	9.003418	8.293888	8.218022
19	H	9.106658	8.243941	9.530264	6.974899	9.370335
20	H	9.781090	9.056264	10.008859	7.870823	9.661344
21	H	9.529495	9.369842	9.105900	8.684689	8.243006
22	H	10.008714	9.661399	9.781019	8.788583	9.056031
23	H	9.203730	8.381865	9.573918	7.141416	9.366018
24	H	8.424043	7.820131	8.529538	6.744606	8.102282

25	H	8.529794	8.102384	8.424747	7.179953	7.820940
26	H	9.574590	9.366707	9.204648	8.636222	8.382735

		6	7	8	9	10
6	C	0.000000				
7	C	4.775297	0.000000			
8	C	1.348078	4.952865	0.000000		
9	C	4.660457	1.220196	4.499304	0.000000	
10	C	2.551300	5.181866	1.215826	4.457063	0.000000
11	C	4.499342	2.539353	3.953816	1.348081	3.579035
12	C	3.933126	5.649008	2.612158	4.686167	1.399008
13	C	4.457083	3.707373	3.579029	2.551290	2.865906
14	C	4.686182	5.053888	3.511405	3.933131	2.438986
15	C	4.893413	7.083251	3.551327	6.105716	2.421705
16	C	6.105680	6.089888	4.891209	4.893396	3.750208
17	N	5.777591	8.293873	4.478666	7.321642	3.466497
18	N	7.321697	6.995658	6.100699	5.777541	4.945278
19	H	5.762636	8.685125	4.540861	7.778127	3.683671
20	H	6.660170	8.788543	5.335635	7.741905	4.246698
21	H	7.777845	6.973965	6.615695	5.761731	5.508407
22	H	7.742016	7.870610	6.456566	6.659951	5.254968
23	H	5.935285	8.635758	4.690648	7.697583	3.773766
24	H	5.587317	7.180212	4.250464	6.115456	3.069125
25	H	6.115003	6.745633	4.827089	5.588381	3.633982
26	H	7.697956	7.142340	6.510943	5.936172	5.388019

		11	12	13	14	15
11	C	0.000000				
12	C	3.511408	0.000000			
13	C	1.215816	2.438993	0.000000		
14	C	2.612168	1.392726	1.399026	0.000000	
15	C	4.891261	1.434451	3.750265	2.458136	0.000000
16	C	3.551302	2.458095	2.421684	1.434402	2.861125
17	N	6.100649	2.646417	4.945225	3.612206	1.217399
18	N	4.478609	3.612288	3.466477	2.646439	3.728236
19	H	6.615874	3.138375	5.508507	4.242937	1.843266
20	H	6.456425	3.203293	5.254813	3.862147	1.836501
21	H	4.540039	4.242981	3.683040	3.138136	4.489917
22	H	5.335438	3.862351	4.246580	3.203309	3.597312
23	H	6.510704	3.108057	5.387859	4.104116	1.834435
24	H	4.827756	1.819778	3.634873	2.270716	1.080955
25	H	4.251451	2.269436	3.069835	1.819596	2.226053
26	H	4.691417	4.104174	3.774408	3.108353	4.255197

		16	17	18	19	20
16	C	0.000000				
17	N	3.728089	0.000000			
18	N	1.217466	4.341846	0.000000		
19	H	4.489476	1.012940	5.127395	0.000000	
20	H	3.596907	1.004630	3.935252	1.632740	0.000000
21	H	1.843310	5.127838	1.012946	5.980160	4.749380

22	H	1.836517	3.935561	1.004574	4.749315	3.353157
23	H	4.255487	1.010722	4.862311	1.634571	1.632120
24	H	2.228449	1.706700	2.919440	2.299796	1.726709
25	H	1.080918	2.916670	1.706793	3.800550	2.774132
26	H	1.834542	4.861727	1.010730	5.520103	4.403308

		21	22	23	24	25
21	H	0.000000				
22	H	1.632698	0.000000			
23	H	5.521293	4.404111	0.000000		
24	H	3.803895	2.777764	2.534384	0.000000	
25	H	2.301986	1.725897	3.309363	1.762581	0.000000
26	H	1.634567	1.632075	5.518016	3.310564	2.533221

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=0 Diff= 8.39D-03
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.727598	-0.673990	0.003907
2	6	0	4.053672	-1.694157	0.010443
3	6	0	4.727671	0.674003	-0.004146
4	6	0	2.844039	-2.286659	0.014404
5	6	0	4.053632	1.694097	-0.010580
6	6	0	1.624618	-2.330190	0.014669
7	6	0	2.844049	2.286692	-0.014403
8	6	0	0.323671	-1.976863	0.011319
9	6	0	1.624628	2.330176	-0.014507
10	6	0	-0.763683	-1.432932	0.005595
11	6	0	0.323667	1.976891	-0.011045
12	6	0	-1.953079	-0.696349	0.003344
13	6	0	-0.763674	1.432953	-0.005440
14	6	0	-1.953087	0.696362	-0.003275
15	6	0	-3.185382	-1.430536	0.010338
16	6	0	-3.185352	1.430514	-0.010291
17	7	0	-4.150407	-2.170292	-0.049235
18	7	0	-4.150358	2.170449	0.048752
19	1	0	-4.074942	-2.924112	0.623154
20	1	0	-5.001668	-1.670590	0.137668
21	1	0	-4.073947	2.924774	-0.622973
22	1	0	-5.001451	1.671090	-0.139530

```
    23        1        0     -4.223148   -2.583665   -0.968686
    24        1        0     -3.676203   -0.659430    0.587358
    25        1        0     -3.677080    0.657591   -0.584030
    26        1        0     -4.224131    2.583161    0.968427
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.7097806           0.2331226           0.1759120
 Leave Link  202 at Fri Sep 25 18:22:04 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1007.2555933825 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0147270021 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1007.2408663803 Hartrees.
 Leave Link  301 at Fri Sep 25 18:22:04 2026, MaxMem=    805306368 cpu:                  0.4 elap:
0.1
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   22941 LenP2D=   51382.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.78D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=           5 IRanWt=          -1 IRanGd=           0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=           0 NUsed=           0 NTot=          32
 NSgBfM=   682   681   682   682   682 MxSgAt=    26 MxSgA2=    26.
 Leave Link  302 at Fri Sep 25 18:22:05 2026, MaxMem=    805306368 cpu:                 10.5 elap:
1.8
 (Enter /home/user/gauss16/g16/l303.exe)
```

Supporting Information file

DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 18:22:06 2026, MaxMem= 805306368 cpu: 1.1 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 -0.000000 0.000000
Rot= 1.000000 0.000136 0.000001 0.000001 Ang= 0.02 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.636010149302
Leave Link 401 at Fri Sep 25 18:22:22 2026, MaxMem= 805306368 cpu: 95.4 elap: 15.9
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.043016403311
DIIS: error= 5.03D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.043016403311 IErMin= 1 ErrMin= 5.03D-03
ErrMax= 5.03D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.64D-02 BMatP= 3.64D-02
IDIUse=3 WtCom= 9.50D-01 WtEn= 5.03D-02

Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.608 Goal=   None   Shift=   0.000
GapD=   0.608 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=1.62D-02 MaxDP=6.21D-01   OVMax= 3.19D-02

Cycle   2 Pass 0 IDiag 1:
RMSU= 1.61D-02   CP: 1.24D+00
E= -723.072241460289   Delta-E=   -0.029225056978 Rises=F Damp=F
DIIS: error= 1.08D-03 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.072241460289   IErMin= 2 ErrMin= 1.08D-03
ErrMax= 1.08D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.43D-03 BMatP= 3.64D-02
IDIUse=3 WtCom= 9.89D-01 WtEn= 1.08D-02
Coeff-Com: -0.156D-01 0.102D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.154D-01 0.102D+01
Gap=   0.190 Goal=   None   Shift=   0.000
RMSDP=3.76D-02 MaxDP=2.39D+00 DE=-2.92D-02 OVMax= 1.77D-02

Cycle   3 Pass 0 IDiag 1:
RMSU= 3.02D-02   CP: 1.80D+00 2.36D+00
E= -723.073952230747   Delta-E=   -0.001710770458 Rises=F Damp=F
DIIS: error= 1.34D-02 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -723.073952230747   IErMin= 2 ErrMin= 1.08D-03
ErrMax= 1.34D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.32D-03 BMatP= 1.43D-03
IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.000D+00 0.000D+00 0.100D+01
Gap=   -1.332 Goal=   None   Shift=   0.000
RMSDP=8.19D+02 MaxDP=3.17D+04 DE=-1.71D-03 OVMax= 9.85D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle   4 Pass 1 IDiag 1:
E= -723.072881712616   Delta-E=   0.001070518131 Rises=F Damp=F
DIIS: error= 2.43D-03 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -723.072881712616   IErMin= 1 ErrMin= 2.43D-03
ErrMax= 2.43D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-03 BMatP= 1.44D-03
IDIUse=3 WtCom= 9.76D-01 WtEn= 2.43D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.946 Goal=   None   Shift=   0.000
GapD=   0.946 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=4.26D-02 MaxDP=2.50D+00 DE= 1.07D-03 OVMax= 1.54D-02

Cycle   5 Pass 1 IDiag 1:

RMSU= 8.78D-03 CP: 1.83D-01
E= -723.073034541228 Delta-E= -0.000152828612 Rises=F Damp=F
DIIS: error= 1.49D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.073034541228 IErMin= 2 ErrMin= 1.49D-03
ErrMax= 1.49D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-03 BMatP= 1.44D-03
IDIUse=3 WtCom= 9.85D-01 WtEn= 1.49D-02
Coeff-Com: 0.488D+00 0.512D+00
Coeff-En: 0.464D+00 0.536D+00
Coeff: 0.488D+00 0.512D+00
Gap= 0.185 Goal= None Shift= 0.000
RMSDP=1.09D-03 MaxDP=7.39D-02 DE=-1.53D-04 OVMax= 1.03D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 4.69D-04 CP: 1.64D-01 9.86D-01
E= -723.074209815065 Delta-E= -0.001175273836 Rises=F Damp=F
DIIS: error= 5.20D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.074209815065 IErMin= 3 ErrMin= 5.20D-04
ErrMax= 5.20D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.01D-05 BMatP= 1.33D-03
IDIUse=3 WtCom= 9.95D-01 WtEn= 5.20D-03
Coeff-Com: 0.590D-01 0.202D+00 0.739D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.587D-01 0.201D+00 0.741D+00
Gap= 0.187 Goal= None Shift= 0.000
RMSDP=9.33D-04 MaxDP=6.44D-02 DE=-1.18D-03 OVMax= 4.01D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.47D-04 CP: 1.49D-01 9.69D-01 1.90D+00
E= -723.074274377655 Delta-E= -0.000064562590 Rises=F Damp=F
DIIS: error= 3.42D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.074274377655 IErMin= 4 ErrMin= 3.42D-04
ErrMax= 3.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.15D-05 BMatP= 8.01D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.42D-03
Coeff-Com: -0.218D-01 0.663D-01 0.470D+00 0.485D+00
Coeff-En: 0.000D+00 0.000D+00 0.241D+00 0.759D+00
Coeff: -0.217D-01 0.660D-01 0.469D+00 0.486D+00
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=1.51D-04 MaxDP=1.06D-02 DE=-6.46D-05 OVMax= 2.47D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 5.75D-05 CP: 1.46D-01 9.69D-01 2.05D+00 1.33D+00
E= -723.074313992477 Delta-E= -0.000039614821 Rises=F Damp=F
DIIS: error= 3.60D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.074313992477 IErMin= 5 ErrMin= 3.60D-05
ErrMax= 3.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.17D-07 BMatP= 3.15D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.853D-02-0.362D-02 0.106D-01 0.531D-01 0.948D+00
Coeff: -0.853D-02-0.362D-02 0.106D-01 0.531D-01 0.948D+00
Gap= 0.186 Goal= None Shift= 0.000

RMSDP=5.87D-05 MaxDP=3.41D-03 DE=-3.96D-05 OVMax= 1.43D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 2.81D-05 CP: 1.46D-01 9.68D-01 2.09D+00 1.56D+00 1.59D+00
E= -723.074317242493 Delta-E= -0.000003250016 Rises=F Damp=F
DIIS: error= 2.04D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.074317242493 IErMin= 6 ErrMin= 2.04D-05
ErrMax= 2.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.29D-07 BMatP= 6.17D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.368D-02-0.185D-01-0.132D+00-0.129D+00 0.295D+00 0.980D+00
Coeff: 0.368D-02-0.185D-01-0.132D+00-0.129D+00 0.295D+00 0.980D+00
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=5.95D-05 MaxDP=2.54D-03 DE=-3.25D-06 OVMax= 1.23D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 8.99D-06 CP: 1.47D-01 9.70D-01 2.06D+00 1.67D+00 2.04D+00
CP: 1.84D+00
E= -723.074318640136 Delta-E= -0.000001397643 Rises=F Damp=F
DIIS: error= 2.44D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.074318640136 IErMin= 6 ErrMin= 2.04D-05
ErrMax= 2.44D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-07 BMatP= 2.29D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.368D-02-0.109D-01-0.841D-01-0.903D-01 0.397D-01 0.609D+00
Coeff-Com: 0.533D+00
Coeff: 0.368D-02-0.109D-01-0.841D-01-0.903D-01 0.397D-01 0.609D+00
Coeff: 0.533D+00
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=3.42D-05 MaxDP=2.03D-03 DE=-1.40D-06 OVMax= 4.12D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 2.32D-06 CP: 1.48D-01 9.70D-01 2.03D+00 1.69D+00 2.19D+00
CP: 2.13D+00 1.69D+00
E= -723.074318963816 Delta-E= -0.000000323680 Rises=F Damp=F
DIIS: error= 7.29D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.074318963816 IErMin= 8 ErrMin= 7.29D-06
ErrMax= 7.29D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-08 BMatP= 1.21D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.105D-02 0.548D-02 0.393D-01 0.380D-01-0.963D-01-0.330D+00
Coeff-Com: 0.253D-01 0.132D+01
Coeff: -0.105D-02 0.548D-02 0.393D-01 0.380D-01-0.963D-01-0.330D+00
Coeff: 0.253D-01 0.132D+01
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=6.00D-05 MaxDP=3.75D-03 DE=-3.24D-07 OVMax= 5.30D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.36D-06 CP: 1.49D-01 9.72D-01 1.98D+00 1.69D+00 2.39D+00
CP: 2.50D+00 2.96D+00 3.00D+00
E= -723.074319127735 Delta-E= -0.000000163919 Rises=F Damp=F

DIIS: error= 2.75D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.074319127735 IErMin= 9 ErrMin= 2.75D-06
ErrMax= 2.75D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.69D-09 BMatP= 1.29D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.108D-02 0.412D-02 0.309D-01 0.324D-01-0.451D-01-0.242D+00
Coeff-Com: -0.884D-01 0.525D+00 0.784D+00
Coeff: -0.108D-02 0.412D-02 0.309D-01 0.324D-01-0.451D-01-0.242D+00
Coeff: -0.884D-01 0.525D+00 0.784D+00
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=1.58D-05 MaxDP=9.29D-04 DE=-1.64D-07 OVMax= 1.69D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 3.80D-06 CP: 1.49D-01 9.72D-01 1.96D+00 1.69D+00 2.44D+00
CP: 2.61D+00 3.00D+00 3.00D+00 1.55D+00
E= -723.074319151299 Delta-E= -0.000000023565 Rises=F Damp=F
DIIS: error= 1.42D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.074319151299 IErMin=10 ErrMin= 1.42D-06
ErrMax= 1.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.91D-10 BMatP= 3.69D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.127D-03-0.470D-04 0.714D-03 0.196D-02 0.113D-01 0.286D-02
Coeff-Com: -0.456D-01-0.201D+00 0.329D+00 0.901D+00
Coeff: -0.127D-03-0.470D-04 0.714D-03 0.196D-02 0.113D-01 0.286D-02
Coeff: -0.456D-01-0.201D+00 0.329D+00 0.901D+00
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=5.81D-06 MaxDP=2.62D-04 DE=-2.36D-08 OVMax= 9.79D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 6.10D-07 CP: 1.49D-01 9.73D-01 1.96D+00 1.69D+00 2.47D+00
CP: 2.67D+00 3.00D+00 3.00D+00 1.87D+00 1.57D+00
E= -723.074319157525 Delta-E= -0.000000006225 Rises=F Damp=F
DIIS: error= 1.18D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.074319157525 IErMin=11 ErrMin= 1.18D-06
ErrMax= 1.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.55D-10 BMatP= 9.91D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.207D-03-0.110D-02-0.751D-02-0.728D-02 0.169D-01 0.643D-01
Coeff-Com: -0.837D-03-0.240D+00-0.196D-01 0.508D+00 0.687D+00
Coeff: 0.207D-03-0.110D-02-0.751D-02-0.728D-02 0.169D-01 0.643D-01
Coeff: -0.837D-03-0.240D+00-0.196D-01 0.508D+00 0.687D+00
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=1.34D-06 MaxDP=5.19D-05 DE=-6.23D-09 OVMax= 3.44D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.17D-07 CP: 1.49D-01 9.73D-01 1.96D+00 1.69D+00 2.48D+00
CP: 2.69D+00 3.00D+00 3.00D+00 1.96D+00 1.73D+00
CP: 1.69D+00
E= -723.074319158519 Delta-E= -0.000000000995 Rises=F Damp=F
DIIS: error= 2.51D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.074319158519 IErMin=12 ErrMin= 2.51D-07

ErrMax= 2.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.41D-11 BMatP= 3.55D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.963D-04-0.381D-03-0.278D-02-0.293D-02 0.365D-02 0.237D-01
Coeff-Com: 0.751D-02-0.544D-01-0.659D-01 0.256D-01 0.240D+00 0.826D+00
Coeff: 0.963D-04-0.381D-03-0.278D-02-0.293D-02 0.365D-02 0.237D-01
Coeff: 0.751D-02-0.544D-01-0.659D-01 0.256D-01 0.240D+00 0.826D+00
Gap=   0.186 Goal=   None   Shift=   0.000
RMSDP=6.32D-07 MaxDP=2.52D-05 DE=-9.95D-10 OVMax= 1.22D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 6.99D-08   CP: 1.49D-01 9.73D-01 1.96D+00 1.69D+00 2.48D+00
               CP: 2.70D+00 3.00D+00 3.00D+00 2.00D+00 1.78D+00
               CP: 2.01D+00 1.89D+00
E= -723.074319158665   Delta-E=   -0.000000000146 Rises=F Damp=F
DIIS: error= 1.26D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.074319158665   IErMin=13 ErrMin= 1.26D-07
ErrMax= 1.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.41D-12 BMatP= 3.41D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.141D-04 0.101D-03 0.661D-03 0.615D-03-0.236D-02-0.534D-02
Coeff-Com: 0.215D-02 0.284D-01-0.912D-02-0.800D-01-0.675D-01 0.189D+00
Coeff-Com: 0.944D+00
Coeff: -0.141D-04 0.101D-03 0.661D-03 0.615D-03-0.236D-02-0.534D-02
Coeff: 0.215D-02 0.284D-01-0.912D-02-0.800D-01-0.675D-01 0.189D+00
Coeff: 0.944D+00
Gap=   0.186 Goal=   None   Shift=   0.000
RMSDP=3.91D-07 MaxDP=1.62D-05 DE=-1.46D-10 OVMax= 4.43D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 3.38D-08   CP: 1.49D-01 9.73D-01 1.96D+00 1.69D+00 2.48D+00
               CP: 2.70D+00 3.00D+00 3.00D+00 2.01D+00 1.79D+00
               CP: 2.11D+00 2.46D+00 1.82D+00
E= -723.074319158660   Delta-E=   0.000000000005 Rises=F Damp=F
DIIS: error= 6.67D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.074319158665   IErMin=14 ErrMin= 6.67D-08
ErrMax= 6.67D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.63D-13 BMatP= 4.41D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.194D-04 0.915D-04 0.651D-03 0.659D-03-0.135D-02-0.532D-02
Coeff-Com: -0.436D-03 0.176D-01 0.774D-02-0.309D-01-0.605D-01-0.607D-01
Coeff-Com: 0.323D+00 0.809D+00
Coeff: -0.194D-04 0.915D-04 0.651D-03 0.659D-03-0.135D-02-0.532D-02
Coeff: -0.436D-03 0.176D-01 0.774D-02-0.309D-01-0.605D-01-0.607D-01
Coeff: 0.323D+00 0.809D+00
Gap=   0.186 Goal=   None   Shift=   0.000
RMSDP=1.57D-07 MaxDP=8.12D-06 DE= 5.00D-12 OVMax= 1.80D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.25D-08   CP: 1.49D-01 9.73D-01 1.96D+00 1.69D+00 2.48D+00
               CP: 2.71D+00 3.00D+00 3.00D+00 2.02D+00 1.80D+00

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               CP:  2.13D+00  2.66D+00  2.16D+00  1.55D+00
E= -723.074319158677     Delta-E=       -0.000000000016 Rises=F Damp=F
DIIS: error= 3.78D-08 at cycle  15 NSaved=  15.
NSaved=15 IEnMin=15 EnMin= -723.074319158677     IErMin=15 ErrMin= 3.78D-08
ErrMax= 3.78D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-13 BMatP= 9.63D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.244D-05-0.188D-04-0.119D-03-0.108D-03 0.448D-03 0.949D-03
Coeff-Com: -0.467D-03-0.529D-02 0.232D-02 0.149D-01 0.107D-01-0.391D-01
Coeff-Com: -0.190D+00 0.188D-01 0.119D+01
Coeff:      0.244D-05-0.188D-04-0.119D-03-0.108D-03 0.448D-03 0.949D-03
Coeff:     -0.467D-03-0.529D-02 0.232D-02 0.149D-01 0.107D-01-0.391D-01
Coeff:     -0.190D+00 0.188D-01 0.119D+01
Gap=     0.186 Goal=   None    Shift=    0.000
RMSDP=9.23D-08 MaxDP=4.76D-06 DE=-1.61D-11 OVMax= 1.55D-06

Cycle  19  Pass 1  IDiag  1:
RMSU=  6.53D-09    CP:  1.49D-01  9.73D-01  1.96D+00  1.69D+00  2.48D+00
               CP:  2.71D+00  3.00D+00  3.00D+00  2.02D+00  1.80D+00
               CP:  2.14D+00  2.75D+00  2.34D+00  2.05D+00  2.44D+00
E= -723.074319158680     Delta-E=       -0.000000000004 Rises=F Damp=F
DIIS: error= 1.48D-08 at cycle  16 NSaved=  16.
NSaved=16 IEnMin=16 EnMin= -723.074319158680     IErMin=16 ErrMin= 1.48D-08
ErrMax= 1.48D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.51D-14 BMatP= 1.57D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.434D-05-0.224D-04-0.154D-03-0.154D-03 0.370D-03 0.124D-02
Coeff-Com: -0.285D-04-0.470D-02-0.851D-03 0.936D-02 0.143D-01 0.416D-02
Coeff-Com: -0.110D+00-0.148D+00 0.302D+00 0.933D+00
Coeff:      0.434D-05-0.224D-04-0.154D-03-0.154D-03 0.370D-03 0.124D-02
Coeff:     -0.285D-04-0.470D-02-0.851D-03 0.936D-02 0.143D-01 0.416D-02
Coeff:     -0.110D+00-0.148D+00 0.302D+00 0.933D+00
Gap=     0.186 Goal=   None    Shift=    0.000
RMSDP=2.85D-08 MaxDP=1.62D-06 DE=-3.64D-12 OVMax= 8.46D-07

Cycle  20  Pass 1  IDiag  1:
RMSU=  5.28D-09    CP:  1.49D-01  9.73D-01  1.96D+00  1.69D+00  2.48D+00
               CP:  2.71D+00  3.00D+00  3.00D+00  2.02D+00  1.80D+00
               CP:  2.14D+00  2.77D+00  2.39D+00  2.25D+00  3.00D+00
               CP:  2.07D+00
E= -723.074319158684     Delta-E=       -0.000000000004 Rises=F Damp=F
DIIS: error= 1.00D-08 at cycle  17 NSaved=  17.
NSaved=17 IEnMin=17 EnMin= -723.074319158684     IErMin=17 ErrMin= 1.00D-08
ErrMax= 1.00D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-14 BMatP= 4.51D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.393D-06 0.374D-05 0.236D-04 0.179D-04-0.974D-04-0.186D-03
Coeff-Com:  0.115D-03 0.120D-02-0.640D-03-0.357D-02-0.214D-02 0.120D-01
Coeff-Com:  0.429D-01-0.134D-01-0.310D+00 0.375D-01 0.124D+01
Coeff:     -0.393D-06 0.374D-05 0.236D-04 0.179D-04-0.974D-04-0.186D-03
Coeff:      0.115D-03 0.120D-02-0.640D-03-0.357D-02-0.214D-02 0.120D-01
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Coeff: 0.429D-01-0.134D-01-0.310D+00 0.375D-01 0.124D+01
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=1.55D-08 MaxDP=7.98D-07 DE=-3.87D-12 OVMax= 7.72D-07

Cycle 21 Pass 1 IDiag 1:
RMSU= 3.83D-09 CP: 1.49D-01 9.73D-01 1.96D+00 1.69D+00 2.48D+00
CP: 2.71D+00 3.00D+00 3.00D+00 2.02D+00 1.80D+00
CP: 2.15D+00 2.78D+00 2.42D+00 2.38D+00 3.00D+00
CP: 3.00D+00 3.00D+00
E= -723.074319158679 Delta-E= 0.000000000005 Rises=F Damp=F
DIIS: error= 5.43D-09 at cycle 18 NSaved= 18.
NSaved=18 IEnMin=17 EnMin= -723.074319158684 IErMin=18 ErrMin= 5.43D-09
ErrMax= 5.43D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.46D-15 BMatP= 1.45D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Large coefficients: NSaved= 18 BigCof= 0.00 CofMax= 10.00 Det=-6.64D-15
Inversion failed. Reducing to 17 matrices.
Large coefficients: NSaved= 17 BigCof= 0.00 CofMax= 10.00 Det=-6.79D-15
Inversion failed. Reducing to 16 matrices.
Large coefficients: NSaved= 16 BigCof= 0.00 CofMax= 10.00 Det=-7.05D-15
Inversion failed. Reducing to 15 matrices.
Coeff-Com: -0.152D-05-0.300D-04-0.963D-05 0.828D-04 0.418D-03-0.384D-03
Coeff-Com: -0.169D-02-0.120D-02 0.502D-02 0.269D-01 0.119D-01-0.162D+00
Coeff-Com: -0.198D+00 0.504D+00 0.816D+00
Coeff: -0.152D-05-0.300D-04-0.963D-05 0.828D-04 0.418D-03-0.384D-03
Coeff: -0.169D-02-0.120D-02 0.502D-02 0.269D-01 0.119D-01-0.162D+00
Coeff: -0.198D+00 0.504D+00 0.816D+00
Gap= 0.186 Goal= None Shift= 0.000
RMSDP=7.92D-09 MaxDP=3.47D-07 DE= 4.55D-12 OVMax= 4.03D-07

SCF Done: E(RwB97XD) = -723.074319159 A.U. after 21 cycles
NFock= 21 Conv=0.79D-08 -V/T= 2.0018
KE= 7.217482640732D+02 PE=-3.696833757161D+03 EE= 1.244770307549D+03
Leave Link 502 at Fri Sep 25 18:43:15 2026, MaxMem= 805306368 cpu: 7518.0 elap: 1253.3
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 22941 LenP2D= 51382.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 18:43:16 2026, MaxMem= 805306368 cpu: 2.9 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 18:43:16 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)

Supporting Information file

Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 18:56:28 2026, MaxMem= 805306368 cpu: 4753.3 elap: 792.5
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-7.60252709D+00 3.05608766D-03-1.25104309D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.003107412	-0.001491652	0.000919931
2	6	-0.002619532	0.001269314	-0.000923146
3	6	0.003082144	0.001493812	-0.000920858
4	6	0.004803357	0.003401360	0.000546859
5	6	-0.002594679	-0.001276305	0.000926114
6	6	-0.004775299	-0.002627201	-0.000857982
7	6	0.004771162	-0.003390243	-0.000552873
8	6	0.005859815	0.007719318	-0.000452313
9	6	-0.004731487	0.002610900	0.000863351
10	6	0.005055930	-0.015210868	0.006845034
11	6	0.005797978	-0.007684433	0.000456096
12	6	0.015798833	0.075624890	0.029316148
13	6	0.005144165	0.015148357	-0.006856990
14	6	0.015688728	-0.075725276	-0.029132545
15	6	0.167875857	-0.272196057	-0.064961799
16	6	0.167734001	0.272467869	0.064608572
17	7	-0.141157868	0.186910780	0.044198402
18	7	-0.141078201	-0.187027689	-0.043880874
19	1	-0.022401746	0.037426948	-0.012524172
20	1	-0.019808812	0.008197104	0.001976752
21	1	-0.022365916	-0.037439140	0.012502788
22	1	-0.019713375	-0.008216122	-0.001950358
23	1	-0.017339560	0.026986048	0.015576213
24	1	0.005609671	-0.027502936	-0.015209035
25	1	0.005648541	0.027539456	0.015084109
26	1	-0.017391120	-0.027008237	-0.015597425

Cartesian Forces: Max 0.272467869 RMS 0.067073731

Supporting Information file

Leave Link 716 at Fri Sep 25 18:56:28 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.319074896 RMS 0.053125197
Search for a local minimum.
Step number 2 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .53125D-01 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2
DE= -1.77D-01 DEPred=-1.91D-01 R= 9.25D-01
TightC=F SS= 1.41D+00 RLast= 3.01D-01 DXNew= 5.0454D-01 9.0173D-01
Trust test= 9.25D-01 RLast= 3.01D-01 DXMaxT set to 5.05D-01
ITU= 1 0
Use linear search instead of GDIIS.
Linear search step of 0.600 exceeds DXMaxT= 0.505 but not scaled.
Quartic linear search produced a step of 2.00000.
Iteration 1 RMS(Cart)= 0.22418807 RMS(Int)= 0.01498790
Iteration 2 RMS(Cart)= 0.05661025 RMS(Int)= 0.00111470
Iteration 3 RMS(Cart)= 0.00160254 RMS(Int)= 0.00067237
Iteration 4 RMS(Cart)= 0.00000109 RMS(Int)= 0.00067237
Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00067237
ITry= 1 IFail=0 DXMaxC= 1.20D+00 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.31054	0.00346	0.00248	0.00000	0.00247	2.31302
R2	2.54738	0.00059	0.00096	0.00000	0.00095	2.54833
R3	2.54537	0.00079	0.00140	0.00000	0.00140	2.54677
R4	2.31054	0.00345	0.00248	0.00000	0.00247	2.31301
R5	2.30584	0.00519	0.00400	0.00000	0.00400	2.30984
R6	2.54537	0.00080	0.00141	0.00000	0.00141	2.54677
R7	2.54750	0.00048	0.00135	0.00000	0.00135	2.54885
R8	2.30584	0.00517	0.00399	0.00000	0.00399	2.30982
R9	2.29758	0.00914	0.00748	0.00000	0.00749	2.30506
R10	2.54750	0.00051	0.00137	0.00000	0.00137	2.54888
R11	2.64374	0.00571	0.00734	0.00000	0.00735	2.65109
R12	2.29756	0.00909	0.00744	0.00000	0.00745	2.30501
R13	2.63187	0.02786	0.03921	0.00000	0.03922	2.67109
R14	2.71072	0.00309	0.00766	0.00000	0.00766	2.71838
R15	2.64378	0.00577	0.00741	0.00000	0.00742	2.65119
R16	2.71063	0.00297	0.00750	0.00000	0.00750	2.71813
R17	2.30055	0.31907	0.26266	0.00000	0.26266	2.56321

R18	2.04271	0.02522	0.04140	0.00000	0.04140	2.08411
R19	2.30068	0.31903	0.26276	0.00000	0.26276	2.56344
R20	2.04264	0.02516	0.04126	0.00000	0.04126	2.08390
R21	1.91418	0.03438	0.04891	0.00000	0.04891	1.96309
R22	1.89848	0.01234	0.01750	0.00000	0.01750	1.91597
R23	1.90999	0.02659	0.04052	0.00000	0.04052	1.95051
R24	1.91419	0.03437	0.04893	0.00000	0.04893	1.96312
R25	1.89837	0.01225	0.01729	0.00000	0.01729	1.91566
R26	1.91000	0.02663	0.04055	0.00000	0.04055	1.95056
A1	2.55786	-0.00361	-0.00538	0.00000	-0.00543	2.55243
A2	2.61006	-0.00030	-0.00114	0.00000	-0.00118	2.60888
A3	2.55764	-0.00360	-0.00536	0.00000	-0.00541	2.55223
A4	2.72180	-0.00163	-0.00254	0.00000	-0.00256	2.71924
A5	2.61025	-0.00032	-0.00116	0.00000	-0.00120	2.60905
A6	2.84070	0.00474	0.00552	0.00000	0.00552	2.84622
A7	2.72168	-0.00162	-0.00252	0.00000	-0.00254	2.71914
A8	2.84077	0.00474	0.00551	0.00000	0.00551	2.84629
A9	2.12529	-0.01710	-0.02946	0.00000	-0.02942	2.09587
A10	2.04978	0.00235	-0.00320	0.00000	-0.00322	2.04656
A11	2.10812	0.01475	0.03265	0.00000	0.03263	2.14075
A12	2.12527	-0.01710	-0.02945	0.00000	-0.02941	2.09586
A13	2.10812	0.01475	0.03265	0.00000	0.03262	2.14075
A14	2.04979	0.00234	-0.00320	0.00000	-0.00322	2.04657
A15	1.59836	0.03966	0.03833	0.00000	0.03833	1.63669
A16	1.67062	0.07923	0.18285	0.00000	0.18285	1.85348
A17	1.59822	0.03964	0.03820	0.00000	0.03820	1.63643
A18	1.67071	0.07931	0.18318	0.00000	0.18318	1.85389
A19	1.93978	0.03127	0.05830	0.00000	0.05631	1.99609
A20	1.93942	0.01258	0.05757	0.00000	0.05538	1.99480
A21	1.92846	0.01965	0.03566	0.00000	0.03417	1.96263
A22	1.88577	-0.02062	-0.04972	0.00000	-0.05204	1.83373
A23	1.88058	-0.02764	-0.06010	0.00000	-0.06124	1.81934
A24	1.88777	-0.01854	-0.04573	0.00000	-0.04719	1.84057
A25	1.93975	0.03125	0.05824	0.00000	0.05625	1.99600
A26	1.93942	0.01252	0.05758	0.00000	0.05539	1.99481
A27	1.92853	0.01972	0.03579	0.00000	0.03430	1.96283
A28	1.88577	-0.02060	-0.04973	0.00000	-0.05205	1.83372
A29	1.88055	-0.02765	-0.06016	0.00000	-0.06130	1.81925
A30	1.88775	-0.01853	-0.04576	0.00000	-0.04722	1.84053
A31	2.94295	0.00432	0.00805	0.00000	0.00807	2.95101
A32	3.05096	0.01357	0.02495	0.00000	0.02499	3.07595
A33	2.94290	0.00432	0.00805	0.00000	0.00807	2.95097
A34	3.05097	0.01356	0.02493	0.00000	0.02497	3.07594
A35	3.26899	0.11889	0.22118	0.00000	0.22118	3.49017
A36	3.26894	0.11895	0.22139	0.00000	0.22139	3.49032
A37	3.14052	-0.00039	-0.00180	0.00000	-0.00172	3.13880
A38	3.14526	0.00308	0.00637	0.00000	0.00645	3.15171
A39	3.14069	-0.00039	-0.00181	0.00000	-0.00172	3.13896

A40	3.14522	0.00309	0.00640	0.00000	0.00647	3.15169
A41	3.15830	0.01717	0.03342	0.00000	0.03342	3.19172
A42	3.15828	0.01711	0.03337	0.00000	0.03337	3.19165
D1	0.00054	0.00038	0.00027	0.00000	0.00031	0.00086
D2	-0.00116	-0.00010	-0.00063	0.00000	-0.00058	-0.00174
D3	0.00051	0.00042	0.00092	0.00000	0.00092	0.00143
D4	0.00048	0.00038	0.00028	0.00000	0.00032	0.00080
D5	0.00236	0.00106	0.00234	0.00000	0.00231	0.00467
D6	0.00059	0.00042	0.00092	0.00000	0.00092	0.00151
D7	-0.00233	-0.00051	-0.00126	0.00000	-0.00111	-0.00344
D8	-3.13991	0.00267	0.00681	0.00000	0.00658	-3.13334
D9	0.00217	0.00106	0.00235	0.00000	0.00232	0.00449
D10	-0.00197	-0.00050	-0.00125	0.00000	-0.00110	-0.00307
D11	-3.13957	0.00266	0.00679	0.00000	0.00656	-3.13300
D12	-0.00217	-0.00274	-0.00613	0.00000	-0.00611	-0.00828
D13	3.13768	-0.00386	-0.00998	0.00000	-0.01002	3.12766
D14	3.13763	-0.00387	-0.01002	0.00000	-0.01006	3.12757
D15	-0.00570	-0.00498	-0.01386	0.00000	-0.01397	-0.01968
D16	2.57406	0.00222	-0.00099	0.00000	-0.00106	2.57300
D17	-0.56581	0.00332	0.00273	0.00000	0.00281	-0.56300
D18	-0.56223	0.00329	0.00267	0.00000	0.00275	-0.55948
D19	2.57769	0.00221	-0.00101	0.00000	-0.00109	2.57661
D20	-1.75986	0.00199	0.00096	0.00000	0.00012	-1.75974
D21	0.34083	0.00545	0.01355	0.00000	0.01416	0.35499
D22	2.43647	0.00343	0.01603	0.00000	0.01627	2.45274
D23	-1.76473	0.00198	0.00089	0.00000	0.00005	-1.76468
D24	0.33594	0.00540	0.01343	0.00000	0.01403	0.34998
D25	2.43161	0.00340	0.01598	0.00000	0.01622	2.44783

Item	Value	Threshold	Converged?
Maximum Force	0.319075	0.000450	NO
RMS Force	0.053125	0.000300	NO
Maximum Displacement	1.195207	0.001800	NO
RMS Displacement	0.276176	0.001200	NO

Predicted change in Energy=-1.232441D-01
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 18:56:28 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.394830	0.673553	-0.026679
2	6	0	3.714701	1.690349	-0.068089
3	6	0	4.394827	-0.673887	0.027288

4	6	0	2.500542	2.274745	-0.092132
5	6	0	3.714491	-1.690550	0.068509
6	6	0	1.278657	2.307207	-0.093092
7	6	0	2.500313	-2.274922	0.092263
8	6	0	-0.021700	1.949416	-0.075869
9	6	0	1.278435	-2.307232	0.092903
10	6	0	-1.115019	1.409263	-0.048181
11	6	0	-0.021913	-1.949357	0.075400
12	6	0	-2.328962	0.706411	-0.026821
13	6	0	-1.115147	-1.409099	0.047679
14	6	0	-2.329053	-0.706073	0.026263
15	6	0	-3.539969	1.481691	-0.067964
16	6	0	-3.540051	-1.481134	0.067234
17	7	0	-4.383542	2.534008	0.076286
18	7	0	-4.383320	-2.534017	-0.075818
19	1	0	-4.211578	3.315176	-0.586550
20	1	0	-5.363726	2.301696	-0.038794
21	1	0	-4.209691	-3.315188	0.586611
22	1	0	-5.363279	-2.302370	0.041017
23	1	0	-4.312132	2.971549	1.008393
24	1	0	-4.097467	0.715655	-0.632494
25	1	0	-4.098383	-0.713326	0.628304
26	1	0	-4.313352	-2.971488	-1.008096

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.223995	0.000000			
3	C	1.348521	2.461967	0.000000		
4	C	2.481215	1.347694	3.506709	0.000000	
5	C	2.461891	3.383658	1.223993	4.150066	0.000000
6	C	3.519057	2.513055	4.314154	1.222316	4.684172
7	C	3.506686	4.150159	2.481273	4.553402	1.347695
8	C	4.597388	3.745379	5.137905	2.543188	5.218173
9	C	4.314081	4.684225	3.519093	4.745767	2.513018
10	C	5.558792	4.837933	5.890977	3.717966	5.739916
11	C	5.137868	5.218269	4.597469	4.922792	3.745362
12	C	6.723872	6.123373	6.864218	5.078193	6.502141
13	C	5.890909	5.739983	5.558845	5.163667	4.837876
14	C	6.864166	6.502207	6.723957	5.676644	6.123349
15	C	7.975953	7.257670	8.222930	6.092396	7.918897
16	C	8.222762	7.918840	7.975934	7.114828	7.257564
17	N	8.973946	8.143349	9.346269	6.891023	9.133734
18	N	9.345952	9.133633	8.973660	8.397143	8.142899
19	H	9.020081	8.107697	9.505767	6.810249	9.397285
20	H	9.893452	9.099034	10.202343	7.864494	9.917840
21	H	9.503892	9.395745	9.018151	8.759867	8.105587
22	H	10.202028	9.917833	9.893067	9.099856	9.098406

23	H	9.064399	8.199410	9.490147	6.936080	9.329803
24	H	8.513982	7.892943	8.630481	6.801212	8.204140
25	H	8.630590	8.204077	8.514539	7.279656	7.893626
26	H	9.491150	9.330915	9.065504	8.648185	8.200375

		6	7	8	9	10
6	C	0.000000				
7	C	4.745809	0.000000			
8	C	1.348792	4.922789	0.000000		
9	C	4.618186	1.222305	4.453975	0.000000	
10	C	2.556953	5.163678	1.219786	4.422767	0.000000
11	C	4.454011	2.543207	3.901707	1.348809	3.534188
12	C	3.947386	5.676657	2.621245	4.702095	1.402895
13	C	4.422787	3.717955	3.534192	2.556936	2.819992
14	C	4.702093	5.078230	3.519366	3.947420	2.440096
15	C	4.888892	7.114972	3.549232	6.131789	2.426112
16	C	6.131654	6.092349	4.916090	4.888855	3.774718
17	N	5.669271	8.397233	4.403472	7.449555	3.458870
18	N	7.449546	6.890558	6.254990	5.668806	5.121719
19	H	5.603765	8.761248	4.436346	7.887545	3.675734
20	H	6.642607	9.099764	5.353757	8.085658	4.341432
21	H	7.886399	6.808135	6.759749	5.601719	5.683344
22	H	8.085883	7.863807	6.828163	6.641919	5.641975
23	H	5.736858	8.647205	4.541826	7.743261	3.711955
24	H	5.632647	7.280078	4.294634	6.210022	3.117292
25	H	6.209395	6.802111	4.919898	5.633592	3.723368
26	H	7.744186	6.937005	6.595652	5.737728	5.508335

		11	12	13	14	15
11	C	0.000000				
12	C	3.519380	0.000000			
13	C	1.219757	2.440140	0.000000		
14	C	2.621272	1.413482	1.402951	0.000000	
15	C	4.916235	1.438502	3.774891	2.502301	0.000000
16	C	3.549168	2.502186	2.426053	1.438371	2.965908
17	N	6.254948	2.751734	5.121652	3.836868	1.356390
18	N	4.403018	3.837077	3.458561	2.751692	4.103317
19	H	6.760679	3.265454	5.684092	4.482174	2.020311
20	H	6.827844	3.428537	5.641622	4.273189	1.999837
21	H	4.434447	4.481819	3.674212	3.264700	4.887437
22	H	5.353129	4.273692	4.341037	3.428543	4.201839
23	H	6.594830	3.183627	5.507610	4.292096	1.993604
24	H	4.920727	1.869368	3.724440	2.362745	1.102864
25	H	4.295473	2.361290	3.117840	1.868966	2.369539
26	H	4.542595	4.292744	3.712713	3.184249	4.616576

		16	17	18	19	20
16	C	0.000000				
17	N	4.102794	0.000000			
18	N	1.356514	5.070307	0.000000		
19	H	4.887020	1.038820	5.873960	0.000000	

20	H	4.200813	1.013889	4.934236	1.629302	0.000000
21	H	2.020378	5.873989	1.038839	6.733352	5.768215
22	H	1.999819	4.934742	1.013721	5.768629	4.604757
23	H	4.616089	1.032165	5.611759	1.634635	1.628236
24	H	2.371964	1.972464	3.309375	2.602430	2.114572
25	H	1.102753	3.306239	1.972788	4.209217	3.337134
26	H	1.993862	5.611710	1.032191	6.301603	5.463451

		21	22	23	24	25
21	H	0.000000				
22	H	1.629183	0.000000			
23	H	6.301703	5.463968	0.000000		
24	H	4.212660	3.341313	2.797794	0.000000	
25	H	2.604576	2.114221	3.710588	1.905675	0.000000
26	H	1.634615	1.628098	6.275820	3.712506	2.797019

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=0 Diff= 1.38D-02
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.723169	-0.674092	0.015169
2	6	0	4.042994	-1.691420	0.039001
3	6	0	4.723228	0.674079	-0.015537
4	6	0	2.828808	-2.276090	0.052912
5	6	0	4.042939	1.691333	-0.039231
6	6	0	1.606922	-2.308508	0.053268
7	6	0	2.828788	2.276082	-0.052940
8	6	0	0.306582	-1.950415	0.042176
9	6	0	1.606912	2.308454	-0.053066
10	6	0	-0.786713	-1.409815	0.023774
11	6	0	0.306547	1.950389	-0.041787
12	6	0	-2.000624	-0.706645	0.014504
13	6	0	-0.786712	1.409782	-0.023433
14	6	0	-2.000650	0.706546	-0.014196
15	6	0	-3.211667	-1.482464	0.042218
16	6	0	-3.211612	1.482252	-0.041828
17	7	0	-4.055281	-2.532097	-0.120201
18	7	0	-4.054839	2.532548	0.119342
19	1	0	-3.883375	-3.324596	0.529062
20	1	0	-5.035458	-2.301761	-0.001164

```
    21        1        0      -3.881152    3.325026   -0.529501
    22        1        0      -5.034804    2.302996   -0.001508
    23        1        0      -3.983856   -2.953491   -1.059717
    24        1        0      -3.769151   -0.726260    0.619864
    25        1        0      -3.769957    0.724266   -0.616086
    26        1        0      -3.984886    2.953862    1.059033
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6554870           0.2356552           0.1738479
 Leave Link  202 at Fri Sep 25 18:56:28 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy       993.6087618201 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.222036 cShort=  0.000000 cLong=
0.777964
  DFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.000000 cShort=  0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0140822130 Hartrees.
 Nuclear repulsion after empirical dispersion term =       993.5946796071 Hartrees.
 Leave Link  301 at Fri Sep 25 18:56:28 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   22863 LenP2D=   51056.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.86D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=           5 IRanWt=          -1 IRanGd=           0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=           0 NUsed=           0 NTot=          32
 NSgBfM=   681   681   681   681   681 MxSgAt=    26 MxSgA2=    26.
```

Supporting Information file

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 Leave Link  302 at Fri Sep 25 18:56:29 2026, MaxMem=    805306368 cpu:                5.7 elap:
1.0
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Sep 25 18:56:29 2026, MaxMem=    805306368 cpu:                0.8 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=    -0.000000    0.000000   -0.000000
       Rot=    0.999999    0.001422    0.000001    0.000007 Ang=   0.16 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Generating alternative initial guess.
 ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn=          5 AccDes=
0.00D+00
 Harris functional with IExCor= 4639 and IRadAn=       5 diagonalized for initial guess.
 HarFok:  IExCor= 4639 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Petite list used in FoFCou.
 Harris En= -691.858915319576
 Leave Link  401 at Fri Sep 25 18:56:40 2026, MaxMem=    805306368 cpu:               63.6 elap:
10.6
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.145434409145
 DIIS: error= 9.88D-03 at cycle   1 NSaved=   1.
```

NSaved= 1 IEnMin= 1 EnMin= -723.145434409145 IErMin= 1 ErrMin= 9.88D-03
ErrMax= 9.88D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-01 BMatP= 1.15D-01
IDIUse=3 WtCom= 9.01D-01 WtEn= 9.88D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.704 Goal= None Shift= 0.000
GapD= 0.704 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=9.14D-03 MaxDP=5.39D-01 OVMax= 6.29D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 8.20D-03 CP: 1.36D+00
E= -723.242891256894 Delta-E= -0.097456847749 Rises=F Damp=F
DIIS: error= 2.08D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.242891256894 IErMin= 2 ErrMin= 2.08D-03
ErrMax= 2.08D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.87D-03 BMatP= 1.15D-01
IDIUse=3 WtCom= 9.79D-01 WtEn= 2.08D-02
Coeff-Com: -0.350D-01 0.103D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.343D-01 0.103D+01
Gap= 0.190 Goal= None Shift= 0.000
RMSDP=1.49D-02 MaxDP=1.21D+00 DE=-9.75D-02 OVMax= 2.61D-02

Cycle 3 Pass 0 IDiag 1:
RMSU= 1.35D-02 CP: 1.60D+00 1.68D+00
E= -723.246820886652 Delta-E= -0.003929629758 Rises=F Damp=F
DIIS: error= 2.62D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.246820886652 IErMin= 2 ErrMin= 2.08D-03
ErrMax= 2.62D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-03 BMatP= 3.87D-03
IDIUse=3 WtCom= 9.74D-01 WtEn= 2.62D-02
Coeff-Com: -0.484D-01 0.501D+00 0.547D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.472D-01 0.488D+00 0.559D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=4.81D+02 MaxDP=2.33D+04 DE=-3.93D-03 OVMax= 9.70D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.246590138249 Delta-E= 0.000230748404 Rises=F Damp=F
DIIS: error= 2.48D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.246590138249 IErMin= 1 ErrMin= 2.48D-03
ErrMax= 2.48D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.09D-03 BMatP= 3.09D-03
IDIUse=3 WtCom= 9.75D-01 WtEn= 2.48D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.178 Goal= None Shift= 0.000

GapD= 0.178 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=1.70D-02 MaxDP=9.59D-01 DE= 2.31D-04 OVMax= 2.35D-02

Cycle 5 Pass 1 IDiag 1:
RMSU= 1.41D-02 CP: 6.35D-01
E= -723.246049153070 Delta-E= 0.000540985179 Rises=F Damp=F
DIIS: error= 2.55D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -723.246590138249 IErMin= 1 ErrMin= 2.48D-03
ErrMax= 2.55D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.83D-03 BMatP= 3.09D-03
IDIUse=3 WtCom= 1.65D-01 WtEn= 8.35D-01
Coeff-Com: 0.528D+00 0.472D+00
Coeff-En: 0.543D+00 0.457D+00
Coeff: 0.541D+00 0.459D+00
Gap= 0.182 Goal= None Shift= 0.000
RMSDP=5.88D-04 MaxDP=3.66D-02 DE= 5.41D-04 OVMax= 1.51D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 4.07D-04 CP: 6.27D-01 1.03D+00
E= -723.249569386540 Delta-E= -0.003520233470 Rises=F Damp=F
DIIS: error= 6.12D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.249569386540 IErMin= 3 ErrMin= 6.12D-04
ErrMax= 6.12D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.27D-05 BMatP= 3.09D-03
IDIUse=3 WtCom= 9.94D-01 WtEn= 6.12D-03
Coeff-Com: 0.149D+00 0.164D+00 0.687D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.148D+00 0.163D+00 0.689D+00
Gap= 0.184 Goal= None Shift= 0.000
RMSDP=6.03D-04 MaxDP=5.03D-02 DE=-3.52D-03 OVMax= 5.25D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.07D-04 CP: 6.15D-01 1.05D+00 1.68D+00
E= -723.249637051865 Delta-E= -0.000067665325 Rises=F Damp=F
DIIS: error= 4.21D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.249637051865 IErMin= 4 ErrMin= 4.21D-04
ErrMax= 4.21D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.24D-05 BMatP= 7.27D-05
IDIUse=3 WtCom= 9.96D-01 WtEn= 4.21D-03
Coeff-Com: -0.377D-01-0.131D-01 0.446D+00 0.604D+00
Coeff-En: 0.000D+00 0.000D+00 0.270D+00 0.730D+00
Coeff: -0.375D-01-0.130D-01 0.446D+00 0.605D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=5.00D-04 MaxDP=1.92D-02 DE=-6.77D-05 OVMax= 4.02D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.46D-04 CP: 6.17D-01 1.08D+00 2.11D+00 1.56D+00
E= -723.249699968488 Delta-E= -0.000062916623 Rises=F Damp=F
DIIS: error= 5.17D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.249699968488 IErMin= 5 ErrMin= 5.17D-05
ErrMax= 5.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-06 BMatP= 4.24D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.234D-01-0.185D-01 0.166D-01 0.994D-01 0.926D+00
Coeff: -0.234D-01-0.185D-01 0.166D-01 0.994D-01 0.926D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=1.95D-04 MaxDP=7.30D-03 DE=-6.29D-05 OVMax= 2.25D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 4.23D-05 CP: 6.20D-01 1.09D+00 2.24D+00 1.77D+00 1.45D+00
E= -723.249707036784 Delta-E= -0.000007068296 Rises=F Damp=F
DIIS: error= 3.42D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.249707036784 IErMin= 6 ErrMin= 3.42D-05
ErrMax= 3.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.92D-07 BMatP= 1.37D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.124D-03-0.336D-02-0.998D-01-0.107D+00 0.348D+00 0.862D+00
Coeff: 0.124D-03-0.336D-02-0.998D-01-0.107D+00 0.348D+00 0.862D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=1.47D-04 MaxDP=7.71D-03 DE=-7.07D-06 OVMax= 1.64D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.43D-05 CP: 6.23D-01 1.09D+00 2.28D+00 1.81D+00 1.80D+00
CP: 1.84D+00
E= -723.249709501114 Delta-E= -0.000002464330 Rises=F Damp=F
DIIS: error= 3.32D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.249709501114 IErMin= 7 ErrMin= 3.32D-05
ErrMax= 3.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-07 BMatP= 4.92D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.551D-02 0.225D-02-0.657D-01-0.898D-01 0.152D-01 0.545D+00
Coeff-Com: 0.588D+00
Coeff: 0.551D-02 0.225D-02-0.657D-01-0.898D-01 0.152D-01 0.545D+00
Coeff: 0.588D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=6.92D-05 MaxDP=4.26D-03 DE=-2.46D-06 OVMax= 7.36D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 3.52D-06 CP: 6.25D-01 1.09D+00 2.30D+00 1.79D+00 1.95D+00
CP: 2.28D+00 1.81D+00
E= -723.249710255316 Delta-E= -0.000000754202 Rises=F Damp=F
DIIS: error= 8.27D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.249710255316 IErMin= 8 ErrMin= 8.27D-06
ErrMax= 8.27D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.66D-08 BMatP= 2.60D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.102D-02 0.104D-02 0.112D-01 0.828D-02-0.771D-01-0.127D+00
Coeff-Com: 0.879D-01 0.109D+01
Coeff: 0.102D-02 0.104D-02 0.112D-01 0.828D-02-0.771D-01-0.127D+00
Coeff: 0.879D-01 0.109D+01
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=7.21D-05 MaxDP=4.12D-03 DE=-7.54D-07 OVMax= 6.56D-04

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Cycle  12  Pass 1  IDiag  1:
RMSU=  3.24D-06    CP:  6.27D-01  1.10D+00  2.32D+00  1.77D+00  2.10D+00
               CP:  2.67D+00  2.80D+00  2.62D+00
E= -723.249710528511     Delta-E=       -0.000000273195 Rises=F Damp=F
DIIS: error= 4.77D-06 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.249710528511     IErMin= 9 ErrMin= 4.77D-06
ErrMax= 4.77D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-08 BMatP= 2.66D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.128D-02-0.331D-03 0.251D-01 0.323D-01-0.375D-01-0.231D+00
Coeff-Com: -0.154D+00 0.505D+00 0.861D+00
Coeff:     -0.128D-02-0.331D-03 0.251D-01 0.323D-01-0.375D-01-0.231D+00
Coeff:     -0.154D+00 0.505D+00 0.861D+00
Gap=     0.183 Goal=   None    Shift=    0.000
RMSDP=4.37D-05 MaxDP=2.04D-03 DE=-2.73D-07 OVMax= 3.77D-04

Cycle  13  Pass 1  IDiag  1:
RMSU=  7.13D-06    CP:  6.28D-01  1.10D+00  2.34D+00  1.76D+00  2.18D+00
               CP:  2.89D+00  3.00D+00  3.00D+00  1.83D+00
E= -723.249710599762     Delta-E=       -0.000000071251 Rises=F Damp=F
DIIS: error= 2.08D-06 at cycle  10 NSaved=  10.
NSaved=10 IEnMin=10 EnMin= -723.249710599762     IErMin=10 ErrMin= 2.08D-06
ErrMax= 2.08D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-09 BMatP= 1.03D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.625D-03-0.313D-03 0.787D-02 0.114D-01-0.339D-02-0.679D-01
Coeff-Com: -0.704D-01 0.403D-01 0.303D+00 0.781D+00
Coeff:     -0.625D-03-0.313D-03 0.787D-02 0.114D-01-0.339D-02-0.679D-01
Coeff:     -0.704D-01 0.403D-01 0.303D+00 0.781D+00
Gap=     0.183 Goal=   None    Shift=    0.000
RMSDP=1.26D-05 MaxDP=5.31D-04 DE=-7.13D-08 OVMax= 1.08D-04

Cycle  14  Pass 1  IDiag  1:
RMSU=  8.36D-07    CP:  6.28D-01  1.10D+00  2.35D+00  1.76D+00  2.21D+00
               CP:  2.94D+00  3.00D+00  3.00D+00  2.20D+00  1.50D+00
E= -723.249710608926     Delta-E=       -0.000000009164 Rises=F Damp=F
DIIS: error= 1.87D-06 at cycle  11 NSaved=  11.
NSaved=11 IEnMin=11 EnMin= -723.249710608926     IErMin=11 ErrMin= 1.87D-06
ErrMax= 1.87D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 9.14D-10 BMatP= 1.79D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.239D-03-0.618D-04-0.752D-02-0.874D-02 0.163D-01 0.731D-01
Coeff-Com:  0.332D-01-0.225D+00-0.250D+00 0.516D+00 0.852D+00
Coeff:      0.239D-03-0.618D-04-0.752D-02-0.874D-02 0.163D-01 0.731D-01
Coeff:      0.332D-01-0.225D+00-0.250D+00 0.516D+00 0.852D+00
Gap=     0.183 Goal=   None    Shift=    0.000
RMSDP=9.73D-06 MaxDP=4.27D-04 DE=-9.16D-09 OVMax= 8.69D-05

Cycle  15  Pass 1  IDiag  1:
RMSU=  1.78D-07    CP:  6.28D-01  1.10D+00  2.36D+00  1.76D+00  2.22D+00
               CP:  2.98D+00  3.00D+00  3.00D+00  2.54D+00  1.90D+00
```

```
               CP:  2.25D+00
E= -723.249710612715     Delta-E=       -0.000000003789 Rises=F Damp=F
DIIS: error= 3.45D-07 at cycle  12 NSaved=  12.
NSaved=12 IEnMin=12 EnMin= -723.249710612715     IErMin=12 ErrMin= 3.45D-07
ErrMax= 3.45D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.62D-11 BMatP= 9.14D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.112D-03 0.251D-04-0.218D-02-0.290D-02 0.292D-02 0.210D-01
Coeff-Com:  0.142D-01-0.446D-01-0.832D-01 0.110D-02 0.157D+00 0.937D+00
Coeff:      0.112D-03 0.251D-04-0.218D-02-0.290D-02 0.292D-02 0.210D-01
Coeff:      0.142D-01-0.446D-01-0.832D-01 0.110D-02 0.157D+00 0.937D+00
Gap=     0.183 Goal=   None    Shift=    0.000
RMSDP=1.95D-06 MaxDP=8.03D-05 DE=-3.79D-09 OVMax= 2.06D-05

Cycle  16  Pass 1  IDiag  1:
RMSU=  1.59D-07    CP:  6.28D-01  1.10D+00  2.36D+00  1.76D+00  2.23D+00
               CP:  2.99D+00  3.00D+00  3.00D+00  2.61D+00  1.98D+00
               CP:  2.57D+00  1.69D+00
E= -723.249710612956     Delta-E=       -0.000000000241 Rises=F Damp=F
DIIS: error= 1.84D-07 at cycle  13 NSaved=  13.
NSaved=13 IEnMin=13 EnMin= -723.249710612956     IErMin=13 ErrMin= 1.84D-07
ErrMax= 1.84D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.46D-12 BMatP= 3.62D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.230D-04 0.126D-04 0.801D-03 0.932D-03-0.199D-02-0.771D-02
Coeff-Com: -0.296D-02 0.257D-01 0.259D-01-0.653D-01-0.964D-01 0.703D-01
Coeff-Com:  0.105D+01
Coeff:     -0.230D-04 0.126D-04 0.801D-03 0.932D-03-0.199D-02-0.771D-02
Coeff:     -0.296D-02 0.257D-01 0.259D-01-0.653D-01-0.964D-01 0.703D-01
Coeff:      0.105D+01
Gap=     0.183 Goal=   None    Shift=    0.000
RMSDP=4.25D-07 MaxDP=2.94D-05 DE=-2.41D-10 OVMax= 4.76D-06

Cycle  17  Pass 1  IDiag  1:
RMSU=  3.96D-08    CP:  6.28D-01  1.10D+00  2.36D+00  1.76D+00  2.23D+00
               CP:  2.99D+00  3.00D+00  3.00D+00  2.63D+00  2.00D+00
               CP:  2.61D+00  2.05D+00  1.63D+00
E= -723.249710612972     Delta-E=       -0.000000000016 Rises=F Damp=F
DIIS: error= 9.07D-08 at cycle  14 NSaved=  14.
NSaved=14 IEnMin=14 EnMin= -723.249710612972     IErMin=14 ErrMin= 9.07D-08
ErrMax= 9.07D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-12 BMatP= 4.46D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.247D-04 0.119D-05 0.615D-03 0.764D-03-0.114D-02-0.588D-02
Coeff-Com: -0.320D-02 0.161D-01 0.210D-01-0.247D-01-0.569D-01-0.102D+00
Coeff-Com:  0.379D+00 0.777D+00
Coeff:     -0.247D-04 0.119D-05 0.615D-03 0.764D-03-0.114D-02-0.588D-02
Coeff:     -0.320D-02 0.161D-01 0.210D-01-0.247D-01-0.569D-01-0.102D+00
Coeff:      0.379D+00 0.777D+00
Gap=     0.183 Goal=   None    Shift=    0.000
RMSDP=1.29D-07 MaxDP=6.97D-06 DE=-1.61D-11 OVMax= 1.44D-06
```

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.21D-08 CP: 6.28D-01 1.10D+00 2.36D+00 1.76D+00 2.23D+00
CP: 2.99D+00 3.00D+00 3.00D+00 2.63D+00 2.00D+00
CP: 2.61D+00 2.12D+00 1.77D+00 1.58D+00
E= -723.249710612990 Delta-E= -0.000000000018 Rises=F Damp=F
DIIS: error= 5.01D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.249710612990 IErMin=15 ErrMin= 5.01D-08
ErrMax= 5.01D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-13 BMatP= 1.09D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.674D-06-0.165D-05-0.563D-04-0.575D-04 0.193D-03 0.450D-03
Coeff-Com: 0.646D-04-0.179D-02-0.183D-02 0.691D-02 0.856D-02-0.226D-01
Coeff-Com: -0.125D+00 0.101D+00 0.103D+01
Coeff: 0.674D-06-0.165D-05-0.563D-04-0.575D-04 0.193D-03 0.450D-03
Coeff: 0.646D-04-0.179D-02-0.183D-02 0.691D-02 0.856D-02-0.226D-01
Coeff: -0.125D+00 0.101D+00 0.103D+01
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=8.29D-08 MaxDP=3.10D-06 DE=-1.80D-11 OVMax= 8.95D-07

Cycle 19 Pass 1 IDiag 1:
RMSU= 4.37D-09 CP: 6.28D-01 1.10D+00 2.36D+00 1.76D+00 2.23D+00
CP: 2.99D+00 3.00D+00 3.00D+00 2.63D+00 2.00D+00
CP: 2.60D+00 2.11D+00 1.75D+00 1.97D+00 1.90D+00
E= -723.249710612975 Delta-E= 0.000000000016 Rises=F Damp=F
DIIS: error= 2.38D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -723.249710612990 IErMin=16 ErrMin= 2.38D-08
ErrMax= 2.38D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.30D-14 BMatP= 1.34D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.458D-05-0.648D-06-0.129D-03-0.155D-03 0.285D-03 0.119D-02
Coeff-Com: 0.566D-03-0.354D-02-0.452D-02 0.693D-02 0.134D-01 0.831D-02
Coeff-Com: -0.116D+00-0.972D-01 0.412D+00 0.779D+00
Coeff: 0.458D-05-0.648D-06-0.129D-03-0.155D-03 0.285D-03 0.119D-02
Coeff: 0.566D-03-0.354D-02-0.452D-02 0.693D-02 0.134D-01 0.831D-02
Coeff: -0.116D+00-0.972D-01 0.412D+00 0.779D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=2.59D-08 MaxDP=1.10D-06 DE= 1.57D-11 OVMax= 3.99D-07

Cycle 20 Pass 1 IDiag 1:
RMSU= 1.69D-09 CP: 6.28D-01 1.10D+00 2.36D+00 1.76D+00 2.23D+00
CP: 2.99D+00 3.00D+00 3.00D+00 2.63D+00 2.00D+00
CP: 2.60D+00 2.11D+00 1.74D+00 2.07D+00 2.20D+00
CP: 1.32D+00
E= -723.249710612985 Delta-E= -0.000000000010 Rises=F Damp=F
DIIS: error= 1.21D-08 at cycle 17 NSaved= 17.
NSaved=17 IEnMin=15 EnMin= -723.249710612990 IErMin=17 ErrMin= 1.21D-08
ErrMax= 1.21D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.61D-15 BMatP= 4.30D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.700D-06 0.266D-06-0.106D-04-0.177D-04 0.128D-04 0.112D-03

Coeff-Com: 0.888D-04-0.184D-03-0.427D-03-0.243D-03 0.626D-03 0.714D-02
Coeff-Com: 0.917D-02-0.420D-01-0.170D+00 0.107D+00 0.109D+01
Coeff: 0.700D-06 0.266D-06-0.106D-04-0.177D-04 0.128D-04 0.112D-03
Coeff: 0.888D-04-0.184D-03-0.427D-03-0.243D-03 0.626D-03 0.714D-02
Coeff: 0.917D-02-0.420D-01-0.170D+00 0.107D+00 0.109D+01
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=1.09D-08 MaxDP=4.81D-07 DE=-1.02D-11 OVMax= 2.49D-07

Cycle 21 Pass 1 IDiag 1:
RMSU= 9.27D-10 CP: 6.28D-01 1.10D+00 2.36D+00 1.76D+00 2.23D+00
CP: 2.99D+00 3.00D+00 3.00D+00 2.63D+00 2.00D+00
CP: 2.60D+00 2.10D+00 1.73D+00 2.06D+00 2.25D+00
CP: 1.52D+00 1.97D+00
E= -723.249710612978 Delta-E= 0.000000000007 Rises=F Damp=F
DIIS: error= 4.75D-09 at cycle 18 NSaved= 18.
NSaved=18 IEnMin=15 EnMin= -723.249710612990 IErMin=18 ErrMin= 4.75D-09
ErrMax= 4.75D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.82D-15 BMatP= 6.61D-15
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Large coefficients: NSaved= 18 BigCof= 0.00 CofMax= 10.00 Det=-3.67D-15
Inversion failed. Reducing to 17 matrices.
Large coefficients: NSaved= 17 BigCof= 0.00 CofMax= 10.00 Det=-3.71D-15
Inversion failed. Reducing to 16 matrices.
Large coefficients: NSaved= 16 BigCof= 0.00 CofMax= 10.00 Det=-3.71D-15
Inversion failed. Reducing to 15 matrices.
Coeff-Com: -0.129D-05-0.666D-05 0.479D-05 0.165D-04 0.661D-04 0.137D-04
Coeff-Com: -0.446D-03-0.412D-03 0.242D-02 0.119D-01-0.710D-02-0.995D-01
Coeff-Com: -0.679D-01 0.379D+00 0.782D+00
Coeff: -0.129D-05-0.666D-05 0.479D-05 0.165D-04 0.661D-04 0.137D-04
Coeff: -0.446D-03-0.412D-03 0.242D-02 0.119D-01-0.710D-02-0.995D-01
Coeff: -0.679D-01 0.379D+00 0.782D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=4.51D-09 MaxDP=1.78D-07 DE= 6.59D-12 OVMax= 8.23D-08

SCF Done: E(RwB97XD) = -723.249710613 A.U. after 21 cycles
NFock= 21 Conv=0.45D-08 -V/T= 2.0041
KE= 7.202622361832D+02 PE=-3.669231409242D+03 EE= 1.232124782838D+03
Leave Link 502 at Fri Sep 25 19:15:57 2026, MaxMem= 805306368 cpu: 6941.9 elap: 1157.3
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 22863 LenP2D= 51056.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 19:15:59 2026, MaxMem= 805306368 cpu: 6.0 elap: 1.0
(Enter /home/user/gauss16/g16/l702.exe)

Supporting Information file

L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 19:15:59 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 19:28:51 2026, MaxMem= 805306368 cpu: 4632.6 elap: 772.2
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-7.60849903D+00 3.95347183D-03-2.05581658D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.002287705	-0.001512137	0.001170664
2	6	-0.003257046	0.000957607	-0.001200539
3	6	0.002259940	0.001516868	-0.001171525
4	6	0.003557787	0.002614157	0.000615617
5	6	-0.003231608	-0.000968826	0.001203338
6	6	-0.003926993	-0.003480574	-0.000791721
7	6	0.003534474	-0.002599919	-0.000621895
8	6	0.002294465	0.005930665	0.000044074
9	6	-0.003898253	0.003463613	0.000797492
10	6	0.005410432	-0.012318795	0.005988949
11	6	0.002264487	-0.005910619	-0.000038839
12	6	0.019555085	0.062346973	0.024879063
13	6	0.005454510	0.012284688	-0.005997098
14	6	0.019510173	-0.062434615	-0.024719388
15	6	-0.013043802	-0.143962309	-0.050191661
16	6	-0.013136506	0.144049811	0.049857108
17	7	0.010369343	0.078874791	0.024070022
18	7	0.010580378	-0.078926015	-0.023916635
19	1	-0.004836035	0.008241886	0.000441558
20	1	-0.000180158	-0.008183656	-0.000365655
21	1	-0.004832221	-0.008209761	-0.000452840
22	1	-0.000248969	0.008249385	0.000400049
23	1	-0.002616661	0.004203977	-0.001782267
24	1	-0.015599146	0.009262149	0.002490776

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    25        1        -0.015656021   -0.009274711   -0.002478720
    26        1        -0.002615361   -0.004214632    0.001770076
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.144049811 RMS     0.030407852
 Leave Link  716 at Fri Sep 25 19:28:51 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.090462273 RMS     0.019954837
 Search for a local minimum.
 Step number   3 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .19955D-01 SwitMx=.10000D-02 MixMth= 1
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    2    3
 ITU=  0  1  0
 Use linear search instead of GDIIS.
 Linear search step of   0.821 exceeds DXMaxT=   0.505 but not scaled.
 Quartic linear search produced a step of  1.36792.
 Iteration  1 RMS(Cart)=  0.25390261 RMS(Int)=  0.03384809
 Iteration  2 RMS(Cart)=  0.13799293 RMS(Int)=  0.00533579
 Iteration  3 RMS(Cart)=  0.01113545 RMS(Int)=  0.00116759
 Iteration  4 RMS(Cart)=  0.00006859 RMS(Int)=  0.00116718
 Iteration  5 RMS(Cart)=  0.00000004 RMS(Int)=  0.00116718
  ITry=  1 IFail=0 DXMaxC=  1.61D+00 DCOld=  1.00D+10 DXMaxT=  5.05D-01 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)    (Quad)   (Total)
    R1        2.31302   0.00259   0.00338   0.00000   0.00337   2.31638
    R2        2.54833   0.00003   0.00130   0.00000   0.00129   2.54962
    R3        2.54677  -0.00063   0.00191   0.00000   0.00191   2.54868
    R4        2.31301   0.00258   0.00338   0.00000   0.00336   2.31638
    R5        2.30984   0.00253   0.00547   0.00000   0.00547   2.31532
    R6        2.54677  -0.00062   0.00192   0.00000   0.00192   2.54869
    R7        2.54885  -0.00168   0.00185   0.00000   0.00185   2.55070
    R8        2.30982   0.00252   0.00545   0.00000   0.00545   2.31527
    R9        2.30506   0.00284   0.01024   0.00000   0.01025   2.31531
   R10        2.54888  -0.00166   0.00188   0.00000   0.00189   2.55077
   R11        2.65109   0.00148   0.01005   0.00000   0.01006   2.66114
   R12        2.30501   0.00283   0.01019   0.00000   0.01020   2.31520
   R13        2.67109   0.00274   0.05365   0.00000   0.05367   2.72477
   R14        2.71838  -0.00526   0.01047   0.00000   0.01047   2.72885
   R15        2.65119   0.00152   0.01015   0.00000   0.01016   2.66135
   R16        2.71813  -0.00531   0.01026   0.00000   0.01026   2.72839
```

R17	2.56321	0.06518	0.35929	0.00000	0.35929	2.92250
R18	2.08411	0.00018	0.05664	0.00000	0.05664	2.14075
R19	2.56344	0.06505	0.35944	0.00000	0.35944	2.92288
R20	2.08390	0.00021	0.05644	0.00000	0.05644	2.14035
R21	1.96309	0.00511	0.06690	0.00000	0.06690	2.02999
R22	1.91597	0.00209	0.02394	0.00000	0.02394	1.93991
R23	1.95051	-0.00001	0.05543	0.00000	0.05543	2.00594
R24	1.96312	0.00508	0.06693	0.00000	0.06693	2.03006
R25	1.91566	0.00217	0.02365	0.00000	0.02365	1.93930
R26	1.95056	0.00001	0.05548	0.00000	0.05548	2.00603
A1	2.55243	-0.00194	-0.00743	0.00000	-0.00754	2.54489
A2	2.60888	0.00041	-0.00162	0.00000	-0.00170	2.60718
A3	2.55223	-0.00192	-0.00741	0.00000	-0.00751	2.54472
A4	2.71924	-0.00200	-0.00350	0.00000	-0.00354	2.71570
A5	2.60905	0.00040	-0.00164	0.00000	-0.00172	2.60733
A6	2.84622	0.00277	0.00755	0.00000	0.00756	2.85378
A7	2.71914	-0.00199	-0.00348	0.00000	-0.00352	2.71562
A8	2.84629	0.00276	0.00754	0.00000	0.00755	2.85383
A9	2.09587	-0.00787	-0.04024	0.00000	-0.04016	2.05571
A10	2.04656	0.01064	-0.00441	0.00000	-0.00445	2.04211
A11	2.14075	-0.00276	0.04463	0.00000	0.04457	2.18532
A12	2.09586	-0.00788	-0.04024	0.00000	-0.04015	2.05571
A13	2.14075	-0.00275	0.04463	0.00000	0.04457	2.18532
A14	2.04657	0.01063	-0.00441	0.00000	-0.00445	2.04211
A15	1.63669	0.06421	0.05243	0.00000	0.05243	1.68913
A16	1.85348	0.02622	0.25013	0.00000	0.25013	2.10360
A17	1.63643	0.06428	0.05226	0.00000	0.05226	1.68869
A18	1.85389	0.02618	0.25058	0.00000	0.25058	2.10447
A19	1.99609	0.01264	0.07703	0.00000	0.07346	2.06955
A20	1.99480	-0.01457	0.07576	0.00000	0.07172	2.06653
A21	1.96263	0.00680	0.04674	0.00000	0.04435	2.00698
A22	1.83373	0.00023	-0.07119	0.00000	-0.07525	1.75847
A23	1.81934	-0.00606	-0.08378	0.00000	-0.08534	1.73400
A24	1.84057	0.00052	-0.06456	0.00000	-0.06684	1.77373
A25	1.99600	0.01263	0.07694	0.00000	0.07338	2.06938
A26	1.99481	-0.01465	0.07577	0.00000	0.07173	2.06654
A27	1.96283	0.00683	0.04692	0.00000	0.04452	2.00735
A28	1.83372	0.00025	-0.07119	0.00000	-0.07525	1.75848
A29	1.81925	-0.00605	-0.08386	0.00000	-0.08542	1.73383
A30	1.84053	0.00054	-0.06460	0.00000	-0.06689	1.77364
A31	2.95101	0.00016	0.01104	0.00000	0.01108	2.96209
A32	3.07595	0.00846	0.03418	0.00000	0.03427	3.11021
A33	2.95097	0.00017	0.01104	0.00000	0.01108	2.96206
A34	3.07594	0.00845	0.03415	0.00000	0.03423	3.11017
A35	3.49017	0.09044	0.30256	0.00000	0.30256	3.79273
A36	3.49032	0.09046	0.30284	0.00000	0.30284	3.79316
A37	3.13880	0.00038	-0.00235	0.00000	-0.00218	3.13662
A38	3.15171	0.00220	0.00882	0.00000	0.00898	3.16068

A39	3.13896	0.00037	-0.00236	0.00000	-0.00219	3.13678
A40	3.15169	0.00221	0.00885	0.00000	0.00901	3.16069
A41	3.19172	0.01930	0.04571	0.00000	0.04571	3.23744
A42	3.19165	0.01923	0.04565	0.00000	0.04565	3.23730
D1	0.00086	0.00058	0.00043	0.00000	0.00050	0.00135
D2	-0.00174	0.00014	-0.00080	0.00000	-0.00070	-0.00245
D3	0.00143	0.00029	0.00126	0.00000	0.00127	0.00270
D4	0.00080	0.00058	0.00043	0.00000	0.00050	0.00130
D5	0.00467	0.00074	0.00317	0.00000	0.00312	0.00779
D6	0.00151	0.00029	0.00126	0.00000	0.00128	0.00279
D7	-0.00344	-0.00010	-0.00152	0.00000	-0.00117	-0.00461
D8	-3.13334	0.00151	0.00900	0.00000	0.00851	-3.12482
D9	0.00449	0.00075	0.00317	0.00000	0.00312	0.00761
D10	-0.00307	-0.00010	-0.00150	0.00000	-0.00115	-0.00423
D11	-3.13300	0.00150	0.00898	0.00000	0.00849	-3.12451
D12	-0.00828	-0.00181	-0.00835	0.00000	-0.00829	-0.01657
D13	3.12766	-0.00177	-0.01371	0.00000	-0.01379	3.11387
D14	3.12757	-0.00178	-0.01376	0.00000	-0.01384	3.11372
D15	-0.01968	-0.00174	-0.01912	0.00000	-0.01934	-0.03902
D16	2.57300	0.00525	-0.00146	0.00000	-0.00162	2.57138
D17	-0.56300	0.00527	0.00385	0.00000	0.00401	-0.55899
D18	-0.55948	0.00525	0.00376	0.00000	0.00392	-0.55556
D19	2.57661	0.00523	-0.00149	0.00000	-0.00165	2.57496
D20	-1.75974	0.00359	0.00016	0.00000	-0.00141	-1.76115
D21	0.35499	0.00234	0.01936	0.00000	0.02046	0.37544
D22	2.45274	-0.00259	0.02225	0.00000	0.02273	2.47547
D23	-1.76468	0.00360	0.00007	0.00000	-0.00150	-1.76618
D24	0.34998	0.00232	0.01920	0.00000	0.02028	0.37026
D25	2.44783	-0.00260	0.02219	0.00000	0.02267	2.47050

Item	Value	Threshold	Converged?
Maximum Force	0.090462	0.000450	NO
RMS Force	0.019955	0.000300	NO
Maximum Displacement	1.606928	0.001800	NO
RMS Displacement	0.386863	0.001200	NO

Predicted change in Energy=-4.858613D-02
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 19:28:51 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.295786	0.672088	-0.053213
2	6	0	3.607065	1.682786	-0.134981

3	6	0	4.295698	-0.672823	0.054281
4	6	0	2.386678	2.255049	-0.181536
5	6	0	3.606672	-1.683331	0.135753
6	6	0	1.161583	2.272051	-0.181914
7	6	0	2.386191	-2.255450	0.181834
8	6	0	-0.137850	1.908487	-0.147587
9	6	0	1.161115	-2.272204	0.181701
10	6	0	-1.239204	1.374364	-0.094026
11	6	0	-0.138283	-1.908431	0.146887
12	6	0	-2.485118	0.719197	-0.054943
13	6	0	-1.239467	-1.374108	0.093105
14	6	0	-2.485308	-0.718582	0.053781
15	6	0	-3.664636	1.547820	-0.140876
16	6	0	-3.664855	-1.546783	0.139298
17	7	0	-4.175281	2.982174	0.130400
18	7	0	-4.174508	-2.982140	-0.129669
19	1	0	-3.827569	3.779254	-0.500244
20	1	0	-5.187600	3.151622	0.112667
21	1	0	-3.824403	-3.778183	0.501025
22	1	0	-5.186265	-3.152720	-0.109469
23	1	0	-3.908001	3.381884	1.076746
24	1	0	-4.312003	0.801845	-0.695631
25	1	0	-4.312974	-0.799051	0.690362
26	1	0	-3.908948	-3.382735	-1.076180

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.225778	0.000000			
3	C	1.349201	2.461490	0.000000		
4	C	2.483329	1.348702	3.503199	0.000000	
5	C	2.461420	3.376987	1.225774	4.135202	0.000000
6	C	3.521316	2.515913	4.307058	1.225212	4.660946
7	C	3.503182	4.135288	2.483384	4.525112	1.348709
8	C	4.603771	3.751731	5.134224	2.548430	5.196429
9	C	4.306995	4.660998	3.521344	4.704249	2.515876
10	C	5.579513	4.856246	5.903229	3.732329	5.734527
11	C	5.134208	5.196531	4.603857	4.880354	3.751731
12	C	6.781068	6.168437	6.923086	5.109723	6.551214
13	C	5.903164	5.734588	5.579548	5.137620	4.856181
14	C	6.923051	6.551275	6.781160	5.712626	6.168442
15	C	8.008927	7.272957	8.266575	6.092637	7.961707
16	C	8.266333	7.961544	8.008835	7.153874	7.272810
17	N	8.782322	7.894540	9.226174	6.609487	9.073354
18	N	9.225243	9.072731	8.781297	8.395237	7.893295
19	H	8.708801	7.733200	9.279869	6.406375	9.247284
20	H	9.803582	8.919919	10.225593	7.632830	10.035762
21	H	9.276291	9.244102	8.705107	8.685811	7.729340

22	H	10.224559	10.035209	9.802261	9.305838	8.918238
23	H	8.713318	7.799451	9.207973	6.517362	9.111101
24	H	8.632704	7.987618	8.765246	6.873749	8.341026
25	H	8.765153	8.340728	8.633063	7.414383	7.988137
26	H	9.209002	9.112399	8.714229	8.498230	7.800083

		6	7	8	9	10
6	C	0.000000				
7	C	4.704279	0.000000			
8	C	1.349772	4.880335	0.000000		
9	C	4.558779	1.225191	4.390207	0.000000	
10	C	2.564633	5.137620	1.225209	4.374359	0.000000
11	C	4.390239	2.548453	3.828261	1.349807	3.470852
12	C	3.965591	5.712639	2.632995	4.722234	1.408217
13	C	4.374375	3.732296	3.470868	2.564609	2.754836
14	C	4.722208	5.109781	3.528824	3.965665	2.440296
15	C	4.880429	7.154126	3.545187	6.163158	2.432078
16	C	6.162887	6.092551	4.945802	4.880371	3.804120
17	N	5.392953	8.395729	4.186996	7.489208	3.354992
18	N	7.488867	6.608168	6.341385	5.391645	5.253229
19	H	5.221555	8.688711	4.151887	7.872240	3.556423
20	H	6.416585	9.306102	5.207024	8.350380	4.334882
21	H	7.869676	6.402506	6.808054	5.217790	5.795351
22	H	8.350363	7.630992	7.148690	6.414774	6.006165
23	H	5.340097	8.496897	4.228940	7.646290	3.538830
24	H	5.690831	7.415039	4.352995	6.338337	3.183049
25	H	6.337454	6.874483	5.046245	5.691623	3.845395
26	H	7.647654	6.517833	6.563574	5.340514	5.542757

		11	12	13	14	15
11	C	0.000000				
12	C	3.528853	0.000000			
13	C	1.225152	2.440388	0.000000		
14	C	2.633046	1.441884	1.408326	0.000000	
15	C	4.946074	1.444044	3.804453	2.562281	0.000000
16	C	3.545075	2.562064	2.431966	1.443802	3.107260
17	N	6.341581	2.830560	5.253341	4.069088	1.546519
18	N	4.185743	4.069339	3.354081	2.830327	4.558578
19	H	6.810240	3.371115	5.797196	4.726430	2.266052
20	H	7.148490	3.639807	6.005862	4.720628	2.226182
21	H	4.148357	4.725380	3.553572	3.369624	5.366924
22	H	5.205391	4.721324	4.333787	3.639622	4.940791
23	H	6.562228	3.224161	5.541488	4.459185	2.214864
24	H	5.047314	1.937736	3.846734	2.492014	1.132835
25	H	4.353635	2.490304	3.183372	1.937028	2.572762
26	H	4.229347	4.460500	3.539483	3.225102	5.024426

		16	17	18	19	20
16	C	0.000000				
17	N	4.557638	0.000000			
18	N	1.546719	5.969982	0.000000		

```
 19  H    5.366764   1.074222   6.780424   0.000000
 20  H    4.939076   1.026556   6.221585   1.618415   0.000000
 21  H    2.266153   6.779595   1.074259   7.623478   7.073283
 22  H    2.226119   6.222262   1.026235   7.074675   6.308254
 23  H    5.022916   1.061498   6.482844   1.628272   1.618593
 24  H    2.575259   2.335563   3.828546   3.022882   2.634666
 25  H    1.132622   3.824942   2.336130   4.755423   4.087361
 26  H    2.215331   6.483737   1.061547   7.185570   6.763589
            21         22         23         24         25
 21  H    0.000000
 22  H    1.618201   0.000000
 23  H    7.183663   6.763291   0.000000
 24  H    4.758823   4.092249   3.156127   0.000000
 25  H    3.024860   2.634791   4.218236   2.117510   0.000000
 26  H    1.628220   1.618325   7.098955   4.221136   3.155841
            26
 26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=2 Diff= 1.44D-02
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.684170   -0.673874    0.034994
    2          6           0        3.995315   -1.686347    0.088932
    3          6           0        4.684261    0.673482   -0.035535
    4          6           0        2.774851   -2.259515    0.119669
    5          6           0        3.995370    1.685934   -0.089281
    6          6           0        1.549754   -2.276362    0.119491
    7          6           0        2.774965    2.259261   -0.119726
    8          6           0        0.250370   -1.911825    0.095065
    9          6           0        1.549891    2.276163   -0.119221
   10          6           0       -0.850912   -1.376290    0.056109
   11          6           0        0.250444    1.911740   -0.094502
   12          6           0       -2.096740   -0.720136    0.034939
   13          6           0       -0.850811    1.376284   -0.055491
   14          6           0       -2.096738    0.720086   -0.034269
   15          6           0       -3.276370   -1.550653    0.098003
   16          6           0       -3.276174    1.550475   -0.097101
   17          7           0       -3.787177   -2.976953   -0.212589
   18          7           0       -3.785665    2.977972    0.211137
   19          1           0       -3.439614   -3.791092    0.395959
```

```
    20        1        0     -4.799519   -3.146693   -0.199588
    21        1        0     -3.435411    3.790986   -0.397437
    22        1        0     -4.797399    3.149173    0.195555
    23        1        0     -3.519876   -3.350564   -1.169533
    24        1        0     -3.923685   -0.820108    0.672983
    25        1        0     -3.924347    0.818239   -0.668534
    26        1        0     -3.520126    3.352395    1.168309
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.5894964           0.2448030           0.1737736
 Leave Link  202 at Fri Sep 25 19:28:51 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy       982.3888966379 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0139839416 Hartrees.
 Nuclear repulsion after empirical dispersion term =      982.3749126963 Hartrees.
 Leave Link  301 at Fri Sep 25 19:28:51 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   22800 LenP2D=   50775.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  2.19D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=         32
 NSgBfM=   681   681   681   681   681 MxSgAt=    26 MxSgA2=    26.
```

Supporting Information file

```
 Leave Link  302 at Fri Sep 25 19:28:52 2026, MaxMem=    805306368 cpu:                5.7 elap:
0.9
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Sep 25 19:28:52 2026, MaxMem=    805306368 cpu:                0.7 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=     0.000000   -0.000000    0.000000
       Rot=    0.999993    0.003606    0.000004    0.000030 Ang=   0.41 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Generating alternative initial guess.
 ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn=          5 AccDes=
0.00D+00
 Harris functional with IExCor= 4639 and IRadAn=       5 diagonalized for initial guess.
 HarFok:  IExCor= 4639 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Petite list used in FoFCou.
 Harris En= -691.958556548014
 Leave Link  401 at Fri Sep 25 19:28:59 2026, MaxMem=    805306368 cpu:               41.2 elap:
6.9
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.130310595167
 DIIS: error= 1.29D-02 at cycle   1 NSaved=   1.
```

NSaved= 1 IEnMin= 1 EnMin= -723.130310595167 IErMin= 1 ErrMin= 1.29D-02
ErrMax= 1.29D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-01 BMatP= 1.46D-01
IDIUse=3 WtCom= 8.71D-01 WtEn= 1.29D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Recover alternate guess density for next cycle.
RMSDP=1.67D-02 MaxDP=9.09D-01 OVMax= 0.00D+00

Cycle 2 Pass 0 IDiag 1:
RMSU= 8.35D-03 CP: 3.48D-01
E= -722.859805751336 Delta-E= 0.270504843831 Rises=F Damp=F
Switch densities from cycles 1 and 2 for lowest energy.
DIIS: error= 6.88D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -723.130310595167 IErMin= 1 ErrMin= 1.29D-02
ErrMax= 6.88D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.74D+00 BMatP= 1.46D-01
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.916D+00 0.842D-01
Coeff: 0.916D+00 0.842D-01
Gap= 0.141 Goal= None Shift= 0.000
RMSDP=6.84D-03 MaxDP=3.34D-01 DE= 2.71D-01 OVMax= 4.67D-01

Cycle 3 Pass 0 IDiag 1:
RMSU= 5.21D-03 CP: 8.52D-01 3.58D-01
E= -723.275872950222 Delta-E= -0.416067198886 Rises=F Damp=F
DIIS: error= 2.47D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.275872950222 IErMin= 3 ErrMin= 2.47D-03
ErrMax= 2.47D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.16D-03 BMatP= 1.46D-01
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.543D-01 0.194D-02 0.105D+01
Coeff: -0.543D-01 0.194D-02 0.105D+01
Gap= 0.170 Goal= None Shift= 0.000
RMSDP=1.19D-02 MaxDP=4.66D-01 DE=-4.16D-01 OVMax= 3.99D-02

Cycle 4 Pass 0 IDiag 1:
RMSU= 5.47D-03 CP: 4.01D-01 5.59D-01 4.04D-01
E= -723.280341348173 Delta-E= -0.004468397951 Rises=F Damp=F
DIIS: error= 2.82D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.280341348173 IErMin= 3 ErrMin= 2.47D-03
ErrMax= 2.82D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.99D-03 BMatP= 4.16D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.521D-01 0.197D-02 0.545D+00 0.505D+00
Coeff: -0.521D-01 0.197D-02 0.545D+00 0.505D+00
Gap= 0.183 Goal= None Shift= 0.000
RMSDP=1.54D-02 MaxDP=5.87D-01 DE=-4.47D-03 OVMax= 2.56D-02

Cycle 5 Pass 0 IDiag 1:
RMSU= 6.45D-03 CP: 9.52D-01 4.69D-01 1.28D+00 4.46D-02

E= -723.283967498831 Delta-E= -0.003626150657 Rises=F Damp=F
DIIS: error= 3.11D-03 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.283967498831 IErMin= 3 ErrMin= 2.47D-03
ErrMax= 3.11D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.06D-03 BMatP= 3.99D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.265D-01 0.156D-02 0.196D+00 0.333D+00 0.496D+00
Coeff: -0.265D-01 0.156D-02 0.196D+00 0.333D+00 0.496D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=1.80D-02 MaxDP=7.15D-01 DE=-3.63D-03 OVMax= 8.21D-03

Cycle 6 Pass 0 IDiag 1:
RMSU= 3.02D-03 CP: 3.12D-01 7.17D-01 2.21D-01 1.52D+00 4.34D-01
E= -723.284606343905 Delta-E= -0.000638845074 Rises=F Damp=F
DIIS: error= 1.95D-03 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.284606343905 IErMin= 6 ErrMin= 1.95D-03
ErrMax= 1.95D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.64D-04 BMatP= 1.06D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.129D-01 0.741D-03 0.637D-01 0.195D+00 0.377D+00 0.376D+00
Coeff: -0.129D-01 0.741D-03 0.637D-01 0.195D+00 0.377D+00 0.376D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.38D+02 MaxDP=1.72D+04 DE=-6.39D-04 OVMax= 9.98D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 7 Pass 1 IDiag 1:
E= -723.284270536555 Delta-E= 0.000335807350 Rises=F Damp=F
DIIS: error= 1.26D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.284270536555 IErMin= 1 ErrMin= 1.26D-03
ErrMax= 1.26D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.79D-04 BMatP= 3.79D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.100D+01
Coeff: 0.100D+01
Gap= 0.179 Goal= None Shift= 0.000
GapD= 0.179 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=1.33D-02 MaxDP=5.90D-01 DE= 3.36D-04 OVMax= 6.77D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.30D-02 CP: 7.78D-01
E= -723.284552273299 Delta-E= -0.000281736744 Rises=F Damp=F
DIIS: error= 2.91D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.284552273299 IErMin= 2 ErrMin= 2.91D-04
ErrMax= 2.91D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.44D-05 BMatP= 3.79D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.160D+00 0.840D+00
Coeff: 0.160D+00 0.840D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=1.60D-03 MaxDP=6.18D-02 DE=-2.82D-04 OVMax= 5.03D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 8.89D-04 CP: 7.90D-01 1.10D+00
E= -723.284554208724 Delta-E= -0.000001935425 Rises=F Damp=F
DIIS: error= 3.22D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.284554208724 IErMin= 2 ErrMin= 2.91D-04
ErrMax= 3.22D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.87D-05 BMatP= 5.44D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.195D-01 0.514D+00 0.505D+00
Coeff: -0.195D-01 0.514D+00 0.505D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=6.47D-04 MaxDP=2.52D-02 DE=-1.94D-06 OVMax= 2.86D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 8.29D-05 CP: 8.00D-01 1.14D+00 1.34D+00
E= -723.284615540635 Delta-E= -0.000061331910 Rises=F Damp=F
DIIS: error= 1.05D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.284615540635 IErMin= 4 ErrMin= 1.05D-04
ErrMax= 1.05D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.17D-06 BMatP= 5.44D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.186D-01 0.244D+00 0.280D+00 0.495D+00
Coeff: -0.186D-01 0.244D+00 0.280D+00 0.495D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.10D-04 MaxDP=4.35D-03 DE=-6.13D-05 OVMax= 6.94D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.56D-05 CP: 8.01D-01 1.15D+00 1.41D+00 1.06D+00
E= -723.284619756615 Delta-E= -0.000004215981 Rises=F Damp=F
DIIS: error= 1.64D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.284619756615 IErMin= 5 ErrMin= 1.64D-05
ErrMax= 1.64D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.44D-07 BMatP= 3.17D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.634D-02-0.169D+00-0.163D+00 0.210D-01 0.130D+01
Coeff: 0.634D-02-0.169D+00-0.163D+00 0.210D-01 0.130D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.72D-04 MaxDP=6.76D-03 DE=-4.22D-06 OVMax= 1.27D-03

Cycle 12 Pass 1 IDiag 1:
RMSU= 8.88D-06 CP: 8.04D-01 1.16D+00 1.51D+00 1.32D+00 2.67D+00
E= -723.284621285996 Delta-E= -0.000001529380 Rises=F Damp=F
DIIS: error= 1.12D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.284621285996 IErMin= 6 ErrMin= 1.12D-05
ErrMax= 1.12D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.90D-08 BMatP= 2.44D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.442D-02-0.985D-01-0.982D-01-0.276D-01 0.599D+00 0.621D+00
Coeff: 0.442D-02-0.985D-01-0.982D-01-0.276D-01 0.599D+00 0.621D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.04D-05 MaxDP=4.90D-04 DE=-1.53D-06 OVMax= 2.78D-04

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Cycle  13  Pass 1  IDiag  1:
RMSU=  2.72D-06    CP:  8.05D-01  1.16D+00  1.51D+00  1.36D+00  2.99D+00
             CP:  1.25D+00
E= -723.284621421379     Delta-E=       -0.000000135384 Rises=F Damp=F
DIIS: error= 5.58D-06 at cycle   7 NSaved=   7.
NSaved= 7 IEnMin= 7 EnMin= -723.284621421379     IErMin= 7 ErrMin= 5.58D-06
ErrMax= 5.58D-06  0.00D+00 EMaxC= 1.00D+00 BMatC= 1.20D-08 BMatP= 4.90D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.158D-03 0.444D-02 0.359D-02-0.162D-01-0.118D+00 0.285D+00
Coeff-Com:  0.841D+00
Coeff:      0.158D-03 0.444D-02 0.359D-02-0.162D-01-0.118D+00 0.285D+00
Coeff:      0.841D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=1.08D-05 MaxDP=5.08D-04 DE=-1.35D-07 OVMax= 2.41D-04

Cycle  14  Pass 1  IDiag  1:
RMSU=  3.04D-06    CP:  8.05D-01  1.16D+00  1.50D+00  1.40D+00  3.00D+00
             CP:  1.50D+00  2.28D+00
E= -723.284621476853     Delta-E=       -0.000000055474 Rises=F Damp=F
DIIS: error= 2.84D-06 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -723.284621476853     IErMin= 8 ErrMin= 2.84D-06
ErrMax= 2.84D-06  0.00D+00 EMaxC= 1.00D+00 BMatC= 3.88D-09 BMatP= 1.20D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.117D-02 0.303D-01 0.302D-01 0.106D-02-0.233D+00-0.179D-01
Coeff-Com:  0.457D+00 0.733D+00
Coeff:     -0.117D-02 0.303D-01 0.302D-01 0.106D-02-0.233D+00-0.179D-01
Coeff:      0.457D+00 0.733D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=4.05D-06 MaxDP=2.20D-04 DE=-5.55D-08 OVMax= 1.40D-04

Cycle  15  Pass 1  IDiag  1:
RMSU=  1.26D-06    CP:  8.05D-01  1.16D+00  1.49D+00  1.41D+00  3.00D+00
             CP:  1.65D+00  3.00D+00  1.47D+00
E= -723.284621493720     Delta-E=       -0.000000016867 Rises=F Damp=F
DIIS: error= 1.37D-06 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.284621493720     IErMin= 9 ErrMin= 1.37D-06
ErrMax= 1.37D-06  0.00D+00 EMaxC= 1.00D+00 BMatC= 4.77D-10 BMatP= 3.88D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.284D-03 0.564D-02 0.597D-02 0.377D-02-0.306D-01-0.578D-01
Coeff-Com: -0.681D-01 0.148D+00 0.993D+00
Coeff:     -0.284D-03 0.564D-02 0.597D-02 0.377D-02-0.306D-01-0.578D-01
Coeff:     -0.681D-01 0.148D+00 0.993D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=7.95D-06 MaxDP=3.20D-04 DE=-1.69D-08 OVMax= 8.59D-05

Cycle  16  Pass 1  IDiag  1:
RMSU=  8.37D-07    CP:  8.05D-01  1.16D+00  1.50D+00  1.42D+00  3.00D+00
             CP:  1.73D+00  3.00D+00  1.72D+00  2.48D+00
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E= -723.284621498061 Delta-E= -0.000000004341 Rises=F Damp=F
DIIS: error= 8.10D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.284621498061 IErMin=10 ErrMin= 8.10D-07
ErrMax= 8.10D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.92D-10 BMatP= 4.77D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.196D-03-0.591D-02-0.564D-02 0.170D-02 0.518D-01-0.202D-01
Coeff-Com: -0.164D+00-0.155D+00 0.467D+00 0.831D+00
Coeff: 0.196D-03-0.591D-02-0.564D-02 0.170D-02 0.518D-01-0.202D-01
Coeff: -0.164D+00-0.155D+00 0.467D+00 0.831D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=5.86D-06 MaxDP=2.42D-04 DE=-4.34D-09 OVMax= 4.81D-05

Cycle 17 Pass 1 IDiag 1:
RMSU= 6.80D-07 CP: 8.05D-01 1.16D+00 1.50D+00 1.43D+00 3.00D+00
CP: 1.77D+00 3.00D+00 1.85D+00 3.00D+00 1.45D+00
E= -723.284621499175 Delta-E= -0.000000001113 Rises=F Damp=F
DIIS: error= 4.41D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.284621499175 IErMin=11 ErrMin= 4.41D-07
ErrMax= 4.41D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.70D-11 BMatP= 1.92D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.159D-03-0.431D-02-0.419D-02 0.299D-03 0.343D-01-0.463D-03
Coeff-Com: -0.803D-01-0.117D+00 0.988D-01 0.463D+00 0.609D+00
Coeff: 0.159D-03-0.431D-02-0.419D-02 0.299D-03 0.343D-01-0.463D-03
Coeff: -0.803D-01-0.117D+00 0.988D-01 0.463D+00 0.609D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.62D-06 MaxDP=6.83D-05 DE=-1.11D-09 OVMax= 1.41D-05

Cycle 18 Pass 1 IDiag 1:
RMSU= 4.47D-08 CP: 8.05D-01 1.16D+00 1.50D+00 1.43D+00 3.00D+00
CP: 1.78D+00 3.00D+00 1.90D+00 3.00D+00 1.55D+00
CP: 1.59D+00
E= -723.284621499353 Delta-E= -0.000000000178 Rises=F Damp=F
DIIS: error= 2.11D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.284621499353 IErMin=12 ErrMin= 2.11D-07
ErrMax= 2.11D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 7.21D-12 BMatP= 5.70D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.409D-04 0.134D-02 0.130D-02-0.625D-03-0.128D-01 0.844D-02
Coeff-Com: 0.465D-01 0.312D-01-0.157D+00-0.226D+00 0.144D+00 0.116D+01
Coeff: -0.409D-04 0.134D-02 0.130D-02-0.625D-03-0.128D-01 0.844D-02
Coeff: 0.465D-01 0.312D-01-0.157D+00-0.226D+00 0.144D+00 0.116D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.76D-07 MaxDP=3.91D-05 DE=-1.78D-10 OVMax= 1.19D-05

Cycle 19 Pass 1 IDiag 1:
RMSU= 4.71D-08 CP: 8.05D-01 1.16D+00 1.50D+00 1.43D+00 3.00D+00
CP: 1.79D+00 3.00D+00 1.95D+00 3.00D+00 1.63D+00
CP: 2.02D+00 2.35D+00
E= -723.284621499421 Delta-E= -0.000000000068 Rises=F Damp=F

DIIS: error= 6.30D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.284621499421 IErMin=13 ErrMin= 6.30D-08
ErrMax= 6.30D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.10D-13 BMatP= 7.21D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.906D-05 0.237D-03 0.243D-03-0.133D-04-0.184D-02 0.363D-04
Coeff-Com: 0.372D-02 0.601D-02-0.105D-02-0.257D-01-0.513D-01-0.200D-01
Coeff-Com: 0.109D+01
Coeff: -0.906D-05 0.237D-03 0.243D-03-0.133D-04-0.184D-02 0.363D-04
Coeff: 0.372D-02 0.601D-02-0.105D-02-0.257D-01-0.513D-01-0.200D-01
Coeff: 0.109D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.84D-08 MaxDP=3.68D-06 DE=-6.82D-11 OVMax= 1.95D-06

Cycle 20 Pass 1 IDiag 1:
RMSU= 1.63D-08 CP: 8.05D-01 1.16D+00 1.50D+00 1.43D+00 3.00D+00
CP: 1.79D+00 3.00D+00 1.96D+00 3.00D+00 1.65D+00
CP: 2.01D+00 2.58D+00 1.27D+00
E= -723.284621499409 Delta-E= 0.000000000012 Rises=F Damp=F
DIIS: error= 4.31D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.284621499421 IErMin=14 ErrMin= 4.31D-08
ErrMax= 4.31D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.67D-13 BMatP= 4.10D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.495D-05-0.189D-03-0.174D-03 0.132D-03 0.192D-02-0.172D-02
Coeff-Com: -0.824D-02-0.426D-02 0.348D-01 0.359D-01-0.516D-01-0.252D+00
Coeff-Com: 0.440D+00 0.806D+00
Coeff: 0.495D-05-0.189D-03-0.174D-03 0.132D-03 0.192D-02-0.172D-02
Coeff: -0.824D-02-0.426D-02 0.348D-01 0.359D-01-0.516D-01-0.252D+00
Coeff: 0.440D+00 0.806D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.41D-08 MaxDP=2.09D-06 DE= 1.21D-11 OVMax= 7.49D-07

Cycle 21 Pass 1 IDiag 1:
RMSU= 3.33D-09 CP: 8.05D-01 1.16D+00 1.50D+00 1.43D+00 3.00D+00
CP: 1.79D+00 3.00D+00 1.96D+00 3.00D+00 1.65D+00
CP: 1.99D+00 2.64D+00 1.35D+00 1.47D+00
E= -723.284621499430 Delta-E= -0.000000000021 Rises=F Damp=F
DIIS: error= 1.45D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.284621499430 IErMin=15 ErrMin= 1.45D-08
ErrMax= 1.45D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.44D-14 BMatP= 1.67D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.328D-05-0.101D-03-0.953D-04 0.381D-04 0.875D-03-0.394D-03
Coeff-Com: -0.295D-02-0.270D-02 0.930D-02 0.130D-01-0.221D-02-0.540D-01
Coeff-Com: -0.121D+00 0.180D+00 0.981D+00
Coeff: 0.328D-05-0.101D-03-0.953D-04 0.381D-04 0.875D-03-0.394D-03
Coeff: -0.295D-02-0.270D-02 0.930D-02 0.130D-01-0.221D-02-0.540D-01
Coeff: -0.121D+00 0.180D+00 0.981D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.08D-08 MaxDP=5.70D-07 DE=-2.11D-11 OVMax= 4.18D-07

Supporting Information file

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 Cycle  22  Pass 1  IDiag  1:
 RMSU=  2.33D-09    CP:  8.05D-01  1.16D+00  1.50D+00  1.43D+00  3.00D+00
                CP:  1.79D+00  3.00D+00  1.96D+00  3.00D+00  1.65D+00
                CP:  1.99D+00  2.62D+00  1.34D+00  1.64D+00  1.86D+00
 E= -723.284621499405     Delta-E=        0.000000000025 Rises=F Damp=F
 DIIS: error= 5.52D-09 at cycle  16 NSaved=  16.
 NSaved=16 IEnMin=15 EnMin= -723.284621499430     IErMin=16 ErrMin= 5.52D-09
 ErrMax= 5.52D-09  0.00D+00 EMaxC= 1.00D+00 BMatC= 5.17D-15 BMatP= 2.44D-14
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.181D-06 0.859D-06 0.125D-05-0.830D-05-0.628D-04 0.198D-03
 Coeff-Com:  0.506D-03-0.108D-03-0.272D-02-0.266D-02 0.743D-02 0.274D-01
 Coeff-Com: -0.106D+00-0.921D-01 0.239D+00 0.929D+00
 Coeff:      0.181D-06 0.859D-06 0.125D-05-0.830D-05-0.628D-04 0.198D-03
 Coeff:      0.506D-03-0.108D-03-0.272D-02-0.266D-02 0.743D-02 0.274D-01
 Coeff:     -0.106D+00-0.921D-01 0.239D+00 0.929D+00
 Gap=     0.180 Goal=   None    Shift=    0.000
 RMSDP=7.49D-09 MaxDP=3.04D-07 DE= 2.48D-11 OVMax= 1.84D-07

 SCF Done:  E(RwB97XD) =  -723.284621499     A.U. after   22 cycles
          NFock= 22  Conv=0.75D-08     -V/T= 2.0060
 KE= 7.189644838602D+02 PE=-3.646042812833D+03 EE= 1.221418794777D+03
 Leave Link  502 at Fri Sep 25 19:51:10 2026, MaxMem=    805306368 cpu:             7981.5 elap:
1330.7
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   22800 LenP2D=   50775.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 Leave Link  701 at Fri Sep 25 19:51:10 2026, MaxMem=    805306368 cpu:                2.6 elap:
0.4
 (Enter /home/user/gauss16/g16/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link  702 at Fri Sep 25 19:51:10 2026, MaxMem=    805306368 cpu:                0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l703.exe)
 Integral derivatives from FoFJK, PRISM(SPDF).
 Compute integral first derivatives, UseDBF=F ICtDFT=          0.
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=         800
        NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
        wScrn=  0.000000 ICntrl=      2527 IOpCl=  0 I1Cent=          0 NGrid=          0
        NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
```

Supporting Information file

Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 20:00:41 2026, MaxMem= 805306368 cpu: 3421.0 elap: 570.3
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-6.75842918D+00 5.07401962D-03-3.23641122D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000869121	-0.000989701	0.001311419
2	6	-0.003604591	0.000222119	-0.001359535
3	6	0.000836120	0.000998456	-0.001312682
4	6	0.001222446	0.001348090	0.000639829
5	6	-0.003576525	-0.000239709	0.001362160
6	6	-0.002090531	-0.004356104	-0.000497013
7	6	0.001208790	-0.001328838	-0.000647030
8	6	-0.002971789	0.003482961	0.000804095
9	6	-0.002078125	0.004337627	0.000503739
10	6	0.005073697	-0.006906182	0.004624325
11	6	-0.002964536	-0.003479300	-0.000795433
12	6	0.022374958	0.045889982	0.017837788
13	6	0.005062382	0.006903315	-0.004636256
14	6	0.022395668	-0.045951329	-0.017702172
15	6	-0.050760635	-0.047797380	-0.017891308
16	6	-0.050643322	0.047728794	0.017658478
17	7	0.046071267	0.015528544	0.003921495
18	7	0.046326430	-0.015467367	-0.003909674
19	1	-0.001845180	-0.026435007	0.007786866
20	1	0.004200279	-0.023145233	-0.003680813
21	1	-0.001908708	0.026471141	-0.007816950
22	1	0.003943083	0.023144541	0.003677070
23	1	-0.001200576	-0.021453703	-0.019723183
24	1	-0.017320810	0.042343513	0.012745958
25	1	-0.017449870	-0.042348399	-0.012599973
26	1	-0.001169044	0.021499172	0.019698803

Cartesian Forces: Max 0.050760635 RMS 0.019665396
Leave Link 716 at Fri Sep 25 20:00:41 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.076139709 RMS 0.020735918
Search for a local minimum.

Supporting Information file

Step number 4 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .20736D-01 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 3 4
ITU= 0 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00436	0.00919	0.01659	0.01660	0.01764
Eigenvalues ---	0.01779	0.02161	0.02402	0.02739	0.02815
Eigenvalues ---	0.03099	0.03295	0.03791	0.03839	0.04440
Eigenvalues ---	0.04465	0.04470	0.04997	0.05026	0.05026
Eigenvalues ---	0.05028	0.08684	0.09040	0.09813	0.10417
Eigenvalues ---	0.10423	0.10825	0.10834	0.14872	0.15897
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16001	0.18853	0.24966	0.24997	0.24998
Eigenvalues ---	0.25000	0.25000	0.25000	0.25000	0.25000
Eigenvalues ---	0.25505	0.37230	0.37505	0.39225	0.40643
Eigenvalues ---	0.41503	0.45815	0.46092	0.47688	0.47688
Eigenvalues ---	0.47688	0.47688	0.47698	0.48391	0.51082
Eigenvalues ---	0.54777	0.55320	0.55521	0.55657	0.55732
Eigenvalues ---	0.93624	0.94067	0.95016	0.95779	0.97652
Eigenvalues ---	0.98122	1.36035			

RFO step: Lambda=-1.11021797D-01 EMin= 4.35529054D-03
Quartic linear search produced a step of -0.29690.
Maximum step size (0.505) exceeded in Quadratic search.
-- Step size scaled by 0.728
Iteration 1 RMS(Cart)= 0.14587788 RMS(Int)= 0.00702820
Iteration 2 RMS(Cart)= 0.01229139 RMS(Int)= 0.00018992
Iteration 3 RMS(Cart)= 0.00005463 RMS(Int)= 0.00018700
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00018700
ITry= 1 IFail=0 DXMaxC= 4.02D-01 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.31638	0.00095	-0.00100	0.00090	-0.00010	2.31628
R2	2.54962	-0.00053	-0.00038	-0.00028	-0.00066	2.54896
R3	2.54868	-0.00238	-0.00057	-0.00192	-0.00248	2.54619
R4	2.31638	0.00095	-0.00100	0.00090	-0.00010	2.31627
R5	2.31532	-0.00154	-0.00163	-0.00041	-0.00204	2.31328
R6	2.54869	-0.00238	-0.00057	-0.00191	-0.00248	2.54621
R7	2.55070	-0.00435	-0.00055	-0.00378	-0.00433	2.54637
R8	2.31527	-0.00154	-0.00162	-0.00042	-0.00203	2.31324
R9	2.31531	-0.00585	-0.00304	-0.00251	-0.00555	2.30976
R10	2.55077	-0.00434	-0.00056	-0.00376	-0.00432	2.54644
R11	2.66114	-0.00460	-0.00299	-0.00374	-0.00673	2.65441
R12	2.31520	-0.00583	-0.00303	-0.00250	-0.00553	2.30967
R13	2.72477	-0.02217	-0.01594	-0.01992	-0.03586	2.68891
R14	2.72885	-0.01694	-0.00311	-0.01810	-0.02121	2.70763

R15	2.66135	-0.00460	-0.00302	-0.00373	-0.00674	2.65461
R16	2.72839	-0.01694	-0.00305	-0.01812	-0.02116	2.70723
R17	2.92250	-0.06912	-0.10667	-0.03961	-0.14629	2.77621
R18	2.14075	-0.02423	-0.01682	-0.02700	-0.04382	2.09693
R19	2.92288	-0.06922	-0.10672	-0.03968	-0.14640	2.77648
R20	2.14035	-0.02410	-0.01676	-0.02685	-0.04361	2.09673
R21	2.02999	-0.02478	-0.01986	-0.02197	-0.04183	1.98816
R22	1.93991	-0.00790	-0.00711	-0.00702	-0.01413	1.92578
R23	2.00594	-0.02596	-0.01646	-0.02432	-0.04078	1.96516
R24	2.03006	-0.02483	-0.01987	-0.02202	-0.04189	1.98816
R25	1.93930	-0.00766	-0.00702	-0.00678	-0.01380	1.92550
R26	2.00603	-0.02597	-0.01647	-0.02432	-0.04079	1.96524
A1	2.54489	0.00043	0.00224	0.00120	0.00343	2.54832
A2	2.60718	0.00135	0.00050	0.00321	0.00371	2.61089
A3	2.54472	0.00046	0.00223	0.00123	0.00346	2.54818
A4	2.71570	-0.00217	0.00105	-0.00350	-0.00246	2.71325
A5	2.60733	0.00133	0.00051	0.00317	0.00368	2.61101
A6	2.85378	0.00020	-0.00224	0.00140	-0.00085	2.85294
A7	2.71562	-0.00216	0.00104	-0.00348	-0.00244	2.71318
A8	2.85383	0.00019	-0.00224	0.00138	-0.00086	2.85298
A9	2.05571	0.00365	0.01192	0.00029	0.01221	2.06792
A10	2.04211	0.01677	0.00132	0.03005	0.03137	2.07347
A11	2.18532	-0.02041	-0.01323	-0.03030	-0.04353	2.14178
A12	2.05571	0.00364	0.01192	0.00027	0.01219	2.06790
A13	2.18532	-0.02039	-0.01323	-0.03025	-0.04349	2.14183
A14	2.04211	0.01675	0.00132	0.03002	0.03134	2.07345
A15	1.68913	0.07605	-0.01557	0.22128	0.20571	1.89484
A16	2.10360	-0.01239	-0.07426	0.01790	-0.05636	2.04724
A17	1.68869	0.07614	-0.01552	0.22152	0.20601	1.89470
A18	2.10447	-0.01247	-0.07440	0.01769	-0.05670	2.04777
A19	2.06955	-0.00568	-0.02181	-0.00205	-0.02399	2.04557
A20	2.06653	-0.02276	-0.02129	-0.06093	-0.08281	1.98371
A21	2.00698	-0.00846	-0.01317	-0.01027	-0.02375	1.98323
A22	1.75847	0.01728	0.02234	0.03547	0.05749	1.81597
A23	1.73400	0.01336	0.02534	0.02584	0.05129	1.78529
A24	1.77373	0.01569	0.01984	0.03135	0.05051	1.82424
A25	2.06938	-0.00570	-0.02179	-0.00207	-0.02398	2.04540
A26	2.06654	-0.02279	-0.02130	-0.06105	-0.08294	1.98360
A27	2.00735	-0.00847	-0.01322	-0.01027	-0.02380	1.98355
A28	1.75848	0.01728	0.02234	0.03550	0.05752	1.81599
A29	1.73383	0.01339	0.02536	0.02591	0.05139	1.78522
A30	1.77364	0.01573	0.01986	0.03144	0.05061	1.82426
A31	2.96209	-0.00525	-0.00329	-0.01807	-0.02136	2.94074
A32	3.11021	0.00177	-0.01017	0.01545	0.00528	3.11549
A33	2.96206	-0.00524	-0.00329	-0.01805	-0.02134	2.94071
A34	3.11017	0.00177	-0.01016	0.01543	0.00527	3.11544
A35	3.79273	0.06366	-0.08983	0.23918	0.14935	3.94208
A36	3.79316	0.06367	-0.08991	0.23922	0.14930	3.94246

A37	3.13662	0.00083	0.00065	0.00376	0.00444	3.14106
A38	3.16068	0.00110	-0.00267	0.00737	0.00463	3.16531
A39	3.13678	0.00083	0.00065	0.00373	0.00442	3.14119
A40	3.16069	0.00111	-0.00267	0.00744	0.00469	3.16538
A41	3.23744	0.02129	-0.01357	0.08669	0.07311	3.31055
A42	3.23730	0.02124	-0.01355	0.08644	0.07289	3.31019
D1	0.00135	0.00058	-0.00015	0.00297	0.00284	0.00419
D2	-0.00245	0.00011	0.00021	0.00126	0.00149	-0.00095
D3	0.00270	0.00017	-0.00038	0.00102	0.00063	0.00333
D4	0.00130	0.00058	-0.00015	0.00298	0.00285	0.00415
D5	0.00779	0.00063	-0.00093	0.00247	0.00151	0.00930
D6	0.00279	0.00017	-0.00038	0.00102	0.00063	0.00342
D7	-0.00461	0.00044	0.00035	0.00197	0.00222	-0.00239
D8	-3.12482	0.00082	-0.00253	0.00445	0.00192	-3.12290
D9	0.00761	0.00063	-0.00093	0.00249	0.00152	0.00913
D10	-0.00423	0.00044	0.00034	0.00196	0.00220	-0.00202
D11	-3.12451	0.00082	-0.00252	0.00446	0.00194	-3.12257
D12	-0.01657	-0.00126	0.00246	-0.00713	-0.00474	-0.02132
D13	3.11387	-0.00005	0.00409	-0.00270	0.00135	3.11522
D14	3.11372	-0.00005	0.00411	-0.00271	0.00136	3.11508
D15	-0.03902	0.00116	0.00574	0.00172	0.00745	-0.03157
D16	2.57138	0.00706	0.00048	0.03608	0.03662	2.60800
D17	-0.55899	0.00593	-0.00119	0.03186	0.03062	-0.52838
D18	-0.55556	0.00593	-0.00116	0.03182	0.03060	-0.52497
D19	2.57496	0.00705	0.00049	0.03605	0.03660	2.61156
D20	-1.76115	0.00315	0.00042	0.01229	0.01239	-1.74876
D21	0.37544	0.00107	-0.00607	0.00347	-0.00289	0.37255
D22	2.47547	-0.00369	-0.00675	-0.01332	-0.01947	2.45600
D23	-1.76618	0.00316	0.00045	0.01234	0.01247	-1.75371
D24	0.37026	0.00106	-0.00602	0.00344	-0.00287	0.36739
D25	2.47050	-0.00369	-0.00673	-0.01336	-0.01948	2.45101

Item	Value	Threshold	Converged?
Maximum Force	0.076140	0.000450	NO
RMS Force	0.020736	0.000300	NO
Maximum Displacement	0.402370	0.001800	NO
RMS Displacement	0.147894	0.001200	NO

Predicted change in Energy=-7.110033D-02
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 20:00:41 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	4.219312	0.672083	-0.051808
2	6	0	3.534097	1.685270	-0.131356
3	6	0	4.219232	-0.672682	0.053117
4	6	0	2.319024	2.265938	-0.174669
5	6	0	3.533754	-1.685714	0.132321
6	6	0	1.095111	2.288952	-0.171431
7	6	0	2.318595	-2.266264	0.175070
8	6	0	-0.203476	1.931366	-0.132555
9	6	0	1.094700	-2.289083	0.171225
10	6	0	-1.292647	1.379241	-0.079550
11	6	0	-0.203860	-1.931325	0.131751
12	6	0	-2.527296	0.710125	-0.048162
13	6	0	-1.292888	-1.379047	0.078403
14	6	0	-2.527474	-0.709616	0.046716
15	6	0	-3.732572	1.481655	-0.119013
16	6	0	-3.732736	-1.480810	0.117096
17	7	0	-4.034494	2.899195	0.121192
18	7	0	-4.033865	-2.899121	-0.120405
19	1	0	-3.624023	3.598633	-0.549023
20	1	0	-5.031338	3.110911	0.119913
21	1	0	-3.621101	-3.597068	0.549959
22	1	0	-5.030370	-3.111689	-0.116323
23	1	0	-3.695076	3.247748	1.040289
24	1	0	-4.512324	0.873449	-0.622392
25	1	0	-4.513414	-0.871092	0.616967
26	1	0	-3.696357	-3.248977	-1.039759

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.225723	0.000000			
3	C	1.348852	2.462393	0.000000		
4	C	2.483257	1.347388	3.506874	0.000000	
5	C	2.462336	3.381281	1.225719	4.145524	0.000000
6	C	3.519831	2.512905	4.310665	1.224133	4.673031
7	C	3.506862	4.145596	2.483304	4.545676	1.347397
8	C	4.599278	3.745666	5.135746	2.544939	5.207717
9	C	4.310620	4.673082	3.519858	4.729358	2.512877
10	C	5.557205	4.836713	5.882924	3.720140	5.721275
11	C	5.135745	5.207812	4.599359	4.906715	3.745675
12	C	6.746716	6.139895	6.887528	5.091499	6.519888
13	C	5.882893	5.721348	5.557252	5.137690	4.836675
14	C	6.887518	6.519956	6.746809	5.691350	6.139917
15	C	7.993271	7.269531	8.240266	6.102459	7.930630
16	C	8.240057	7.930489	7.993182	7.123695	7.269394
17	N	8.550746	7.669482	8.993716	6.391849	8.848723
18	N	8.992949	8.848210	8.549898	8.187794	7.668448
19	H	8.386287	7.421191	8.951165	6.102132	8.923134

20	H	9.568275	8.686902	9.994653	7.404632	9.816750
21	H	8.947616	8.919873	8.382702	8.377649	7.417523
22	H	9.993883	9.816370	9.567267	9.106912	8.685588
23	H	8.394299	7.488326	8.887100	6.213651	8.798831
24	H	8.752575	8.102164	8.893082	6.986186	8.476926
25	H	8.893208	8.476875	8.753079	7.559752	8.102802
26	H	8.888676	8.800650	8.395726	8.206550	7.489464

		6	7	8	9	10
6	C	0.000000				
7	C	4.729374	0.000000			
8	C	1.347481	4.906687	0.000000		
9	C	4.590841	1.224114	4.426029	0.000000	
10	C	2.556835	5.137666	1.222271	4.383938	0.000000
11	C	4.426058	2.544964	3.871724	1.347518	3.491411
12	C	3.953444	5.691343	2.626536	4.707678	1.404656
13	C	4.383968	3.720122	3.491441	2.556825	2.762806
14	C	4.707666	5.091563	3.522484	3.953524	2.429828
15	C	4.894997	7.123904	3.557660	6.132312	2.442392
16	C	6.132085	6.102369	4.915379	4.894933	3.764650
17	N	5.174057	8.188200	3.959518	7.295845	3.141382
18	N	7.295554	6.390741	6.164872	5.172946	5.081371
19	H	4.912033	8.380694	3.827972	7.579597	3.252909
20	H	6.188205	9.107062	4.976276	8.166450	4.125079
21	H	7.576826	6.098489	6.535256	4.908466	5.530066
22	H	8.166485	7.403171	6.980801	6.186747	5.842976
23	H	5.033234	8.204704	3.911483	7.372497	3.242996
24	H	5.800891	7.560106	4.463777	6.486151	3.304061
25	H	6.485600	6.986997	5.195299	5.801752	3.990298
26	H	7.374335	6.214594	6.313414	5.034094	5.302850

		11	12	13	14	15
11	C	0.000000				
12	C	3.522497	0.000000			
13	C	1.222227	2.429902	0.000000		
14	C	2.626592	1.422908	1.404757	0.000000	
15	C	4.915600	1.432818	3.764923	2.506272	0.000000
16	C	3.557548	2.506111	2.442276	1.432603	2.971859
17	N	6.165046	2.663147	5.081495	3.911544	1.469107
18	N	3.958428	3.911730	3.140558	2.662908	4.391125
19	H	6.537691	3.130039	5.532192	4.485347	2.162935
20	H	6.980604	3.473075	5.842727	4.568493	2.097226
21	H	3.824543	4.483980	3.250009	3.128363	5.123805
22	H	4.974937	4.569058	4.124165	3.472898	4.773163
23	H	6.311642	2.997993	5.301222	4.243962	2.112930
24	H	5.195994	2.072861	3.991193	2.625535	1.109647
25	H	4.464503	2.624369	3.304521	2.072492	2.585885
26	H	3.912311	4.245522	3.244008	2.999178	4.819539

		16	17	18	19	20
16	C	0.000000				

```
  17  N    4.390389   0.000000
  18  N    1.469249   5.803348   0.000000
  19  H    5.124087   1.052087   6.524760   0.000000
  20  H    4.771821   1.019080   6.096982   1.632753   0.000000
  21  H    2.162957   6.523509   1.052090   7.279140   6.868093
  22  H    2.097166   6.097451   1.018932   6.869749   6.227082
  23  H    4.817983   1.039920   6.264662   1.629135   1.628316
  24  H    2.587882   2.210177   3.835779   2.867243   2.413841
  25  H    1.109543   3.832783   2.210563   4.704146   4.046191
  26  H    2.113304   6.265952   1.039963   6.865552   6.601150
                21         22         23         24         25
  21  H    0.000000
  22  H    1.632656   0.000000
  23  H    6.862754   6.600242   0.000000
  24  H    4.706826   4.050407   3.011593   0.000000
  25  H    2.869087   2.413551   4.220630   2.139962   0.000000
  26  H    1.629121   1.628242   6.821585   4.223079   3.011090
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=2 Diff= 4.75D-04
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.636838   -0.673723    0.033920
    2          6           0        3.951506   -1.688620    0.085892
    3          6           0        4.636913    0.673393   -0.034494
    4          6           0        2.736367   -2.270115    0.113320
    5          6           0        3.951552    1.688276   -0.086262
    6          6           0        1.512452   -2.292898    0.109338
    7          6           0        2.736460    2.269906   -0.113370
    8          6           0        0.213908   -1.934247    0.080045
    9          6           0        1.512567    2.292746   -0.109029
   10          6           0       -0.875199   -1.380767    0.041926
   11          6           0        0.213965    1.934192   -0.079401
   12          6           0       -2.109773   -0.710911    0.028575
   13          6           0       -0.875128    1.380790   -0.041159
   14          6           0       -2.109789    0.710882   -0.027762
   15          6           0       -3.315139   -1.483945    0.078356
   16          6           0       -3.314961    1.483833   -0.077321
   17          7           0       -3.617188   -2.894416   -0.200237
```

```
    18        7        0       -3.615963    2.895215    0.198531
    19        1        0       -3.206861   -3.611819    0.450802
    20        1        0       -4.614056   -3.105979   -0.204800
    21        1        0       -3.203055    3.611041   -0.452617
    22        1        0       -4.612444    3.107924    0.200116
    23        1        0       -3.277714   -3.217950   -1.128416
    24        1        0       -4.094877   -0.889530    0.597967
    25        1        0       -4.095654    0.887983   -0.593622
    26        1        0       -3.278511    3.219970    1.127068
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6026251           0.2523287           0.1786145
 Leave Link  202 at Fri Sep 25 20:00:41 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy       993.7397150279 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.222036 cShort=  0.000000 cLong=
0.777964
  DFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.000000 cShort=  0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0145743959 Hartrees.
 Nuclear repulsion after empirical dispersion term =      993.7251406319 Hartrees.
 Leave Link  301 at Fri Sep 25 20:00:41 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   22935 LenP2D=   51168.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.89D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
```

Supporting Information file

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 681 681 681 681 681 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Fri Sep 25 20:00:42 2026, MaxMem= 805306368 cpu: 6.2 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 20:00:42 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 0.999999 -0.001057 0.000005 -0.000006 Ang= -0.12 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.985932277937
Leave Link 401 at Fri Sep 25 20:00:50 2026, MaxMem= 805306368 cpu: 45.9 elap: 7.7
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.

E= -723.339075459089
DIIS: error= 3.74D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.339075459089 IErMin= 1 ErrMin= 3.74D-03
ErrMax= 3.74D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-02 BMatP= 2.22D-02
IDIUse=3 WtCom= 9.63D-01 WtEn= 3.74D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.730 Goal= None Shift= 0.000
GapD= 0.730 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=5.30D-03 MaxDP=1.75D-01 OVMax= 3.95D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 4.96D-03 CP: 9.00D-01
E= -723.359124881677 Delta-E= -0.020049422588 Rises=F Damp=F
DIIS: error= 1.19D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.359124881677 IErMin= 2 ErrMin= 1.19D-03
ErrMax= 1.19D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.43D-03 BMatP= 2.22D-02
IDIUse=3 WtCom= 9.88D-01 WtEn= 1.19D-02
Coeff-Com: 0.251D-01 0.975D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.248D-01 0.975D+00
Gap= 0.172 Goal= None Shift= 0.000
RMSDP=3.70D-01 MaxDP=1.42D+01 DE=-2.00D-02 OVMax= 3.18D-02

Cycle 3 Pass 0 IDiag 1:
RMSU= 3.41D-01 CP: 3.00D+00 3.00D+00
E= -723.361758574799 Delta-E= -0.002633693122 Rises=F Damp=F
DIIS: error= 1.22D-02 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.361758574799 IErMin= 2 ErrMin= 1.19D-03
ErrMax= 1.22D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.33D-03 BMatP= 1.43D-03
IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.000D+00 0.000D+00 0.100D+01
Gap= -1.984 Goal= None Shift= 0.000
RMSDP=6.92D+02 MaxDP=2.58D+04 DE=-2.63D-03 OVMax= 9.91D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.358847872151 Delta-E= 0.002910702648 Rises=F Damp=F
DIIS: error= 3.97D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.358847872151 IErMin= 1 ErrMin= 3.97D-03
ErrMax= 3.97D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-03 BMatP= 2.15D-03
IDIUse=3 WtCom= 9.60D-01 WtEn= 3.97D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01

Gap= 0.963 Goal= None Shift= 0.000
GapD= 0.963 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=3.54D-01 MaxDP=1.36D+01 DE= 2.91D-03 OVMax= 2.23D-02

Cycle 5 Pass 1 IDiag 1:
RMSU= 1.44D-02 CP: 7.84D-02
E= -723.359686516611 Delta-E= -0.000838644459 Rises=F Damp=F
DIIS: error= 1.45D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.359686516611 IErMin= 2 ErrMin= 1.45D-03
ErrMax= 1.45D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.41D-03 BMatP= 2.15D-03
IDIUse=3 WtCom= 9.86D-01 WtEn= 1.45D-02
Coeff-Com: 0.436D+00 0.564D+00
Coeff-En: 0.314D+00 0.686D+00
Coeff: 0.434D+00 0.566D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=7.53D-03 MaxDP=2.81D-01 DE=-8.39D-04 OVMax= 1.41D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.03D-03 CP: 5.91D-02 9.43D-01
E= -723.360877847144 Delta-E= -0.001191330533 Rises=F Damp=F
DIIS: error= 7.90D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.360877847144 IErMin= 3 ErrMin= 7.90D-04
ErrMax= 7.90D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-04 BMatP= 1.41D-03
IDIUse=3 WtCom= 9.92D-01 WtEn= 7.90D-03
Coeff-Com: 0.286D-01 0.236D+00 0.735D+00
Coeff-En: 0.000D+00 0.427D-01 0.957D+00
Coeff: 0.284D-01 0.235D+00 0.737D+00
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=5.72D-03 MaxDP=2.28D-01 DE=-1.19D-03 OVMax= 5.77D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.17D-04 CP: 4.46D-02 8.72D-01 1.81D+00
E= -723.361006032431 Delta-E= -0.000128185287 Rises=F Damp=F
DIIS: error= 4.67D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.361006032431 IErMin= 4 ErrMin= 4.67D-04
ErrMax= 4.67D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.29D-05 BMatP= 1.46D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.67D-03
Coeff-Com: -0.230D-01 0.994D-01 0.471D+00 0.452D+00
Coeff-En: 0.000D+00 0.000D+00 0.210D+00 0.790D+00
Coeff: -0.229D-01 0.990D-01 0.470D+00 0.454D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=8.92D-04 MaxDP=3.55D-02 DE=-1.28D-04 OVMax= 2.99D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.51D-05 CP: 4.23D-02 8.61D-01 1.96D+00 1.08D+00
E= -723.361069910168 Delta-E= -0.000063877737 Rises=F Damp=F
DIIS: error= 5.41D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.361069910168 IErMin= 5 ErrMin= 5.41D-05

ErrMax= 5.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.62D-07 BMatP= 5.29D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.110D-02-0.170D-01-0.586D-01-0.986D-02 0.109D+01
Coeff: -0.110D-02-0.170D-01-0.586D-01-0.986D-02 0.109D+01
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=3.09D-04 MaxDP=1.38D-02 DE=-6.39D-05 OVMax= 2.67D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 4.84D-05 CP: 4.16D-02 8.56D-01 2.03D+00 1.10D+00 1.39D+00
E= -723.361076436422 Delta-E= -0.000006526254 Rises=F Damp=F
DIIS: error= 4.66D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.361076436422 IErMin= 6 ErrMin= 4.66D-05
ErrMax= 4.66D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.10D-07 BMatP= 8.62D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.662D-02-0.417D-01-0.185D+00-0.154D+00 0.651D+00 0.724D+00
Coeff: 0.662D-02-0.417D-01-0.185D+00-0.154D+00 0.651D+00 0.724D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=4.35D-05 MaxDP=1.85D-03 DE=-6.53D-06 OVMax= 1.98D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.10D-05 CP: 4.15D-02 8.56D-01 2.05D+00 1.07D+00 1.77D+00
CP: 1.68D+00
E= -723.361079268551 Delta-E= -0.000002832129 Rises=F Damp=F
DIIS: error= 2.33D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.361079268551 IErMin= 7 ErrMin= 2.33D-05
ErrMax= 2.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-07 BMatP= 6.10D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.330D-02-0.150D-01-0.696D-01-0.704D-01-0.148D-02 0.360D+00
Coeff-Com: 0.793D+00
Coeff: 0.330D-02-0.150D-01-0.696D-01-0.704D-01-0.148D-02 0.360D+00
Coeff: 0.793D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.28D-04 MaxDP=4.93D-03 DE=-2.83D-06 OVMax= 1.07D-03

Cycle 11 Pass 1 IDiag 1:
RMSU= 4.79D-06 CP: 4.18D-02 8.59D-01 2.03D+00 1.04D+00 2.00D+00
CP: 2.12D+00 2.43D+00
E= -723.361080050596 Delta-E= -0.000000782045 Rises=F Damp=F
DIIS: error= 1.03D-05 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.361080050596 IErMin= 8 ErrMin= 1.03D-05
ErrMax= 1.03D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.05D-08 BMatP= 1.42D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.970D-03 0.838D-02 0.368D-01 0.255D-01-0.241D+00-0.858D-01
Coeff-Com: 0.345D+00 0.912D+00
Coeff: -0.970D-03 0.838D-02 0.368D-01 0.255D-01-0.241D+00-0.858D-01
Coeff: 0.345D+00 0.912D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.29D-04 MaxDP=5.05D-03 DE=-7.82D-07 OVMax= 6.82D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 8.63D-06 CP: 4.21D-02 8.61D-01 2.00D+00 1.02D+00 2.14D+00
CP: 2.40D+00 3.00D+00 1.98D+00
E= -723.361080246813 Delta-E= -0.000000196217 Rises=F Damp=F
DIIS: error= 5.91D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.361080246813 IErMin= 9 ErrMin= 5.91D-06
ErrMax= 5.91D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.89D-09 BMatP= 3.05D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.852D-03 0.555D-02 0.254D-01 0.202D-01-0.113D+00-0.792D-01
Coeff-Com: 0.579D-01 0.382D+00 0.702D+00
Coeff: -0.852D-03 0.555D-02 0.254D-01 0.202D-01-0.113D+00-0.792D-01
Coeff: 0.579D-01 0.382D+00 0.702D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=2.01D-05 MaxDP=8.39D-04 DE=-1.96D-07 OVMax= 1.57D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 7.23D-07 CP: 4.22D-02 8.61D-01 2.00D+00 1.02D+00 2.16D+00
CP: 2.46D+00 3.00D+00 2.33D+00 1.43D+00
E= -723.361080264537 Delta-E= -0.000000017723 Rises=F Damp=F
DIIS: error= 2.62D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.361080264537 IErMin=10 ErrMin= 2.62D-06
ErrMax= 2.62D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-09 BMatP= 4.89D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.194D-03 0.742D-03 0.401D-02 0.398D-02-0.445D-03-0.152D-01
Coeff-Com: -0.486D-01-0.366D-01 0.365D+00 0.728D+00
Coeff: -0.194D-03 0.742D-03 0.401D-02 0.398D-02-0.445D-03-0.152D-01
Coeff: -0.486D-01-0.366D-01 0.365D+00 0.728D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=2.05D-06 MaxDP=1.15D-04 DE=-1.77D-08 OVMax= 5.83D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 3.72D-07 CP: 4.22D-02 8.61D-01 2.00D+00 1.02D+00 2.16D+00
CP: 2.48D+00 3.00D+00 2.48D+00 1.57D+00 1.78D+00
E= -723.361080269109 Delta-E= -0.000000004572 Rises=F Damp=F
DIIS: error= 1.48D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.361080269109 IErMin=11 ErrMin= 1.48D-06
ErrMax= 1.48D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.47D-10 BMatP= 1.54D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.163D-03-0.133D-02-0.567D-02-0.409D-02 0.335D-01 0.188D-01
Coeff-Com: -0.400D-01-0.142D+00-0.384D-01 0.354D+00 0.825D+00
Coeff: 0.163D-03-0.133D-02-0.567D-02-0.409D-02 0.335D-01 0.188D-01
Coeff: -0.400D-01-0.142D+00-0.384D-01 0.354D+00 0.825D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=3.73D-06 MaxDP=1.88D-04 DE=-4.57D-09 OVMax= 3.19D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.17D-07 CP: 4.22D-02 8.61D-01 2.00D+00 1.02D+00 2.16D+00

```
              CP:  2.49D+00  3.00D+00  2.54D+00  1.59D+00  2.30D+00
              CP:  1.85D+00
E= -723.361080270506     Delta-E=       -0.000000001397 Rises=F Damp=F
DIIS: error= 5.44D-07 at cycle  12 NSaved=  12.
NSaved=12 IEnMin=12 EnMin= -723.361080270506     IErMin=12 ErrMin= 5.44D-07
ErrMax= 5.44D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.65D-11 BMatP= 3.47D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.525D-04-0.308D-03-0.141D-02-0.115D-02 0.383D-02 0.574D-02
Coeff-Com:  0.157D-02-0.185D-01-0.605D-01-0.436D-01 0.116D+00 0.999D+00
Coeff:      0.525D-04-0.308D-03-0.141D-02-0.115D-02 0.383D-02 0.574D-02
Coeff:      0.157D-02-0.185D-01-0.605D-01-0.436D-01 0.116D+00 0.999D+00
Gap=     0.177 Goal=   None    Shift=    0.000
RMSDP=1.57D-06 MaxDP=7.14D-05 DE=-1.40D-09 OVMax= 1.43D-05

Cycle  16  Pass 1  IDiag  1:
RMSU=  8.84D-08    CP:  4.22D-02  8.61D-01  2.00D+00  1.02D+00  2.16D+00
              CP:  2.49D+00  3.00D+00  2.54D+00  1.57D+00  2.42D+00
              CP:  2.11D+00  1.68D+00
E= -723.361080270785     Delta-E=       -0.000000000279 Rises=F Damp=F
DIIS: error= 2.24D-07 at cycle  13 NSaved=  13.
NSaved=13 IEnMin=13 EnMin= -723.361080270785     IErMin=13 ErrMin= 2.24D-07
ErrMax= 2.24D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 9.86D-12 BMatP= 3.65D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.293D-04 0.268D-03 0.114D-02 0.761D-03-0.763D-02-0.263D-02
Coeff-Com:  0.119D-01 0.317D-01-0.563D-02-0.100D+00-0.192D+00 0.258D+00
Coeff-Com:  0.101D+01
Coeff:     -0.293D-04 0.268D-03 0.114D-02 0.761D-03-0.763D-02-0.263D-02
Coeff:      0.119D-01 0.317D-01-0.563D-02-0.100D+00-0.192D+00 0.258D+00
Coeff:      0.101D+01
Gap=     0.177 Goal=   None    Shift=    0.000
RMSDP=7.51D-07 MaxDP=3.27D-05 DE=-2.79D-10 OVMax= 1.05D-05

Cycle  17  Pass 1  IDiag  1:
RMSU=  3.51D-08    CP:  4.22D-02  8.61D-01  2.00D+00  1.02D+00  2.15D+00
              CP:  2.48D+00  3.00D+00  2.53D+00  1.55D+00  2.41D+00
              CP:  2.22D+00  2.16D+00  1.75D+00
E= -723.361080270890     Delta-E=       -0.000000000105 Rises=F Damp=F
DIIS: error= 1.25D-07 at cycle  14 NSaved=  14.
NSaved=14 IEnMin=14 EnMin= -723.361080270890     IErMin=14 ErrMin= 1.25D-07
ErrMax= 1.25D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.12D-12 BMatP= 9.86D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.210D-04 0.155D-03 0.677D-03 0.501D-03-0.343D-02-0.200D-02
Coeff-Com:  0.333D-02 0.136D-01 0.999D-02-0.226D-01-0.884D-01-0.153D+00
Coeff-Com:  0.387D+00 0.855D+00
Coeff:     -0.210D-04 0.155D-03 0.677D-03 0.501D-03-0.343D-02-0.200D-02
Coeff:      0.333D-02 0.136D-01 0.999D-02-0.226D-01-0.884D-01-0.153D+00
Coeff:      0.387D+00 0.855D+00
Gap=     0.177 Goal=   None    Shift=    0.000
```

RMSDP=1.07D-07 MaxDP=4.17D-06 DE=-1.05D-10 OVMax= 4.00D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.61D-08 CP: 4.22D-02 8.61D-01 2.00D+00 1.02D+00 2.15D+00
CP: 2.48D+00 3.00D+00 2.53D+00 1.54D+00 2.39D+00
CP: 2.18D+00 2.26D+00 2.17D+00 1.76D+00
E= -723.361080270916 Delta-E= -0.000000000026 Rises=F Damp=F
DIIS: error= 5.84D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.361080270916 IErMin=15 ErrMin= 5.84D-08
ErrMax= 5.84D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-13 BMatP= 3.12D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.413D-05-0.448D-04-0.188D-03-0.114D-03 0.144D-02 0.430D-03
Coeff-Com: -0.254D-02-0.613D-02 0.337D-02 0.236D-01 0.352D-01-0.106D+00
Coeff-Com: -0.156D+00 0.719D-01 0.114D+01
Coeff: 0.413D-05-0.448D-04-0.188D-03-0.114D-03 0.144D-02 0.430D-03
Coeff: -0.254D-02-0.613D-02 0.337D-02 0.236D-01 0.352D-01-0.106D+00
Coeff: -0.156D+00 0.719D-01 0.114D+01
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.19D-07 MaxDP=5.03D-06 DE=-2.59D-11 OVMax= 2.29D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 6.18D-09 CP: 4.22D-02 8.61D-01 2.00D+00 1.02D+00 2.15D+00
CP: 2.48D+00 3.00D+00 2.53D+00 1.54D+00 2.37D+00
CP: 2.13D+00 2.26D+00 2.40D+00 2.41D+00 1.80D+00
E= -723.361080270912 Delta-E= 0.000000000004 Rises=F Damp=F
DIIS: error= 1.86D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -723.361080270916 IErMin=16 ErrMin= 1.86D-08
ErrMax= 1.86D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.24D-14 BMatP= 3.61D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.438D-05-0.378D-04-0.160D-03-0.114D-03 0.992D-03 0.437D-03
Coeff-Com: -0.135D-02-0.407D-02 0.256D-04 0.119D-01 0.249D-01-0.176D-01
Coeff-Com: -0.105D+00-0.107D+00 0.429D+00 0.767D+00
Coeff: 0.438D-05-0.378D-04-0.160D-03-0.114D-03 0.992D-03 0.437D-03
Coeff: -0.135D-02-0.407D-02 0.256D-04 0.119D-01 0.249D-01-0.176D-01
Coeff: -0.105D+00-0.107D+00 0.429D+00 0.767D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=6.07D-08 MaxDP=2.42D-06 DE= 3.87D-12 OVMax= 5.20D-07

Cycle 20 Pass 1 IDiag 1:
RMSU= 2.30D-09 CP: 4.22D-02 8.61D-01 2.00D+00 1.02D+00 2.15D+00
CP: 2.48D+00 3.00D+00 2.53D+00 1.54D+00 2.36D+00
CP: 2.12D+00 2.25D+00 2.45D+00 2.56D+00 1.98D+00
CP: 1.43D+00
E= -723.361080270916 Delta-E= -0.000000000004 Rises=F Damp=F
DIIS: error= 8.39D-09 at cycle 17 NSaved= 17.
NSaved=17 IEnMin=17 EnMin= -723.361080270916 IErMin=17 ErrMin= 8.39D-09
ErrMax= 8.39D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.19D-15 BMatP= 8.24D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.374D-06 0.452D-05 0.194D-04 0.101D-04-0.158D-03-0.425D-04
Coeff-Com: 0.296D-03 0.669D-03-0.459D-03-0.289D-02-0.401D-02 0.152D-01
Coeff-Com: 0.176D-01-0.255D-01-0.138D+00 0.686D-01 0.107D+01
Coeff: -0.374D-06 0.452D-05 0.194D-04 0.101D-04-0.158D-03-0.425D-04
Coeff: 0.296D-03 0.669D-03-0.459D-03-0.289D-02-0.401D-02 0.152D-01
Coeff: 0.176D-01-0.255D-01-0.138D+00 0.686D-01 0.107D+01
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=3.19D-08 MaxDP=1.31D-06 DE=-4.32D-12 OVMax= 1.96D-07

Cycle 21 Pass 1 IDiag 1:
RMSU= 1.19D-09 CP: 4.22D-02 8.61D-01 2.00D+00 1.02D+00 2.15D+00
CP: 2.48D+00 3.00D+00 2.53D+00 1.54D+00 2.36D+00
CP: 2.13D+00 2.25D+00 2.46D+00 2.58D+00 2.00D+00
CP: 1.75D+00 1.71D+00
E= -723.361080270918 Delta-E= -0.000000000001 Rises=F Damp=F
DIIS: error= 3.62D-09 at cycle 18 NSaved= 18.
NSaved=18 IEnMin=18 EnMin= -723.361080270918 IErMin=18 ErrMin= 3.62D-09
ErrMax= 3.62D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-15 BMatP= 7.19D-15
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Large coefficients: NSaved= 18 BigCof= 0.00 CofMax= 10.00 Det=-6.21D-15
Inversion failed. Reducing to 17 matrices.
Large coefficients: NSaved= 17 BigCof= 0.00 CofMax= 10.00 Det=-6.43D-15
Inversion failed. Reducing to 16 matrices.
Large coefficients: NSaved= 16 BigCof= 0.00 CofMax= 10.00 Det=-6.73D-15
Inversion failed. Reducing to 15 matrices.
Coeff-Com: -0.181D-05-0.338D-04 0.667D-05 0.109D-03 0.174D-03-0.321D-03
Coeff-Com: -0.125D-02-0.142D-02 0.749D-02 0.818D-02-0.958D-02-0.747D-01
Coeff-Com: -0.948D-02 0.477D+00 0.604D+00
Coeff: -0.181D-05-0.338D-04 0.667D-05 0.109D-03 0.174D-03-0.321D-03
Coeff: -0.125D-02-0.142D-02 0.749D-02 0.818D-02-0.958D-02-0.747D-01
Coeff: -0.948D-02 0.477D+00 0.604D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=6.04D-09 MaxDP=2.41D-07 DE=-1.14D-12 OVMax= 4.53D-08

SCF Done: E(RwB97XD) = -723.361080271 A.U. after 21 cycles
NFock= 21 Conv=0.60D-08 -V/T= 2.0052
KE= 7.195845484697D+02 PE=-3.669032122253D+03 EE= 1.232361352880D+03
Leave Link 502 at Fri Sep 25 20:25:51 2026, MaxMem= 805306368 cpu: 9006.0 elap: 1501.3
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 22935 LenP2D= 51168.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 20:25:52 2026, MaxMem= 805306368 cpu: 2.9 elap: 0.5

Supporting Information file

(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 20:25:52 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 20:36:15 2026, MaxMem= 805306368 cpu: 3739.5 elap: 623.3
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-6.33036187D+00 3.90848757D-03-3.52634751D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001414567	-0.003408574	0.001384717
2	6	-0.003998404	0.001972893	-0.001352476
3	6	0.001385495	0.003416427	-0.001385502
4	6	0.004566182	0.000257393	0.000671445
5	6	-0.003976274	-0.001989859	0.001354762
6	6	-0.004328179	-0.002665777	-0.000327620
7	6	0.004556192	-0.000239512	-0.000677046
8	6	0.003411513	0.004972546	0.000955589
9	6	-0.004323297	0.002651349	0.000332378
10	6	-0.005006401	-0.005615970	0.002635435
11	6	0.003415059	-0.004965777	-0.000944336
12	6	0.009518225	0.040244612	0.008321806
13	6	-0.005021874	0.005611863	-0.002639858
14	6	0.009507229	-0.040247262	-0.008252707
15	6	-0.032694007	-0.046446551	-0.008375596
16	6	-0.032623177	0.046357850	0.008240955
17	7	0.031638026	0.014116743	-0.001109268
18	7	0.031742813	-0.014037776	0.001112653
19	1	-0.001920555	-0.010143488	0.003786461
20	1	0.000459084	-0.011860988	-0.001593988
21	1	-0.001949342	0.010181785	-0.003801939
22	1	0.000341651	0.011850000	0.001582326
23	1	-0.001644790	-0.010228933	-0.008692986

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    24        1        -0.001398037    0.023742644    0.009782878
    25        1        -0.001436663   -0.023770571   -0.009691779
    26        1        -0.001635036    0.010244935    0.008683697
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.046446551 RMS     0.013927897
 Leave Link  716 at Fri Sep 25 20:36:15 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.045806298 RMS     0.012109360
 Search for a local minimum.
 Step number   5 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .12109D-01 SwitMx=.10000D-02 MixMth= 1
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    4    5
 DE= -7.65D-02 DEPred=-7.11D-02 R= 1.08D+00
 TightC=F SS=  1.41D+00  RLast= 4.99D-01 DXNew= 8.4853D-01 1.4958D+00
 Trust test= 1.08D+00 RLast= 4.99D-01 DXMaxT set to 8.49D-01
 ITU=  1  0  0  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.00437   0.00949   0.01636   0.01660   0.01715
    Eigenvalues ---    0.01761   0.02161   0.02404   0.02740   0.02808
    Eigenvalues ---    0.03101   0.03296   0.03792   0.03838   0.04440
    Eigenvalues ---    0.04462   0.04469   0.04559   0.05026   0.05026
    Eigenvalues ---    0.05028   0.08684   0.09856   0.10208   0.10856
    Eigenvalues ---    0.10927   0.11160   0.11180   0.14934   0.15718
    Eigenvalues ---    0.15975   0.16000   0.16000   0.16000   0.16000
    Eigenvalues ---    0.16502   0.17832   0.24935   0.24992   0.24993
    Eigenvalues ---    0.24997   0.24999   0.25000   0.25000   0.25000
    Eigenvalues ---    0.26100   0.31115   0.37230   0.38698   0.40643
    Eigenvalues ---    0.41033   0.45822   0.46140   0.47674   0.47688
    Eigenvalues ---    0.47688   0.47688   0.47689   0.48503   0.51171
    Eigenvalues ---    0.54786   0.55328   0.55495   0.55658   0.55722
    Eigenvalues ---    0.93648   0.94061   0.95018   0.95822   0.97662
    Eigenvalues ---    0.98345   1.36035
 RFO step:  Lambda=-4.14636274D-02 EMin= 4.36769386D-03
 Quartic linear search produced a step of  1.00690.
 Iteration  1 RMS(Cart)=  0.27883605 RMS(Int)=  0.04707050
 Iteration  2 RMS(Cart)=  0.18825745 RMS(Int)=  0.01157180
 Iteration  3 RMS(Cart)=  0.02703388 RMS(Int)=  0.00073966
 Iteration  4 RMS(Cart)=  0.00029270 RMS(Int)=  0.00072402
 Iteration  5 RMS(Cart)=  0.00000016 RMS(Int)=  0.00072402
```

Supporting Information file

ITry= 1 IFail=0 DXMaxC= 1.15D+00 DCOld= 1.00D+10 DXMaxT= 8.49D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.31628	0.00230	-0.00010	0.00375	0.00363	2.31991
R2	2.54896	-0.00169	-0.00066	-0.00476	-0.00544	2.54352
R3	2.54619	-0.00244	-0.00250	-0.00435	-0.00686	2.53933
R4	2.31627	0.00230	-0.00010	0.00375	0.00363	2.31990
R5	2.31328	0.00197	-0.00205	0.00548	0.00342	2.31670
R6	2.54621	-0.00244	-0.00250	-0.00434	-0.00685	2.53936
R7	2.54637	-0.00284	-0.00436	-0.00266	-0.00701	2.53936
R8	2.31324	0.00196	-0.00205	0.00547	0.00342	2.31667
R9	2.30976	0.00217	-0.00559	0.00981	0.00423	2.31399
R10	2.54644	-0.00284	-0.00435	-0.00265	-0.00700	2.53944
R11	2.65441	-0.00491	-0.00678	-0.01011	-0.01688	2.63754
R12	2.30967	0.00217	-0.00557	0.00980	0.00424	2.31392
R13	2.68891	-0.00378	-0.03611	0.02824	-0.00784	2.68106
R14	2.70763	-0.01700	-0.02136	-0.03937	-0.06073	2.64691
R15	2.65461	-0.00491	-0.00679	-0.01014	-0.01692	2.63769
R16	2.70723	-0.01700	-0.02131	-0.03939	-0.06070	2.64652
R17	2.77621	-0.02459	-0.14730	0.07035	-0.07695	2.69926
R18	2.09693	-0.01647	-0.04412	-0.01967	-0.06379	2.03314
R19	2.77648	-0.02467	-0.14741	0.07033	-0.07708	2.69940
R20	2.09673	-0.01642	-0.04391	-0.01972	-0.06363	2.03310
R21	1.98816	-0.00990	-0.04212	0.01140	-0.03072	1.95744
R22	1.92578	-0.00291	-0.01422	0.00493	-0.00930	1.91649
R23	1.96516	-0.01165	-0.04106	0.00631	-0.03475	1.93042
R24	1.98816	-0.00994	-0.04218	0.01135	-0.03083	1.95733
R25	1.92550	-0.00280	-0.01389	0.00490	-0.00899	1.91651
R26	1.96524	-0.01165	-0.04107	0.00630	-0.03477	1.93048
A1	2.54832	0.00075	0.00345	0.00287	0.00618	2.55450
A2	2.61089	0.00110	0.00373	0.00304	0.00667	2.61755
A3	2.54818	0.00077	0.00348	0.00294	0.00629	2.55446
A4	2.71325	-0.00117	-0.00247	0.00032	-0.00220	2.71104
A5	2.61101	0.00108	0.00371	0.00299	0.00659	2.61760
A6	2.85294	-0.00007	-0.00085	0.00159	0.00074	2.85367
A7	2.71318	-0.00116	-0.00245	0.00038	-0.00213	2.71106
A8	2.85298	-0.00008	-0.00087	0.00157	0.00070	2.85368
A9	2.06792	0.00250	0.01229	0.00888	0.02125	2.08917
A10	2.07347	0.00406	0.03158	-0.02895	0.00256	2.07604
A11	2.14178	-0.00656	-0.04383	0.02009	-0.02381	2.11797
A12	2.06790	0.00250	0.01227	0.00888	0.02124	2.08914
A13	2.14183	-0.00653	-0.04379	0.02017	-0.02368	2.11814
A14	2.07345	0.00404	0.03155	-0.02904	0.00245	2.07590
A15	1.89484	0.04446	0.20713	0.07598	0.28311	2.17795
A16	2.04724	0.00134	-0.05675	0.10342	0.04667	2.09391
A17	1.89470	0.04449	0.20743	0.07573	0.28316	2.17786
A18	2.04777	0.00131	-0.05710	0.10355	0.04646	2.09422

A19	2.04557	-0.00100	-0.02415	0.01646	-0.00876	2.03681
A20	1.98371	-0.01279	-0.08338	0.00564	-0.08006	1.90365
A21	1.98323	-0.00519	-0.02392	-0.01314	-0.03858	1.94465
A22	1.81597	0.00819	0.05789	-0.00490	0.05139	1.86735
A23	1.78529	0.00633	0.05165	-0.00493	0.04634	1.83163
A24	1.82424	0.00788	0.05086	-0.00103	0.04719	1.87143
A25	2.04540	-0.00105	-0.02415	0.01612	-0.00911	2.03629
A26	1.98360	-0.01280	-0.08351	0.00579	-0.08004	1.90356
A27	1.98355	-0.00517	-0.02396	-0.01294	-0.03843	1.94512
A28	1.81599	0.00820	0.05791	-0.00487	0.05143	1.86742
A29	1.78522	0.00635	0.05174	-0.00490	0.04646	1.83168
A30	1.82426	0.00789	0.05096	-0.00109	0.04723	1.87149
A31	2.94074	-0.00379	-0.02151	-0.01452	-0.03597	2.90477
A32	3.11549	0.00068	0.00531	-0.00205	0.00337	3.11886
A33	2.94071	-0.00379	-0.02149	-0.01447	-0.03590	2.90481
A34	3.11544	0.00067	0.00530	-0.00215	0.00326	3.11870
A35	3.94208	0.04581	0.15038	0.17940	0.32978	4.27186
A36	3.94246	0.04580	0.15033	0.17929	0.32962	4.27208
A37	3.14106	0.00076	0.00447	0.00598	0.01073	3.15180
A38	3.16531	-0.00072	0.00466	-0.04443	-0.03969	3.12562
A39	3.14119	0.00075	0.00445	0.00586	0.01058	3.15177
A40	3.16538	-0.00070	0.00472	-0.04418	-0.03939	3.12600
A41	3.31055	0.02663	0.07362	0.31715	0.39076	3.70131
A42	3.31019	0.02651	0.07339	0.31541	0.38881	3.69900
D1	0.00419	0.00025	0.00286	-0.00377	-0.00081	0.00338
D2	-0.00095	-0.00017	0.00150	-0.01010	-0.00847	-0.00942
D3	0.00333	-0.00010	0.00063	-0.00668	-0.00606	-0.00273
D4	0.00415	0.00025	0.00287	-0.00375	-0.00079	0.00336
D5	0.00930	0.00031	0.00152	-0.00029	0.00109	0.01038
D6	0.00342	-0.00010	0.00064	-0.00665	-0.00603	-0.00261
D7	-0.00239	0.00069	0.00224	0.01719	0.01961	0.01722
D8	-3.12290	0.00005	0.00194	-0.01346	-0.01207	-3.13497
D9	0.00913	0.00031	0.00153	-0.00025	0.00114	0.01026
D10	-0.00202	0.00068	0.00222	0.01713	0.01953	0.01751
D11	-3.12257	0.00005	0.00196	-0.01335	-0.01194	-3.13450
D12	-0.02132	-0.00013	-0.00478	0.01668	0.01186	-0.00945
D13	3.11522	0.00052	0.00136	0.02058	0.02176	3.13699
D14	3.11508	0.00052	0.00137	0.02061	0.02180	3.13688
D15	-0.03157	0.00118	0.00750	0.02450	0.03170	0.00013
D16	2.60800	0.00780	0.03687	0.12471	0.16150	2.76950
D17	-0.52838	0.00714	0.03083	0.12067	0.15158	-0.37680
D18	-0.52497	0.00711	0.03081	0.11978	0.15067	-0.37430
D19	2.61156	0.00776	0.03685	0.12379	0.16055	2.77211
D20	-1.74876	0.00150	0.01248	-0.00361	0.00794	-1.74082
D21	0.37255	0.00095	-0.00291	0.00811	0.00427	0.37682
D22	2.45600	-0.00208	-0.01960	0.00113	-0.01660	2.43940
D23	-1.75371	0.00151	0.01255	-0.00355	0.00807	-1.74564
D24	0.36739	0.00094	-0.00289	0.00806	0.00425	0.37164

Supporting Information file

D25 2.45101 -0.00208 -0.01962 0.00126 -0.01649 2.43452
Item Value Threshold Converged?
Maximum Force 0.045806 0.000450 NO
RMS Force 0.012109 0.000300 NO
Maximum Displacement 1.148547 0.001800 NO
RMS Displacement 0.466376 0.001200 NO
Predicted change in Energy=-6.639591D-02
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 20:36:15 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.971657	0.671635	0.045872
2	6	0	3.291595	1.691618	0.111091
3	6	0	3.971697	-0.671306	-0.044399
4	6	0	2.087308	2.286643	0.147448
5	6	0	3.291654	-1.691280	-0.109882
6	6	0	0.861888	2.322489	0.145824
7	6	0	2.087393	-2.286360	-0.146694
8	6	0	-0.437129	1.979379	0.122235
9	6	0	0.861993	-2.322268	-0.145590
10	6	0	-1.514214	1.399107	0.071288
11	6	0	-0.437092	-1.979220	-0.122544
12	6	0	-2.726592	0.708654	0.032992
13	6	0	-1.514226	-1.399072	-0.072082
14	6	0	-2.726643	-0.708530	-0.033810
15	6	0	-3.922746	1.436632	0.067306
16	6	0	-3.922552	-1.436513	-0.068282
17	7	0	-3.611726	2.826416	-0.042518
18	7	0	-3.612455	-2.826528	0.042192
19	1	0	-3.016238	3.108350	-0.841800
20	1	0	-4.474589	3.354360	-0.115073
21	1	0	-3.015190	-3.107631	0.840365
22	1	0	-4.475643	-3.353533	0.117823
23	1	0	-3.118685	3.164953	0.785632
24	1	0	-4.874435	1.070099	-0.275449
25	1	0	-4.874684	-1.069203	0.272339
26	1	0	-3.121830	-3.166816	-0.786713

Distance matrix (angstroms):

	1	2	3	4	5
1 C	0.000000				

Supporting Information file

2	C	1.227642	0.000000			
3	C	1.345971	2.463763	0.000000		
4	C	2.483817	1.343757	3.512434	0.000000	
5	C	2.463743	3.390108	1.227638	4.164198	0.000000
6	C	3.522212	2.510513	4.320868	1.225945	4.698882
7	C	3.512445	4.164237	2.483841	4.582453	1.343771
8	C	4.599285	3.739828	5.147003	2.543192	5.237503
9	C	4.320894	4.698950	3.522240	4.778004	2.510512
10	C	5.533955	4.814867	5.864744	3.710051	5.716615
11	C	5.147084	5.237628	4.599366	4.964180	3.739868
12	C	6.698364	6.098433	6.839397	5.067226	6.480692
13	C	5.864866	5.716802	5.534055	5.157881	4.814903
14	C	6.839476	6.480810	6.698452	5.672569	6.098482
15	C	7.931412	7.218978	8.171788	6.070394	7.865290
16	C	8.171649	7.865195	7.931285	7.072965	7.218822
17	N	7.884073	6.997657	8.351190	5.727690	8.250501
18	N	8.352001	8.251321	7.884913	7.657865	6.998474
19	H	7.453605	6.534821	7.984540	5.263078	7.960003
20	H	8.863521	7.945405	9.356855	6.653377	9.261373
21	H	7.983114	7.958654	7.452186	7.457467	6.533399
22	H	9.357566	9.261943	8.864436	8.653600	7.946435
23	H	7.552274	6.611914	8.104280	5.317995	8.091810
24	H	8.860890	8.198765	9.018865	7.079879	8.621928
25	H	9.018845	8.621847	8.860988	7.729595	8.198912
26	H	8.108296	8.095829	7.556237	7.599209	6.615744

		6	7	8	9	10
6	C	0.000000				
7	C	4.777961	0.000000			
8	C	1.343774	4.964077	0.000000		
9	C	4.653890	1.225926	4.501512	0.000000	
10	C	2.550305	5.157689	1.224510	4.420636	0.000000
11	C	4.501564	2.543215	3.966160	1.343813	3.551177
12	C	3.936291	5.672463	2.619989	4.700672	1.395726
13	C	4.420794	3.710054	3.551313	2.550315	2.801850
14	C	4.700734	5.067271	3.534272	3.936363	2.433755
15	C	4.866583	7.073064	3.528047	6.088381	2.408827
16	C	6.088251	6.070240	4.883931	4.866457	3.722943
17	N	4.505845	7.657107	3.289785	6.821564	2.539630
18	N	6.822233	5.728501	5.760715	4.506687	4.717992
19	H	4.078338	7.458761	2.975860	6.709470	2.451798
20	H	5.441582	8.653226	4.271764	7.791286	3.552684
21	H	6.708229	5.261665	5.748024	4.076941	4.811974
22	H	7.791486	6.654492	6.689511	5.442725	5.599983
23	H	4.118745	7.595346	3.006065	6.842701	2.490547
24	H	5.886541	7.729776	4.546936	6.665705	3.394047
25	H	6.665422	7.080083	5.385933	5.886790	4.174414
26	H	6.846320	5.321731	5.875127	4.122516	4.916121

		11	12	13	14	15

```
 11  C    0.000000
 12  C    3.534214   0.000000
 13  C    1.224473   2.433800   0.000000
 14  C    2.620033   1.418758   1.395804   0.000000
 15  C    4.884043   1.400684   3.723120   2.458172   0.000000
 16  C    3.527875   2.458113   2.408620   1.400480   2.876343
 17  N    5.760108   2.296537   4.717535   3.644076   1.428388
 18  N    3.290592   3.644496   2.540326   2.297031   4.274511
 19  H    5.749147   2.570544   4.813041   3.912197   2.107811
 20  H    6.689433   3.174457   5.600064   4.423685   2.003864
 21  H    2.974406   3.911416   2.450434   2.569655   4.698043
 22  H    4.272752   4.423544   3.553305   3.174592   4.822233
 23  H    5.871818   2.598771   4.913277   3.978574   2.037057
 24  H    5.386255   2.199775   4.174826   2.799093   1.075890
 25  H    4.547119   2.798636   3.394131   2.199521   2.688389
 26  H    3.009870   3.980879   2.493994   2.601193   4.750005
                16         17         18         19         20
 16  C    0.000000
 17  N    4.274323   0.000000
 18  N    1.428462   5.653578   0.000000
 19  H    4.698459   1.035830   6.029899   0.000000
 20  H    4.822800   1.014160   6.242706   1.647859   0.000000
 21  H    2.107506   6.028951   1.035773   6.439573   6.693283
 22  H    2.003874   6.242102   1.014174   6.693778   6.711935
 23  H    4.748564   1.021533   6.057587   1.631635   1.638786
 24  H    2.689257   2.175624   4.108185   2.815691   2.324531
 25  H    1.075870   4.107316   2.175863   4.706068   4.458483
 26  H    2.037461   6.059097   1.021564   6.276296   6.693788
                21         22         23         24         25
 21  H    0.000000
 22  H    1.647865   0.000000
 23  H    6.273677   6.691634   0.000000
 24  H    4.706938   4.458948   2.932058   0.000000
 25  H    2.817013   2.324064   4.612492   2.208322   0.000000
 26  H    1.631642   1.638859   6.524077   4.613509   2.931564
                26
 26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=3 Diff= 7.99D-02
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
```

Supporting Information file

```
 ---------------------------------------------------------------------
    1        6        0        4.498804   -0.672257   -0.025481
    2        6        0        3.818827   -1.693771   -0.060779
    3        6        0        4.498730    0.672757    0.025267
    4        6        0        2.614590   -2.289703   -0.079795
    5        6        0        3.818601    1.694162    0.060638
    6        6        0        1.389173   -2.325583   -0.077289
    7        6        0        2.614290    2.289971    0.079769
    8        6        0        0.090127   -1.982030   -0.063980
    9        6        0        1.388888    2.325734    0.077438
   10        6        0       -0.987009   -1.400596   -0.030267
   11        6        0        0.089832    1.982055    0.064306
   12        6        0       -2.199444   -0.709412   -0.012457
   13        6        0       -0.987251    1.400589    0.030772
   14        6        0       -2.199611    0.709123    0.012648
   15        6        0       -3.395539   -1.438179   -0.025521
   16        6        0       -3.395579    1.437711    0.025535
   17        7        0       -3.084430   -2.824108    0.125159
   18        7        0       -3.085571    2.823901   -0.125715
   19        1        0       -2.489035   -3.082374    0.932468
   20        1        0       -3.947264   -3.349759    0.213084
   21        1        0       -2.488213    3.081463   -0.931725
   22        1        0       -3.948788    3.348386   -0.216929
   23        1        0       -2.591245   -3.186809   -0.692610
   24        1        0       -4.347304   -1.061802    0.306175
   25        1        0       -4.347636    1.060470   -0.304273
   26        1        0       -2.595089    3.188451    0.692895
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6086943           0.2768518           0.1908687
 Leave Link  202 at Fri Sep 25 20:36:15 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1018.5255748499 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
```

Supporting Information file

Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0154735012 Hartrees.
Nuclear repulsion after empirical dispersion term = 1018.5101013487 Hartrees.
Leave Link 301 at Fri Sep 25 20:36:15 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23308 LenP2D= 52233.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.79D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Fri Sep 25 20:36:16 2026, MaxMem= 805306368 cpu: 5.7 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 20:36:16 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 0.999999 0.001066 0.000011 -0.000067 Ang= 0.12 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.964836753737
Leave Link 401 at Fri Sep 25 20:36:26 2026, MaxMem= 805306368 cpu: 55.8 elap: 9.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.

Supporting Information file

Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.069826752879
DIIS: error= 1.88D-02 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.069826752879 IErMin= 1 ErrMin= 1.88D-02
ErrMax= 1.88D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.31D-01 BMatP= 3.31D-01
IDIUse=3 WtCom= 8.12D-01 WtEn= 1.88D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Recover alternate guess density for next cycle.
RMSDP=8.25D-03 MaxDP=3.36D-01 OVMax= 0.00D+00

Cycle 2 Pass 0 IDiag 1:
RMSU= 8.08D-03 CP: 9.21D-01
E= -723.085032251966 Delta-E= -0.015205499087 Rises=F Damp=F
DIIS: error= 5.80D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.085032251966 IErMin= 1 ErrMin= 1.88D-02
ErrMax= 5.80D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D+00 BMatP= 3.31D-01
IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.000D+00 0.100D+01
Gap= 0.225 Goal= None Shift= 0.000
RMSDP=7.13D+02 MaxDP=2.42D+04 DE=-1.52D-02 OVMax= 9.95D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 3 Pass 1 IDiag 1:
E= -723.085084534730 Delta-E= -0.000052282764 Rises=F Damp=F
DIIS: error= 5.80D-02 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.085084534730 IErMin= 1 ErrMin= 5.80D-02
ErrMax= 5.80D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D+00 BMatP= 1.66D+00

IDIUse=3 WtCom= 4.20D-01 WtEn= 5.80D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.225 Goal=   None   Shift=   0.000
GapD=   0.225 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.
Damping current iteration by 5.00D-01
RMSDP=6.00D-03 MaxDP=1.84D-01 DE=-5.23D-05 OVMax= 3.16D-01

Cycle   4 Pass 1 IDiag 1:
RMSU= 2.90D-03   CP: 9.64D-01
E= -723.235750951236   Delta-E=   -0.150666416507 Rises=F Damp=T
DIIS: error= 2.76D-02 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.235750951236   IErMin= 2 ErrMin= 2.76D-02
ErrMax= 2.76D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-01 BMatP= 1.66D+00
IDIUse=3 WtCom= 7.24D-01 WtEn= 2.76D-01
Coeff-Com: -0.701D+00 0.170D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.507D+00 0.151D+01
Gap=   0.271 Goal=   None   Shift=   0.000
GapD=   0.271 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.
Damping current iteration by 5.00D-01
RMSDP=5.46D-03 MaxDP=3.58D-01 DE=-1.51D-01 OVMax= 2.86D-01

Cycle   5 Pass 1 IDiag 1:
RMSU= 1.51D-03   CP: 8.54D-01 9.61D-01
E= -723.283765835674   Delta-E=   -0.048014884438 Rises=F Damp=T
DIIS: error= 1.33D-02 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -723.283765835674   IErMin= 3 ErrMin= 1.33D-02
ErrMax= 1.33D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.91D-02 BMatP= 3.57D-01
IDIUse=3 WtCom= 8.67D-01 WtEn= 1.33D-01
Coeff-Com: -0.409D+00 0.388D+00 0.102D+01
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.354D+00 0.336D+00 0.102D+01
Gap=   0.191 Goal=   None   Shift=   0.000
RMSDP=2.99D-03 MaxDP=1.23D-01 DE=-4.80D-02 OVMax= 2.30D-01

Cycle   6 Pass 1 IDiag 1:
RMSU= 1.25D-03   CP: 7.27D-01 1.07D+00 1.42D+00
E= -723.385076922567   Delta-E=   -0.101311086893 Rises=F Damp=F
DIIS: error= 7.27D-03 at cycle   4 NSaved=   4.
NSaved= 4 IEnMin= 4 EnMin= -723.385076922567   IErMin= 4 ErrMin= 7.27D-03
ErrMax= 7.27D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-02 BMatP= 9.91D-02
IDIUse=3 WtCom= 9.27D-01 WtEn= 7.27D-02
Coeff-Com: -0.195D+00 0.914D-01 0.659D+00 0.444D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.180D+00 0.847D-01 0.611D+00 0.485D+00
Gap=   0.172 Goal=   None   Shift=   0.000

RMSDP=9.25D-04 MaxDP=3.35D-02 DE=-1.01D-01 OVMax= 4.08D-02

Cycle 7 Pass 1 IDiag 1:
RMSU= 4.37D-04 CP: 7.59D-01 1.09D+00 1.62D+00 7.12D-01
E= -723.399770818560 Delta-E= -0.014693895993 Rises=F Damp=F
DIIS: error= 1.78D-03 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.399770818560 IErMin= 5 ErrMin= 1.78D-03
ErrMax= 1.78D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.17D-04 BMatP= 1.24D-02
IDIUse=3 WtCom= 9.82D-01 WtEn= 1.78D-02
Coeff-Com: -0.412D-01 0.660D-02 0.165D+00 0.222D+00 0.648D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.405D-01 0.649D-02 0.162D+00 0.218D+00 0.654D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.98D-04 MaxDP=6.83D-03 DE=-1.47D-02 OVMax= 1.99D-02

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.38D-04 CP: 7.56D-01 1.09D+00 1.65D+00 7.84D-01 1.16D+00
E= -723.400683103694 Delta-E= -0.000912285134 Rises=F Damp=F
DIIS: error= 6.56D-04 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.400683103694 IErMin= 6 ErrMin= 6.56D-04
ErrMax= 6.56D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.40D-05 BMatP= 6.17D-04
IDIUse=3 WtCom= 9.93D-01 WtEn= 6.56D-03
Coeff-Com: 0.313D-01-0.230D-01-0.897D-01-0.467D-01 0.168D+00 0.960D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.310D-01-0.229D-01-0.891D-01-0.464D-01 0.167D+00 0.960D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=2.44D-04 MaxDP=8.59D-03 DE=-9.12D-04 OVMax= 1.59D-02

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.70D-05 CP: 7.63D-01 1.09D+00 1.69D+00 8.13D-01 1.55D+00
CP: 1.50D+00
E= -723.400969688759 Delta-E= -0.000286585064 Rises=F Damp=F
DIIS: error= 4.53D-04 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.400969688759 IErMin= 7 ErrMin= 4.53D-04
ErrMax= 4.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-05 BMatP= 5.40D-05
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.53D-03
Coeff-Com: 0.174D-01-0.107D-01-0.545D-01-0.532D-01-0.541D-01 0.413D+00
Coeff-Com: 0.742D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
Coeff-En: 0.100D+01
Coeff: 0.173D-01-0.106D-01-0.542D-01-0.529D-01-0.538D-01 0.412D+00
Coeff: 0.743D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=1.09D-04 MaxDP=3.78D-03 DE=-2.87D-04 OVMax= 7.60D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.10D-05 CP: 7.66D-01 1.10D+00 1.70D+00 8.18D-01 1.70D+00
CP: 1.86D+00 1.32D+00

E= -723.401046514296 Delta-E= -0.000076825537 Rises=F Damp=F
DIIS: error= 3.25D-04 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.401046514296 IErMin= 8 ErrMin= 3.25D-04
ErrMax= 3.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.52D-06 BMatP= 2.16D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.25D-03
Coeff-Com: -0.423D-02 0.282D-02 0.128D-01-0.447D-02-0.768D-01-0.111D+00
Coeff-Com: 0.241D+00 0.940D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.422D-02 0.281D-02 0.128D-01-0.445D-02-0.766D-01-0.111D+00
Coeff: 0.240D+00 0.940D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=1.58D-04 MaxDP=5.90D-03 DE=-7.68D-05 OVMax= 6.24D-03

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.66D-05 CP: 7.72D-01 1.11D+00 1.70D+00 8.09D-01 1.86D+00
CP: 2.03D+00 1.77D+00 1.75D+00
E= -723.401081500849 Delta-E= -0.000034986554 Rises=F Damp=F
DIIS: error= 2.14D-04 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.401081500849 IErMin= 9 ErrMin= 2.14D-04
ErrMax= 2.14D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.87D-06 BMatP= 4.52D-06
IDIUse=3 WtCom= 9.98D-01 WtEn= 2.14D-03
Coeff-Com: -0.810D-02 0.462D-02 0.261D-01 0.127D-01-0.311D-01-0.181D+00
Coeff-Com: -0.112D+00 0.579D+00 0.710D+00
Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.808D-02 0.461D-02 0.260D-01 0.127D-01-0.310D-01-0.181D+00
Coeff: -0.112D+00 0.578D+00 0.710D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=9.79D-05 MaxDP=3.73D-03 DE=-3.50D-05 OVMax= 3.90D-03

Cycle 12 Pass 1 IDiag 1:
RMSU= 6.35D-06 CP: 7.76D-01 1.12D+00 1.70D+00 8.03D-01 1.95D+00
CP: 2.12D+00 2.01D+00 2.33D+00 1.54D+00
E= -723.401095131875 Delta-E= -0.000013631026 Rises=F Damp=F
DIIS: error= 9.45D-05 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.401095131875 IErMin=10 ErrMin= 9.45D-05
ErrMax= 9.45D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.78D-07 BMatP= 2.87D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.186D-02 0.751D-03 0.650D-02 0.577D-02 0.166D-01-0.332D-01
Coeff-Com: -0.174D+00-0.143D+00 0.243D+00 0.108D+01
Coeff: -0.186D-02 0.751D-03 0.650D-02 0.577D-02 0.166D-01-0.332D-01
Coeff: -0.174D+00-0.143D+00 0.243D+00 0.108D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=8.49D-05 MaxDP=3.27D-03 DE=-1.36D-05 OVMax= 3.17D-03

Cycle 13 Pass 1 IDiag 1:
RMSU= 4.17D-06 CP: 7.79D-01 1.13D+00 1.70D+00 7.97D-01 2.03D+00

```
              CP:  2.19D+00  2.23D+00  2.78D+00  2.14D+00  1.80D+00
E= -723.401100474576     Delta-E=       -0.000005342701 Rises=F Damp=F
DIIS: error= 2.19D-05 at cycle  11 NSaved=  11.
NSaved=11 IEnMin=11 EnMin= -723.401100474576     IErMin=11 ErrMin= 2.19D-05
ErrMax= 2.19D-05  0.00D+00 EMaxC= 1.00D-01 BMatC= 8.75D-08 BMatP= 5.78D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.773D-03-0.510D-03-0.240D-02-0.550D-03 0.114D-01 0.211D-01
Coeff-Com: -0.279D-01-0.147D+00-0.632D-01 0.386D+00 0.822D+00
Coeff:      0.773D-03-0.510D-03-0.240D-02-0.550D-03 0.114D-01 0.211D-01
Coeff:     -0.279D-01-0.147D+00-0.632D-01 0.386D+00 0.822D+00
Gap=     0.174 Goal=   None    Shift=    0.000
RMSDP=2.53D-05 MaxDP=1.07D-03 DE=-5.34D-06 OVMax= 6.71D-04

Cycle  14  Pass 1  IDiag  1:
RMSU=  1.67D-06    CP:  7.80D-01  1.13D+00  1.70D+00  7.95D-01  2.06D+00
              CP:  2.19D+00  2.29D+00  2.85D+00  2.34D+00  2.26D+00
              CP:  1.38D+00
E= -723.401100873244     Delta-E=       -0.000000398668 Rises=F Damp=F
DIIS: error= 1.36D-05 at cycle  12 NSaved=  12.
NSaved=12 IEnMin=12 EnMin= -723.401100873244     IErMin=12 ErrMin= 1.36D-05
ErrMax= 1.36D-05  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.18D-08 BMatP= 8.75D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.653D-03-0.307D-03-0.223D-02-0.112D-02 0.320D-02 0.153D-01
Coeff-Com:  0.220D-01-0.476D-01-0.844D-01-0.574D-02 0.435D+00 0.665D+00
Coeff:      0.653D-03-0.307D-03-0.223D-02-0.112D-02 0.320D-02 0.153D-01
Coeff:      0.220D-01-0.476D-01-0.844D-01-0.574D-02 0.435D+00 0.665D+00
Gap=     0.174 Goal=   None    Shift=    0.000
RMSDP=9.68D-06 MaxDP=4.07D-04 DE=-3.99D-07 OVMax= 1.74D-04

Cycle  15  Pass 1  IDiag  1:
RMSU=  7.50D-07    CP:  7.81D-01  1.13D+00  1.70D+00  7.94D-01  2.06D+00
              CP:  2.18D+00  2.31D+00  2.87D+00  2.41D+00  2.44D+00
              CP:  1.59D+00  1.56D+00
E= -723.401100941372     Delta-E=       -0.000000068128 Rises=F Damp=F
DIIS: error= 3.57D-06 at cycle  13 NSaved=  13.
NSaved=13 IEnMin=13 EnMin= -723.401100941372     IErMin=13 ErrMin= 3.57D-06
ErrMax= 3.57D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.28D-09 BMatP= 3.18D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.133D-03-0.189D-04-0.535D-03-0.346D-03-0.443D-03 0.243D-02
Coeff-Com:  0.157D-01 0.378D-02-0.290D-01-0.759D-01 0.438D-01 0.292D+00
Coeff-Com:  0.748D+00
Coeff:      0.133D-03-0.189D-04-0.535D-03-0.346D-03-0.443D-03 0.243D-02
Coeff:      0.157D-01 0.378D-02-0.290D-01-0.759D-01 0.438D-01 0.292D+00
Coeff:      0.748D+00
Gap=     0.174 Goal=   None    Shift=    0.000
RMSDP=4.02D-06 MaxDP=1.61D-04 DE=-6.81D-08 OVMax= 8.81D-05

Cycle  16  Pass 1  IDiag  1:
```

RMSU= 2.87D-07 CP: 7.81D-01 1.13D+00 1.70D+00 7.94D-01 2.07D+00
CP: 2.18D+00 2.32D+00 2.88D+00 2.43D+00 2.52D+00
CP: 1.70D+00 1.88D+00 1.38D+00
E= -723.401100953793 Delta-E= -0.000000012420 Rises=F Damp=F
DIIS: error= 1.90D-06 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.401100953793 IErMin=14 ErrMin= 1.90D-06
ErrMax= 1.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.21D-10 BMatP= 4.28D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.775D-04 0.532D-04 0.234D-03 0.581D-04-0.909D-03-0.232D-02
Coeff-Com: 0.188D-02 0.114D-01 0.709D-02-0.298D-01-0.783D-01-0.201D-01
Coeff-Com: 0.344D+00 0.767D+00
Coeff: -0.775D-04 0.532D-04 0.234D-03 0.581D-04-0.909D-03-0.232D-02
Coeff: 0.188D-02 0.114D-01 0.709D-02-0.298D-01-0.783D-01-0.201D-01
Coeff: 0.344D+00 0.767D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.16D-06 MaxDP=4.65D-05 DE=-1.24D-08 OVMax= 3.35D-05

Cycle 17 Pass 1 IDiag 1:
RMSU= 1.32D-07 CP: 7.81D-01 1.13D+00 1.70D+00 7.94D-01 2.07D+00
CP: 2.18D+00 2.32D+00 2.88D+00 2.43D+00 2.55D+00
CP: 1.74D+00 2.01D+00 1.61D+00 1.59D+00
E= -723.401100955920 Delta-E= -0.000000002128 Rises=F Damp=F
DIIS: error= 7.00D-07 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.401100955920 IErMin=15 ErrMin= 7.00D-07
ErrMax= 7.00D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.59D-11 BMatP= 8.21D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.132D-04 0.568D-06 0.557D-04 0.189D-04-0.308D-04-0.174D-03
Coeff-Com: -0.169D-02-0.619D-03 0.353D-02 0.680D-02-0.798D-02-0.261D-01
Coeff-Com: -0.587D-01-0.215D-01 0.111D+01
Coeff: -0.132D-04 0.568D-06 0.557D-04 0.189D-04-0.308D-04-0.174D-03
Coeff: -0.169D-02-0.619D-03 0.353D-02 0.680D-02-0.798D-02-0.261D-01
Coeff: -0.587D-01-0.215D-01 0.111D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=4.33D-07 MaxDP=2.00D-05 DE=-2.13D-09 OVMax= 1.26D-05

Cycle 18 Pass 1 IDiag 1:
RMSU= 4.95D-08 CP: 7.81D-01 1.13D+00 1.70D+00 7.94D-01 2.07D+00
CP: 2.18D+00 2.32D+00 2.88D+00 2.43D+00 2.55D+00
CP: 1.75D+00 2.06D+00 1.72D+00 1.96D+00 1.41D+00
E= -723.401100956172 Delta-E= -0.000000000252 Rises=F Damp=F
DIIS: error= 2.50D-07 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.401100956172 IErMin=16 ErrMin= 2.50D-07
ErrMax= 2.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.37D-12 BMatP= 3.59D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.345D-05-0.332D-05-0.860D-05 0.394D-05 0.842D-04 0.211D-03
Coeff-Com: -0.566D-03-0.119D-02 0.242D-03 0.486D-02 0.506D-02-0.342D-02
Coeff-Com: -0.459D-01-0.917D-01 0.206D+00 0.926D+00
Coeff: 0.345D-05-0.332D-05-0.860D-05 0.394D-05 0.842D-04 0.211D-03

Coeff: -0.566D-03-0.119D-02 0.242D-03 0.486D-02 0.506D-02-0.342D-02
Coeff: -0.459D-01-0.917D-01 0.206D+00 0.926D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.23D-07 MaxDP=6.22D-06 DE=-2.52D-10 OVMax= 5.38D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.39D-08 CP: 7.81D-01 1.13D+00 1.70D+00 7.94D-01 2.07D+00
CP: 2.18D+00 2.32D+00 2.88D+00 2.43D+00 2.55D+00
CP: 1.75D+00 2.07D+00 1.75D+00 2.08D+00 1.58D+00
CP: 1.42D+00
E= -723.401100956187 Delta-E= -0.000000000015 Rises=F Damp=F
DIIS: error= 1.34D-07 at cycle 17 NSaved= 17.
NSaved=17 IEnMin=17 EnMin= -723.401100956187 IErMin=17 ErrMin= 1.34D-07
ErrMax= 1.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-12 BMatP= 7.37D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.323D-05-0.817D-06-0.124D-04 0.131D-06 0.412D-04 0.944D-04
Coeff-Com: 0.751D-04-0.365D-03-0.420D-03 0.658D-03 0.280D-02 0.266D-02
Coeff-Com: -0.480D-02-0.265D-01-0.119D+00 0.294D+00 0.851D+00
Coeff: 0.323D-05-0.817D-06-0.124D-04 0.131D-06 0.412D-04 0.944D-04
Coeff: 0.751D-04-0.365D-03-0.420D-03 0.658D-03 0.280D-02 0.266D-02
Coeff: -0.480D-02-0.265D-01-0.119D+00 0.294D+00 0.851D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=6.17D-08 MaxDP=2.98D-06 DE=-1.48D-11 OVMax= 1.92D-06

Cycle 20 Pass 1 IDiag 1:
RMSU= 5.70D-09 CP: 7.81D-01 1.13D+00 1.70D+00 7.94D-01 2.07D+00
CP: 2.18D+00 2.32D+00 2.88D+00 2.43D+00 2.55D+00
CP: 1.75D+00 2.07D+00 1.75D+00 2.12D+00 1.63D+00
CP: 1.62D+00 1.49D+00
E= -723.401100956207 Delta-E= -0.000000000020 Rises=F Damp=F
DIIS: error= 4.48D-08 at cycle 18 NSaved= 18.
NSaved=18 IEnMin=18 EnMin= -723.401100956207 IErMin=18 ErrMin= 4.48D-08
ErrMax= 4.48D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.14D-13 BMatP= 1.63D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.443D-06 0.472D-06 0.964D-06-0.176D-06-0.693D-05-0.393D-04
Coeff-Com: 0.964D-04 0.132D-03-0.730D-04-0.735D-03-0.680D-03 0.493D-03
Coeff-Com: 0.790D-02 0.160D-01-0.396D-01-0.169D+00 0.612D-01 0.112D+01
Coeff: -0.443D-06 0.472D-06 0.964D-06-0.176D-06-0.693D-05-0.393D-04
Coeff: 0.964D-04 0.132D-03-0.730D-04-0.735D-03-0.680D-03 0.493D-03
Coeff: 0.790D-02 0.160D-01-0.396D-01-0.169D+00 0.612D-01 0.112D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.94D-08 MaxDP=7.65D-07 DE=-2.00D-11 OVMax= 9.47D-07

Cycle 21 Pass 1 IDiag 1:
RMSU= 3.69D-09 CP: 7.81D-01 1.13D+00 1.70D+00 7.94D-01 2.07D+00
CP: 2.18D+00 2.32D+00 2.88D+00 2.43D+00 2.55D+00
CP: 1.75D+00 2.07D+00 1.75D+00 2.12D+00 1.64D+00
CP: 1.71D+00 1.87D+00 1.62D+00

Supporting Information file

E= -723.401100956191 Delta-E= 0.000000000016 Rises=F Damp=F
DIIS: error= 1.54D-08 at cycle 19 NSaved= 19.
NSaved=19 IEnMin=18 EnMin= -723.401100956207 IErMin=19 ErrMin= 1.54D-08
ErrMax= 1.54D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-14 BMatP= 2.14D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.230D-06 0.531D-07 0.886D-06-0.777D-06-0.488D-05-0.120D-04
Coeff-Com: 0.130D-04 0.491D-04 0.276D-04-0.136D-03-0.240D-03-0.243D-03
Coeff-Com: 0.958D-03 0.389D-02 0.956D-02-0.506D-01-0.818D-01 0.105D+00
Coeff-Com: 0.101D+01
Coeff: -0.230D-06 0.531D-07 0.886D-06-0.777D-06-0.488D-05-0.120D-04
Coeff: 0.130D-04 0.491D-04 0.276D-04-0.136D-03-0.240D-03-0.243D-03
Coeff: 0.958D-03 0.389D-02 0.956D-02-0.506D-01-0.818D-01 0.105D+00
Coeff: 0.101D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=9.75D-09 MaxDP=3.95D-07 DE= 1.57D-11 OVMax= 3.36D-07

SCF Done: E(RwB97XD) = -723.401100956 A.U. after 21 cycles
NFock= 21 Conv=0.98D-08 -V/T= 2.0043
KE= 7.203349317775D+02 PE=-3.718347667723D+03 EE= 1.256101533641D+03
Leave Link 502 at Fri Sep 25 21:02:59 2026, MaxMem= 805306368 cpu: 9556.3 elap: 1593.2
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23308 LenP2D= 52233.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 21:02:59 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 21:02:59 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 21:15:22 2026, MaxMem= 805306368 cpu: 4452.9 elap: 742.3

Supporting Information file

(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.97324250D+00 2.27989797D-03-3.42246512D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.002156332	-0.009081201	-0.000492390
2	6	-0.006637441	0.006378012	0.000136166
3	6	0.002144698	0.009084516	0.000493521
4	6	0.009446039	-0.003197053	-0.000043357
5	6	-0.006631829	-0.006385626	-0.000137377
6	6	-0.009434961	0.000177248	0.000015109
7	6	0.009449121	0.003204008	0.000044627
8	6	0.011410455	0.003461335	0.000131738
9	6	-0.009447873	-0.000178745	-0.000020248
10	6	-0.005464473	-0.008841138	-0.000345038
11	6	0.011421930	-0.003470338	-0.000128651
12	6	0.007514249	-0.003800585	-0.000410402
13	6	-0.005479386	0.008833641	0.000366476
14	6	0.007600839	0.003733154	0.000362460
15	6	0.009277451	-0.019281253	0.006650166
16	6	0.009211545	0.019264990	-0.006603959
17	7	-0.019390172	0.033400866	-0.003723513
18	7	-0.019347391	-0.033266617	0.003710083
19	1	0.000718380	-0.004340098	0.000437126
20	1	-0.001509456	0.004165848	0.000993857
21	1	0.000715851	0.004337880	-0.000435339
22	1	-0.001502965	-0.004162479	-0.000996203
23	1	0.001846751	0.000226865	0.000211169
24	1	0.000059449	0.006165814	-0.004921742
25	1	0.000036235	-0.006194500	0.004916100
26	1	0.001836622	-0.000234546	-0.000210377

Cartesian Forces: Max 0.033400866 RMS 0.008457654
Leave Link 716 at Fri Sep 25 21:15:22 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.031553630 RMS 0.008655841
Search for a local minimum.
Step number 6 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .86558D-02 SwitMx=.10000D-02 MixMth= 1

Supporting Information file

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 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    5    6
 DE= -4.00D-02 DEPred=-6.64D-02 R= 6.03D-01
 TightC=F SS=  1.41D+00  RLast= 9.27D-01 DXNew= 1.4270D+00 2.7795D+00
 Trust test= 6.03D-01 RLast= 9.27D-01 DXMaxT set to 1.43D+00
 ITU=  1  1  0  0  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.00444   0.00990   0.01660   0.01692   0.01745
    Eigenvalues ---    0.01764   0.02171   0.02410   0.02744   0.02801
    Eigenvalues ---    0.03101   0.03306   0.03788   0.03850   0.04439
    Eigenvalues ---    0.04462   0.04468   0.05025   0.05026   0.05026
    Eigenvalues ---    0.06220   0.08684   0.09968   0.10967   0.11075
    Eigenvalues ---    0.11602   0.11626   0.14372   0.15011   0.15914
    Eigenvalues ---    0.16000   0.16000   0.16000   0.16000   0.16090
    Eigenvalues ---    0.16759   0.18216   0.24994   0.24999   0.24999
    Eigenvalues ---    0.25000   0.25000   0.25000   0.25000   0.25074
    Eigenvalues ---    0.25881   0.33685   0.37230   0.40068   0.40643
    Eigenvalues ---    0.41564   0.45835   0.46153   0.47664   0.47688
    Eigenvalues ---    0.47688   0.47688   0.47721   0.48809   0.51206
    Eigenvalues ---    0.54803   0.55350   0.55549   0.55659   0.55784
    Eigenvalues ---    0.93693   0.94051   0.95024   0.95835   0.97679
    Eigenvalues ---    0.98403   1.36035
 RFO step:  Lambda=-1.02976930D-02 EMin= 4.43976909D-03
 Quartic linear search produced a step of -0.21643.
 Iteration  1 RMS(Cart)=  0.15157290 RMS(Int)=  0.00728591
 Iteration  2 RMS(Cart)=  0.01537423 RMS(Int)=  0.00013236
 Iteration  3 RMS(Cart)=  0.00015503 RMS(Int)=  0.00011782
 Iteration  4 RMS(Cart)=  0.00000002 RMS(Int)=  0.00011782
  ITry=  1 IFail=0 DXMaxC= 4.91D-01 DCOld= 1.00D+10 DXMaxT= 1.43D+00 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
    R1        2.31991   0.00410  -0.00079   0.00448   0.00370   2.32361
    R2        2.54352  -0.00560   0.00118  -0.00848  -0.00730   2.53621
    R3        2.53933  -0.00530   0.00148  -0.00852  -0.00704   2.53229
    R4        2.31990   0.00410  -0.00078   0.00448   0.00370   2.32360
    R5        2.31670   0.00497  -0.00074   0.00508   0.00433   2.32103
    R6        2.53936  -0.00530   0.00148  -0.00852  -0.00704   2.53232
    R7        2.53936  -0.00436   0.00152  -0.00761  -0.00609   2.53328
    R8        2.31667   0.00497  -0.00074   0.00508   0.00433   2.32100
    R9        2.31399   0.00768  -0.00092   0.00746   0.00654   2.32053
   R10        2.53944  -0.00437   0.00152  -0.00762  -0.00610   2.53334
   R11        2.63754  -0.00145   0.00365  -0.00563  -0.00198   2.63556
   R12        2.31392   0.00769  -0.00092   0.00746   0.00654   2.32046
   R13        2.68106   0.01096   0.00170   0.01828   0.01998   2.70104
   R14        2.64691   0.01825   0.01314   0.01977   0.03291   2.67982
   R15        2.63769  -0.00146   0.00366  -0.00564  -0.00198   2.63571
   R16        2.64652   0.01825   0.01314   0.01976   0.03290   2.67942
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R17	2.69926	0.02872	0.01665	0.02962	0.04627	2.74554
R18	2.03314	-0.00059	0.01381	-0.01319	0.00061	2.03375
R19	2.69940	0.02862	0.01668	0.02955	0.04623	2.74564
R20	2.03310	-0.00059	0.01377	-0.01317	0.00060	2.03370
R21	1.95744	-0.00111	0.00665	-0.00429	0.00235	1.95979
R22	1.91649	0.00338	0.00201	0.00490	0.00691	1.92340
R23	1.93042	0.00114	0.00752	-0.00275	0.00477	1.93519
R24	1.95733	-0.00110	0.00667	-0.00431	0.00236	1.95969
R25	1.91651	0.00337	0.00195	0.00494	0.00688	1.92339
R26	1.93048	0.00113	0.00752	-0.00276	0.00476	1.93524
A1	2.55450	-0.00051	-0.00134	0.00007	-0.00128	2.55322
A2	2.61755	-0.00084	-0.00144	-0.00077	-0.00222	2.61533
A3	2.55446	-0.00050	-0.00136	0.00012	-0.00126	2.55321
A4	2.71104	0.00067	0.00048	-0.00064	-0.00017	2.71087
A5	2.61760	-0.00085	-0.00143	-0.00083	-0.00226	2.61534
A6	2.85367	0.00028	-0.00016	-0.00082	-0.00098	2.85269
A7	2.71106	0.00067	0.00046	-0.00063	-0.00018	2.71088
A8	2.85368	0.00027	-0.00015	-0.00086	-0.00102	2.85266
A9	2.08917	-0.00447	-0.00460	-0.01547	-0.02010	2.06906
A10	2.07604	0.00811	-0.00055	0.02938	0.02877	2.10481
A11	2.11797	-0.00364	0.00515	-0.01399	-0.00889	2.10909
A12	2.08914	-0.00443	-0.00460	-0.01539	-0.02002	2.06912
A13	2.11814	-0.00364	0.00513	-0.01394	-0.00887	2.10927
A14	2.07590	0.00808	-0.00053	0.02925	0.02867	2.10457
A15	2.17795	-0.00938	-0.06127	0.05034	-0.01093	2.16702
A16	2.09391	-0.02217	-0.01010	-0.08937	-0.09947	1.99444
A17	2.17786	-0.00928	-0.06128	0.05109	-0.01020	2.16766
A18	2.09422	-0.02213	-0.01005	-0.08896	-0.09901	1.99521
A19	2.03681	-0.00687	0.00189	-0.02877	-0.02683	2.00998
A20	1.90365	0.00579	0.01733	0.00195	0.01955	1.92321
A21	1.94465	0.00014	0.00835	-0.01010	-0.00169	1.94296
A22	1.86735	0.00170	-0.01112	0.02321	0.01231	1.87966
A23	1.83163	0.00020	-0.01003	0.00706	-0.00311	1.82852
A24	1.87143	-0.00077	-0.01021	0.01080	0.00088	1.87231
A25	2.03629	-0.00687	0.00197	-0.02889	-0.02688	2.00941
A26	1.90356	0.00579	0.01732	0.00193	0.01953	1.92309
A27	1.94512	0.00015	0.00832	-0.00999	-0.00161	1.94352
A28	1.86742	0.00170	-0.01113	0.02322	0.01230	1.87973
A29	1.83168	0.00020	-0.01006	0.00713	-0.00306	1.82861
A30	1.87149	-0.00078	-0.01022	0.01076	0.00082	1.87231
A31	2.90477	0.00285	0.00779	-0.00487	0.00292	2.90768
A32	3.11886	0.00199	-0.00073	0.02232	0.02160	3.14046
A33	2.90481	0.00285	0.00777	-0.00492	0.00285	2.90766
A34	3.11870	0.00201	-0.00071	0.02246	0.02176	3.14045
A35	4.27186	-0.03155	-0.07137	-0.03903	-0.11040	4.16146
A36	4.27208	-0.03140	-0.07134	-0.03787	-0.10921	4.16287
A37	3.15180	-0.00006	-0.00232	0.00825	0.00582	3.15761
A38	3.12562	0.00053	0.00859	-0.02553	-0.01682	3.10881

A39	3.15177	-0.00006	-0.00229	0.00812	0.00572	3.15749
A40	3.12600	0.00052	0.00852	-0.02544	-0.01679	3.10921
A41	3.70131	-0.01756	-0.08457	0.03085	-0.05372	3.64759
A42	3.69900	-0.01744	-0.08415	0.03109	-0.05306	3.64594
D1	0.00338	0.00009	0.00018	0.00063	0.00079	0.00417
D2	-0.00942	0.00009	0.00183	-0.00610	-0.00432	-0.01374
D3	-0.00273	-0.00003	0.00131	-0.00700	-0.00565	-0.00838
D4	0.00336	0.00009	0.00017	0.00063	0.00078	0.00413
D5	0.01038	0.00008	-0.00023	0.00096	0.00083	0.01121
D6	-0.00261	-0.00003	0.00131	-0.00702	-0.00568	-0.00829
D7	0.01722	0.00010	-0.00424	0.02957	0.02551	0.04272
D8	-3.13497	0.00016	0.00261	-0.00420	-0.00153	-3.13650
D9	0.01026	0.00008	-0.00025	0.00098	0.00084	0.01110
D10	0.01751	0.00010	-0.00423	0.02943	0.02539	0.04290
D11	-3.13450	0.00016	0.00258	-0.00400	-0.00135	-3.13586
D12	-0.00945	-0.00043	-0.00257	-0.01093	-0.01311	-0.02257
D13	3.13699	-0.00025	-0.00471	0.00926	0.00465	-3.14155
D14	3.13688	-0.00024	-0.00472	0.00957	0.00495	-3.14136
D15	0.00013	-0.00007	-0.00686	0.02975	0.02272	0.02285
D16	2.76950	-0.00124	-0.03495	0.16312	0.12830	2.89780
D17	-0.37680	-0.00146	-0.03281	0.14266	0.10973	-0.26707
D18	-0.37430	-0.00148	-0.03261	0.14112	0.10839	-0.26591
D19	2.77211	-0.00127	-0.03475	0.16128	0.12665	2.89876
D20	-1.74082	-0.00137	-0.00172	0.00140	-0.00005	-1.74087
D21	0.37682	0.00062	-0.00092	0.01328	0.01243	0.38925
D22	2.43940	0.00341	0.00359	0.02172	0.02497	2.46437
D23	-1.74564	-0.00136	-0.00175	0.00158	0.00011	-1.74554
D24	0.37164	0.00063	-0.00092	0.01337	0.01252	0.38416
D25	2.43452	0.00342	0.00357	0.02182	0.02505	2.45957

Item	Value	Threshold	Converged?
Maximum Force	0.031554	0.000450	NO
RMS Force	0.008656	0.000300	NO
Maximum Displacement	0.491052	0.001800	NO
RMS Displacement	0.158549	0.001200	NO

Predicted change in Energy=-1.068491D-02
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 21:15:22 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.059923	0.665986	0.078856
2	6	0	3.377593	1.682495	0.193094

3	6	0	4.059804	-0.667004	-0.077298
4	6	0	2.174648	2.269549	0.256158
5	6	0	3.377279	-1.683351	-0.191760
6	6	0	0.946842	2.301725	0.251105
7	6	0	2.174211	-2.270139	-0.255193
8	6	0	-0.347473	1.955934	0.203605
9	6	0	0.946414	-2.302040	-0.250554
10	6	0	-1.426457	1.376943	0.111511
11	6	0	-0.347861	-1.955914	-0.203467
12	6	0	-2.651544	0.713195	0.050470
13	6	0	-1.426686	-1.376628	-0.111867
14	6	0	-2.651680	-0.712539	-0.050840
15	6	0	-3.868957	1.437504	0.115980
16	6	0	-3.868913	-1.436753	-0.116145
17	7	0	-3.754661	2.869458	-0.101487
18	7	0	-3.753582	-2.868830	0.100306
19	1	0	-3.276092	3.145374	-0.979193
20	1	0	-4.677312	3.299181	-0.103902
21	1	0	-3.271864	-3.144454	0.976317
22	1	0	-4.676210	-3.298565	0.106115
23	1	0	-3.212645	3.317109	0.643175
24	1	0	-4.830855	1.026867	-0.137725
25	1	0	-4.831178	-1.026440	0.136578
26	1	0	-3.214232	-3.316583	-0.646265

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229599	0.000000			
3	C	1.342105	2.461436	0.000000		
4	C	2.481353	1.340032	3.505474	0.000000	
5	C	2.461426	3.387776	1.229594	4.156004	0.000000
6	C	3.520879	2.509056	4.314132	1.228239	4.688708
7	C	3.505471	4.156008	2.481360	4.568397	1.340044
8	C	4.593981	3.735103	5.136419	2.542088	5.222498
9	C	4.314120	4.688707	3.520875	4.760751	2.509052
10	C	5.532349	4.814448	5.857680	3.712900	5.703792
11	C	5.136402	5.222479	4.593987	4.942555	3.735117
12	C	6.711693	6.108222	6.852989	5.075104	6.492212
13	C	5.857604	5.703712	5.532299	5.138060	4.814410
14	C	6.852938	6.492135	6.711690	5.681596	6.108247
15	C	7.966413	7.251099	8.205580	6.102222	7.895718
16	C	8.205240	7.895389	7.966089	7.099290	7.250781
17	N	8.121301	7.236346	8.577471	5.970302	8.461725
18	N	8.575910	8.460308	8.119641	7.846728	7.234628
19	H	7.815621	6.912727	8.316430	5.657184	8.258570
20	H	9.127233	8.220910	9.595234	6.938238	9.471524
21	H	8.311437	8.253977	7.810327	7.713271	6.907266

22	H	9.593665	9.470071	9.125606	8.829534	8.219266
23	H	7.761260	6.804834	8.323506	5.501826	8.314374
24	H	8.900735	8.241232	9.050783	7.125762	8.644170
25	H	9.050929	8.644387	8.900814	7.743348	8.241244
26	H	8.324662	8.315495	7.762448	7.814044	6.806030

		6	7	8	9	10
6	C	0.000000				
7	C	4.760747	0.000000			
8	C	1.340552	4.942578	0.000000		
9	C	4.631017	1.228220	4.473337	0.000000	
10	C	2.550932	5.138140	1.227973	4.392781	0.000000
11	C	4.473296	2.542098	3.932971	1.340585	3.517174
12	C	3.938536	5.681692	2.622326	4.703994	1.394678
13	C	4.392683	3.712865	3.517128	2.550927	2.762616
14	C	4.703862	5.075145	3.534806	3.938614	2.427646
15	C	4.894594	7.099596	3.560519	6.107891	2.443255
16	C	6.107584	6.101902	4.900316	4.894299	3.732868
17	N	4.748765	7.847968	3.540697	6.990473	2.773717
18	N	6.989375	5.968545	5.906826	4.747032	4.841718
19	H	4.478676	7.717367	3.374994	6.930714	2.781750
20	H	5.722941	8.830831	4.543828	7.938606	3.782785
21	H	6.927068	5.651617	5.929848	4.473113	4.959481
22	H	7.937441	6.936603	6.808614	5.721378	5.693971
23	H	4.299541	7.812978	3.202379	7.047791	2.690238
24	H	5.929438	7.743061	4.591338	6.668673	3.431414
25	H	6.668981	7.125710	5.385411	5.929384	4.167614
26	H	7.048773	5.503027	6.061355	4.300798	5.079327

		11	12	13	14	15
11	C	0.000000				
12	C	3.534909	0.000000			
13	C	1.227936	2.427754	0.000000		
14	C	2.622376	1.429329	1.394757	0.000000	
15	C	4.900555	1.418100	3.733086	2.476343	0.000000
16	C	3.560191	2.476292	2.442970	1.417888	2.883614
17	N	5.907698	2.426814	4.842398	3.748311	1.452876
18	N	3.539015	3.748050	2.772387	2.426237	4.307908
19	H	5.932910	2.713994	4.961961	4.016868	2.113697
20	H	6.809557	3.288600	5.694718	4.494429	2.041477
21	H	3.369615	4.015401	2.777415	2.711806	4.700111
22	H	4.542373	4.494061	3.781635	3.287991	4.804384
23	H	6.060409	2.728828	5.078474	4.127275	2.059513
24	H	5.385029	2.209797	4.167232	2.789604	1.076214
25	H	4.591261	2.790080	3.431460	2.209948	2.645243
26	H	3.203681	4.128095	2.691529	2.729843	4.859118

		16	17	18	19	20
16	C	0.000000				
17	N	4.307751	0.000000			
18	N	1.452928	5.741836	0.000000		

```
 19  H    4.700231   1.037076   6.128945   0.000000
 20  H    4.804448   1.017817   6.240139   1.659279   0.000000
 21  H    2.113336   6.128776   1.037023   6.586804   6.683008
 22  H    2.041439   6.239941   1.017815   6.683007   6.601088
 23  H    4.858647   1.024057   6.233231   1.632665   1.644291
 24  H    2.644848   2.134162   4.048906   2.759244   2.277746
 25  H    1.076187   4.048899   2.134697   4.589910   4.335032
 26  H    2.059951   6.233454   1.024084   6.470824   6.797286
            21         22         23         24         25
 21  H    0.000000
 22  H    1.659274   0.000000
 23  H    6.470417   6.796882   0.000000
 24  H    4.590367   4.335059   2.910948   0.000000
 25  H    2.760907   2.277607   4.662908   2.071549   0.000000
 26  H    1.632704   1.644316   6.757850   4.662365   2.910689
            26
 26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 2.44D-02
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.546109   -0.669857   -0.046909
    2          6           0        3.863582   -1.690449   -0.113715
    3          6           0        4.546248    0.668966    0.046895
    4          6           0        2.660523   -2.279561   -0.149517
    5          6           0        3.863921    1.689684    0.113714
    6          6           0        1.432709   -2.311216   -0.143163
    7          6           0        2.660967    2.279038    0.149517
    8          6           0        0.138460   -1.963321   -0.112050
    9          6           0        1.433178    2.310939    0.143200
   10          6           0       -0.940415   -1.380445   -0.047235
   11          6           0        0.138837    1.963257    0.112104
   12          6           0       -2.165372   -0.714322   -0.017416
   13          6           0       -0.940097    1.380548    0.047455
   14          6           0       -2.165221    0.714586    0.017277
   15          6           0       -3.382927   -1.440650   -0.049261
   16          6           0       -3.382311    1.441305    0.048537
   17          7           0       -3.268966   -2.860925    0.234783
   18          7           0       -3.266645    2.861704   -0.234462
   19          1           0       -2.790586   -3.095696    1.124480
```

```
    20        1        0     -4.191708   -3.289879    0.257095
    21        1        0     -2.784739    3.096067   -1.122300
    22        1        0     -4.189182    3.290888   -0.260456
    23        1        0     -2.726934   -3.342935   -0.488101
    24        1        0     -4.344777   -1.018430    0.184861
    25        1        0     -4.344625    1.019847   -0.184924
    26        1        0     -2.727313    3.343685    0.490495
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6058630           0.2675919           0.1865089
 Leave Link  202 at Fri Sep 25 21:15:22 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1008.6410939589 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000  wLong=    0.200000  cFull=    0.222036  cShort=    0.000000  cLong=
0.777964
  DFx    wShort=    0.000000  wLong=    0.200000  cFull=    0.000000  cShort=    0.000000  cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0153355405 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1008.6257584184 Hartrees.
 Leave Link  301 at Fri Sep 25 21:15:22 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23211 LenP2D=   51848.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.88D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=         32
 NSgBfM=   683   683   683   683   683 MxSgAt=    26 MxSgA2=    26.
```

Supporting Information file

```
 Leave Link  302 at Fri Sep 25 21:15:23 2026, MaxMem=    805306368 cpu:                5.7 elap:
1.0
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Sep 25 21:15:23 2026, MaxMem=    805306368 cpu:                0.7 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=    -0.000000    0.000000    0.000000
       Rot=    1.000000    0.000097    0.000006    0.000110 Ang=   0.02 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Generating alternative initial guess.
 ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn=          5 AccDes=
0.00D+00
 Harris functional with IExCor= 4639 and IRadAn=       5 diagonalized for initial guess.
 HarFok:  IExCor= 4639 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Petite list used in FoFCou.
 Harris En= -691.989929697438
 Leave Link  401 at Fri Sep 25 21:15:31 2026, MaxMem=    805306368 cpu:               47.4 elap:
7.9
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.370900765108
 DIIS: error= 5.90D-03 at cycle   1 NSaved=   1.
```

NSaved= 1 IEnMin= 1 EnMin= -723.370900765108 IErMin= 1 ErrMin= 5.90D-03
ErrMax= 5.90D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-02 BMatP= 3.98D-02
IDIUse=3 WtCom= 9.41D-01 WtEn= 5.90D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.697 Goal= None Shift= 0.000
GapD= 0.697 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=5.18D-03 MaxDP=2.32D-01 OVMax= 4.57D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 4.11D-03 CP: 8.14D-01
E= -723.405660392632 Delta-E= -0.034759627524 Rises=F Damp=F
DIIS: error= 1.02D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.405660392632 IErMin= 2 ErrMin= 1.02D-03
ErrMax= 1.02D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.99D-04 BMatP= 3.98D-02
IDIUse=3 WtCom= 9.90D-01 WtEn= 1.02D-02
Coeff-Com: -0.722D-01 0.107D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.715D-01 0.107D+01
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.92D-01 MaxDP=8.05D+00 DE=-3.48D-02 OVMax= 2.02D-02

Cycle 3 Pass 0 IDiag 1:
RMSU= 1.63D-01 CP: 3.00D+00 -2.67D+00
E= -723.405071927828 Delta-E= 0.000588464804 Rises=F Damp=F
DIIS: error= 2.11D-02 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.405660392632 IErMin= 2 ErrMin= 1.02D-03
ErrMax= 2.11D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-02 BMatP= 8.99D-04
IDIUse=2 WtCom= 0.00D+00 WtEn= 1.00D+00
Coeff-En: 0.000D+00 0.670D+00 0.330D+00
Coeff: 0.000D+00 0.670D+00 0.330D+00
Gap= 1.350 Goal= None Shift= 0.000
RMSDP=1.87D-01 MaxDP=7.91D+00 DE= 5.88D-04 OVMax= 1.31D-02

Cycle 4 Pass 0 IDiag 1:
RMSU= 9.44D-03 CP: 1.10D+00 1.95D+00 1.49D-02
E= -723.407444507359 Delta-E= -0.002372579531 Rises=F Damp=F
DIIS: error= 4.16D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.407444507359 IErMin= 2 ErrMin= 1.02D-03
ErrMax= 4.16D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.39D-04 BMatP= 8.99D-04
IDIUse=3 WtCom= 9.58D-01 WtEn= 4.16D-02
Coeff-Com: -0.267D-01 0.238D+00 0.158D+00 0.631D+00
Coeff-En: 0.000D+00 0.000D+00 0.509D-01 0.949D+00
Coeff: -0.256D-01 0.228D+00 0.153D+00 0.644D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=7.41D+02 MaxDP=3.09D+04 DE=-2.37D-03 OVMax= 9.67D-01

Supporting Information file

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 5 Pass 1 IDiag 1:
E= -723.407179619840 Delta-E= 0.000264887520 Rises=F Damp=F
DIIS: error= 2.19D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.407179619840 IErMin= 1 ErrMin= 2.19D-03
ErrMax= 2.19D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.06D-04 BMatP= 3.06D-04
IDIUse=3 WtCom= 9.78D-01 WtEn= 2.19D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.175 Goal= None Shift= 0.000
GapD= 0.175 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=1.38D-02 MaxDP=4.59D-01 DE= 2.65D-04 OVMax= 5.82D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 7.58D-03 CP: 4.88D-01
E= -723.407460800831 Delta-E= -0.000281180991 Rises=F Damp=F
DIIS: error= 1.20D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.407460800831 IErMin= 2 ErrMin= 1.20D-04
ErrMax= 1.20D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-05 BMatP= 3.06D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.20D-03
Coeff-Com: 0.256D-02 0.997D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.256D-02 0.997D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=5.16D-04 MaxDP=1.91D-02 DE=-2.81D-04 OVMax= 2.82D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.77D-04 CP: 4.86D-01 1.05D+00
E= -723.407474590751 Delta-E= -0.000013789920 Rises=F Damp=F
DIIS: error= 1.67D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.407474590751 IErMin= 2 ErrMin= 1.20D-04
ErrMax= 1.67D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.52D-06 BMatP= 1.02D-05
IDIUse=3 WtCom= 9.98D-01 WtEn= 1.67D-03
Coeff-Com: -0.282D-01 0.503D+00 0.525D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.281D-01 0.502D+00 0.526D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=8.75D-05 MaxDP=3.59D-03 DE=-1.38D-05 OVMax= 1.29D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 2.53D-05 CP: 4.87D-01 1.05D+00 1.15D+00
E= -723.407485521247 Delta-E= -0.000010930496 Rises=F Damp=F
DIIS: error= 5.64D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.407485521247 IErMin= 4 ErrMin= 5.64D-05
ErrMax= 5.64D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.40D-07 BMatP= 9.52D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.967D-02 0.635D-01 0.181D+00 0.765D+00
Coeff: -0.967D-02 0.635D-01 0.181D+00 0.765D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=6.01D-05 MaxDP=2.69D-03 DE=-1.09D-05 OVMax= 1.09D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 1.61D-05 CP: 4.89D-01 1.06D+00 1.24D+00 1.61D+00
E= -723.407487844711 Delta-E= -0.000002323464 Rises=F Damp=F
DIIS: error= 3.97D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.407487844711 IErMin= 5 ErrMin= 3.97D-05
ErrMax= 3.97D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.36D-07 BMatP= 7.40D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.608D-02-0.176D+00-0.102D+00 0.459D+00 0.813D+00
Coeff: 0.608D-02-0.176D+00-0.102D+00 0.459D+00 0.813D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=4.64D-05 MaxDP=2.03D-03 DE=-2.32D-06 OVMax= 1.19D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 3.95D-06 CP: 4.90D-01 1.06D+00 1.32D+00 2.14D+00 1.83D+00
E= -723.407489316457 Delta-E= -0.000001471745 Rises=F Damp=F
DIIS: error= 1.88D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.407489316457 IErMin= 6 ErrMin= 1.88D-05
ErrMax= 1.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.75D-08 BMatP= 3.36D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.354D-02-0.673D-01-0.581D-01 0.101D-01 0.280D+00 0.832D+00
Coeff: 0.354D-02-0.673D-01-0.581D-01 0.101D-01 0.280D+00 0.832D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=1.21D-05 MaxDP=4.31D-04 DE=-1.47D-06 OVMax= 5.60D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 2.19D-06 CP: 4.90D-01 1.06D+00 1.33D+00 2.31D+00 2.07D+00
CP: 1.59D+00
E= -723.407489628265 Delta-E= -0.000000311808 Rises=F Damp=F
DIIS: error= 9.77D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.407489628265 IErMin= 7 ErrMin= 9.77D-06
ErrMax= 9.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-08 BMatP= 4.75D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.814D-03 0.356D-01 0.165D-01-0.160D+00-0.176D+00 0.311D+00
Coeff-Com: 0.973D+00
Coeff: -0.814D-03 0.356D-01 0.165D-01-0.160D+00-0.176D+00 0.311D+00
Coeff: 0.973D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=8.27D-06 MaxDP=2.54D-04 DE=-3.12D-07 OVMax= 4.11D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.27D-06 CP: 4.90D-01 1.06D+00 1.34D+00 2.44D+00 2.17D+00
CP: 2.02D+00 2.05D+00
E= -723.407489739165 Delta-E= -0.000000110901 Rises=F Damp=F

DIIS: error= 5.45D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.407489739165 IErMin= 8 ErrMin= 5.45D-06
ErrMax= 5.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.87D-09 BMatP= 1.57D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.148D-02 0.411D-01 0.273D-01-0.109D+00-0.189D+00-0.831D-02
Coeff-Com: 0.617D+00 0.623D+00
Coeff: -0.148D-02 0.411D-01 0.273D-01-0.109D+00-0.189D+00-0.831D-02
Coeff: 0.617D+00 0.623D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=4.05D-06 MaxDP=1.28D-04 DE=-1.11D-07 OVMax= 1.62D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 3.73D-07 CP: 4.91D-01 1.06D+00 1.34D+00 2.50D+00 2.18D+00
CP: 2.12D+00 2.52D+00 1.54D+00
E= -723.407489760998 Delta-E= -0.000000021833 Rises=F Damp=F
DIIS: error= 2.17D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.407489760998 IErMin= 9 ErrMin= 2.17D-06
ErrMax= 2.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-10 BMatP= 6.87D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.113D-03 0.835D-03 0.265D-02 0.830D-02 0.113D-02-0.464D-01
Coeff-Com: -0.785D-01 0.116D+00 0.996D+00
Coeff: -0.113D-03 0.835D-03 0.265D-02 0.830D-02 0.113D-02-0.464D-01
Coeff: -0.785D-01 0.116D+00 0.996D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=2.17D-06 MaxDP=8.57D-05 DE=-2.18D-08 OVMax= 6.60D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 2.92D-07 CP: 4.91D-01 1.06D+00 1.34D+00 2.52D+00 2.16D+00
CP: 2.11D+00 2.67D+00 1.82D+00 1.93D+00
E= -723.407489764758 Delta-E= -0.000000003760 Rises=F Damp=F
DIIS: error= 1.38D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.407489764758 IErMin=10 ErrMin= 1.38D-06
ErrMax= 1.38D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.47D-10 BMatP= 5.26D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.316D-03-0.982D-02-0.539D-02 0.291D-01 0.472D-01-0.152D-01
Coeff-Com: -0.204D+00-0.115D+00 0.485D+00 0.788D+00
Coeff: 0.316D-03-0.982D-02-0.539D-02 0.291D-01 0.472D-01-0.152D-01
Coeff: -0.204D+00-0.115D+00 0.485D+00 0.788D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=1.08D-06 MaxDP=3.99D-05 DE=-3.76D-09 OVMax= 3.22D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.26D-07 CP: 4.91D-01 1.06D+00 1.35D+00 2.53D+00 2.17D+00
CP: 2.10D+00 2.71D+00 1.94D+00 2.31D+00 1.46D+00
E= -723.407489765986 Delta-E= -0.000000001228 Rises=F Damp=F
DIIS: error= 6.61D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.407489765986 IErMin=11 ErrMin= 6.61D-07
ErrMax= 6.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.47D-11 BMatP= 2.47D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.176D-03-0.491D-02-0.299D-02 0.122D-01 0.232D-01 0.401D-02
Coeff-Com: -0.862D-01-0.741D-01 0.616D-01 0.264D+00 0.803D+00
Coeff: 0.176D-03-0.491D-02-0.299D-02 0.122D-01 0.232D-01 0.401D-02
Coeff: -0.862D-01-0.741D-01 0.616D-01 0.264D+00 0.803D+00
Gap=   0.175 Goal=   None   Shift=   0.000
RMSDP=1.77D-07 MaxDP=6.51D-06 DE=-1.23D-09 OVMax= 1.70D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 8.23D-08   CP: 4.91D-01 1.06D+00 1.35D+00 2.53D+00 2.17D+00
               CP: 2.09D+00 2.70D+00 1.96D+00 2.39D+00 1.59D+00
               CP: 1.23D+00
E= -723.407489766244   Delta-E=   -0.000000000259 Rises=F Damp=F
DIIS: error= 4.99D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.407489766244   IErMin=12 ErrMin= 4.99D-07
ErrMax= 4.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.63D-11 BMatP= 4.47D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.270D-04 0.116D-02 0.567D-03-0.532D-02-0.555D-02 0.107D-01
Coeff-Com: 0.317D-01 0.304D-02-0.152D+00-0.196D+00 0.513D+00 0.799D+00
Coeff: -0.270D-04 0.116D-02 0.567D-03-0.532D-02-0.555D-02 0.107D-01
Coeff: 0.317D-01 0.304D-02-0.152D+00-0.196D+00 0.513D+00 0.799D+00
Gap=   0.175 Goal=   None   Shift=   0.000
RMSDP=1.38D-07 MaxDP=5.51D-06 DE=-2.59D-10 OVMax= 1.13D-05

Cycle 17 Pass 1 IDiag 1:
RMSU= 2.72D-08   CP: 4.91D-01 1.06D+00 1.35D+00 2.53D+00 2.17D+00
               CP: 2.08D+00 2.69D+00 1.97D+00 2.36D+00 1.57D+00
               CP: 1.56D+00 1.84D+00
E= -723.407489766388   Delta-E=   -0.000000000143 Rises=F Damp=F
DIIS: error= 2.19D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.407489766388   IErMin=13 ErrMin= 2.19D-07
ErrMax= 2.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.24D-12 BMatP= 2.63D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.567D-04 0.178D-02 0.106D-02-0.573D-02-0.818D-02 0.456D-02
Coeff-Com: 0.349D-01 0.212D-01-0.757D-01-0.189D+00 0.428D-01 0.422D+00
Coeff-Com: 0.750D+00
Coeff: -0.567D-04 0.178D-02 0.106D-02-0.573D-02-0.818D-02 0.456D-02
Coeff: 0.349D-01 0.212D-01-0.757D-01-0.189D+00 0.428D-01 0.422D+00
Coeff: 0.750D+00
Gap=   0.175 Goal=   None   Shift=   0.000
RMSDP=7.70D-08 MaxDP=4.50D-06 DE=-1.43D-10 OVMax= 5.36D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.76D-08   CP: 4.91D-01 1.06D+00 1.35D+00 2.53D+00 2.17D+00
               CP: 2.08D+00 2.69D+00 1.97D+00 2.32D+00 1.54D+00
               CP: 1.64D+00 2.30D+00 1.52D+00
E= -723.407489766419   Delta-E=   -0.000000000031 Rises=F Damp=F
DIIS: error= 9.24D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -723.407489766419 IErMin=14 ErrMin= 9.24D-08
ErrMax= 9.24D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.23D-13 BMatP= 6.24D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.821D-05 0.167D-03 0.168D-03-0.120D-03-0.700D-03-0.171D-02
Coeff-Com: -0.286D-04 0.595D-02 0.261D-01-0.161D-01-0.134D+00-0.104D+00
Coeff-Com: 0.233D+00 0.992D+00
Coeff: -0.821D-05 0.167D-03 0.168D-03-0.120D-03-0.700D-03-0.171D-02
Coeff: -0.286D-04 0.595D-02 0.261D-01-0.161D-01-0.134D+00-0.104D+00
Coeff: 0.233D+00 0.992D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=3.54D-08 MaxDP=1.90D-06 DE=-3.09D-11 OVMax= 3.02D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 9.04D-09 CP: 4.91D-01 1.06D+00 1.35D+00 2.53D+00 2.17D+00
CP: 2.08D+00 2.68D+00 1.97D+00 2.30D+00 1.52D+00
CP: 1.67D+00 2.52D+00 2.08D+00 1.91D+00
E= -723.407489766427 Delta-E= -0.000000000008 Rises=F Damp=F
DIIS: error= 1.45D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.407489766427 IErMin=15 ErrMin= 1.45D-08
ErrMax= 1.45D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.67D-14 BMatP= 9.23D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.672D-05-0.238D-03-0.112D-03 0.874D-03 0.114D-02-0.118D-02
Coeff-Com: -0.582D-02-0.125D-02 0.222D-01 0.217D-01-0.419D-01-0.953D-01
Coeff-Com: -0.482D-01 0.273D+00 0.875D+00
Coeff: 0.672D-05-0.238D-03-0.112D-03 0.874D-03 0.114D-02-0.118D-02
Coeff: -0.582D-02-0.125D-02 0.222D-01 0.217D-01-0.419D-01-0.953D-01
Coeff: -0.482D-01 0.273D+00 0.875D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=1.20D-08 MaxDP=4.83D-07 DE=-7.96D-12 OVMax= 6.62D-07

Cycle 20 Pass 1 IDiag 1:
RMSU= 2.67D-09 CP: 4.91D-01 1.06D+00 1.35D+00 2.53D+00 2.17D+00
CP: 2.08D+00 2.68D+00 1.97D+00 2.30D+00 1.51D+00
CP: 1.66D+00 2.55D+00 2.24D+00 2.29D+00 1.47D+00
E= -723.407489766442 Delta-E= -0.000000000015 Rises=F Damp=F
DIIS: error= 2.63D-09 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.407489766442 IErMin=16 ErrMin= 2.63D-09
ErrMax= 2.63D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.98D-15 BMatP= 8.67D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.134D-05-0.386D-04-0.228D-04 0.104D-03 0.176D-03-0.106D-04
Coeff-Com: -0.676D-03-0.509D-03 0.928D-03 0.265D-02 0.432D-02-0.290D-02
Coeff-Com: -0.175D-01-0.444D-01 0.931D-01 0.965D+00
Coeff: 0.134D-05-0.386D-04-0.228D-04 0.104D-03 0.176D-03-0.106D-04
Coeff: -0.676D-03-0.509D-03 0.928D-03 0.265D-02 0.432D-02-0.290D-02
Coeff: -0.175D-01-0.444D-01 0.931D-01 0.965D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=6.94D-09 MaxDP=3.37D-07 DE=-1.55D-11 OVMax= 1.37D-07

Supporting Information file

SCF Done: E(RwB97XD) = -723.407489766 A.U. after 20 cycles
NFock= 20 Conv=0.69D-08 -V/T= 2.0047
KE= 7.200144242950D+02 PE=-3.698592312953D+03 EE= 1.246544640473D+03
Leave Link 502 at Fri Sep 25 21:38:35 2026, MaxMem= 805306368 cpu: 8299.4 elap: 1383.7
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23211 LenP2D= 51848.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 21:38:35 2026, MaxMem= 805306368 cpu: 3.1 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 21:38:35 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 21:48:46 2026, MaxMem= 805306368 cpu: 3661.6 elap: 610.4
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-5.47928107D+00 2.11893376D-03 1.31285658D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000682081	-0.002901985	-0.000476261
2	6	-0.001854472	0.002153982	0.000228311
3	6	0.000671274	0.002908704	0.000476678
4	6	0.002335563	-0.001120097	-0.000131795
5	6	-0.001850963	-0.002166562	-0.000228467
6	6	-0.002324072	0.000126643	0.000129324
7	6	0.002348389	0.001129138	0.000132435
8	6	0.001380732	0.000051933	-0.001313085
9	6	-0.002347089	-0.000129959	-0.000131335

```
    10        6       -0.005676647   0.002124344   0.000035110
    11        6        0.001420458  -0.000062404   0.001297589
    12        6       -0.002416373   0.005287322  -0.001276200
    13        6       -0.005703380  -0.002080892  -0.000004313
    14        6       -0.002376670  -0.005199256   0.001247709
    15        6        0.003234503  -0.013824870   0.004786258
    16        6        0.003292507   0.013728270  -0.004765564
    17        7        0.002875308   0.012510615  -0.002289146
    18        7        0.002759619  -0.012485345   0.002271436
    19        1       -0.001591901  -0.002337957   0.002258272
    20        1        0.001756159  -0.001081085   0.000569419
    21        1       -0.001594259   0.002331711  -0.002257730
    22        1        0.001749563   0.001061569  -0.000569860
    23        1        0.000031304  -0.000703201  -0.000625109
    24        1        0.001584169   0.001924332  -0.004480921
    25        1        0.001580938  -0.001959178   0.004480051
    26        1        0.000033258   0.000714230   0.000637195
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.013824870 RMS     0.003729006
 Leave Link  716 at Fri Sep 25 21:48:46 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.008556657 RMS     0.002856364
 Search for a local minimum.
 Step number   7 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .28564D-02 SwitMx=.10000D-02 MixMth= 1
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    6    7
 DE= -6.39D-03 DEPred=-1.07D-02 R= 5.98D-01
 TightC=F SS=  1.41D+00  RLast= 3.52D-01 DXNew= 2.4000D+00 1.0557D+00
 Trust test= 5.98D-01 RLast= 3.52D-01 DXMaxT set to 1.43D+00
 ITU=  1  1  1  0  0  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.00441   0.00967   0.01660   0.01681   0.01751
    Eigenvalues ---    0.02018   0.02195   0.02404   0.02744   0.02794
    Eigenvalues ---    0.03100   0.03304   0.03796   0.03845   0.04439
    Eigenvalues ---    0.04462   0.04469   0.04988   0.05026   0.05026
    Eigenvalues ---    0.06193   0.08684   0.09909   0.11019   0.11207
    Eigenvalues ---    0.11521   0.11566   0.14554   0.15147   0.15279
    Eigenvalues ---    0.15971   0.16000   0.16000   0.16000   0.16000
    Eigenvalues ---    0.16573   0.20999   0.24992   0.24995   0.24996
    Eigenvalues ---    0.25000   0.25000   0.25000   0.25000   0.25106
```

```
    Eigenvalues ---    0.27673   0.33354   0.37230   0.38017   0.40643
    Eigenvalues ---    0.45150   0.45826   0.47129   0.47473   0.47688
    Eigenvalues ---    0.47688   0.47688   0.47729   0.49512   0.50775
    Eigenvalues ---    0.54797   0.55197   0.55384   0.55659   0.55674
    Eigenvalues ---    0.93679   0.93924   0.95022   0.95699   0.97678
    Eigenvalues ---    0.98227   1.36034
 RFO step:  Lambda=-6.04338287D-03 EMin= 4.40701864D-03
 Quartic linear search produced a step of -0.22407.
 Iteration  1 RMS(Cart)=  0.18938915 RMS(Int)=  0.00961964
 Iteration  2 RMS(Cart)=  0.02417902 RMS(Int)=  0.00021272
 Iteration  3 RMS(Cart)=  0.00030445 RMS(Int)=  0.00017269
 Iteration  4 RMS(Cart)=  0.00000006 RMS(Int)=  0.00017269
  ITry=  1 IFail=0 DXMaxC= 5.36D-01 DCOld= 1.00D+10 DXMaxT= 1.43D+00 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)   (Quad)   (Total)
    R1        2.32361   0.00160  -0.00083   0.00295   0.00206   2.32567
    R2        2.53621  -0.00146   0.00164  -0.00547  -0.00390   2.53231
    R3        2.53229  -0.00136   0.00158  -0.00507  -0.00352   2.52877
    R4        2.32360   0.00161  -0.00083   0.00296   0.00207   2.32566
    R5        2.32103   0.00117  -0.00097   0.00305   0.00207   2.32311
    R6        2.53232  -0.00136   0.00158  -0.00507  -0.00353   2.52879
    R7        2.53328  -0.00120   0.00136  -0.00426  -0.00288   2.53040
    R8        2.32100   0.00118  -0.00097   0.00306   0.00208   2.32308
    R9        2.32053  -0.00002  -0.00147   0.00328   0.00185   2.32238
   R10        2.53334  -0.00121   0.00137  -0.00428  -0.00289   2.53044
   R11        2.63556  -0.00396   0.00044  -0.00757  -0.00709   2.62847
   R12        2.32046   0.00001  -0.00147   0.00330   0.00187   2.32233
   R13        2.70104   0.00347  -0.00448   0.01597   0.01157   2.71261
   R14        2.67982  -0.00856  -0.00737  -0.00372  -0.01109   2.66873
   R15        2.63571  -0.00398   0.00044  -0.00760  -0.00712   2.62859
   R16        2.67942  -0.00844  -0.00737  -0.00350  -0.01087   2.66855
   R17        2.74554   0.00852  -0.01037   0.04244   0.03207   2.77761
   R18        2.03375  -0.00109  -0.00014  -0.00140  -0.00154   2.03221
   R19        2.74564   0.00850  -0.01036   0.04242   0.03206   2.77770
   R20        2.03370  -0.00111  -0.00013  -0.00145  -0.00158   2.03212
   R21        1.95979  -0.00327  -0.00053  -0.00277  -0.00330   1.95649
   R22        1.92340  -0.00205  -0.00155   0.00016  -0.00139   1.92200
   R23        1.93519  -0.00075  -0.00107   0.00214   0.00107   1.93626
   R24        1.95969  -0.00327  -0.00053  -0.00277  -0.00330   1.95639
   R25        1.92339  -0.00204  -0.00154   0.00015  -0.00139   1.92200
   R26        1.93524  -0.00076  -0.00107   0.00212   0.00105   1.93629
    A1        2.55322   0.00062   0.00029   0.00044   0.00023   2.55345
    A2        2.61533   0.00003   0.00050  -0.00107  -0.00098   2.61436
    A3        2.55321   0.00063   0.00028   0.00048   0.00027   2.55347
    A4        2.71087   0.00029   0.00004   0.00174   0.00154   2.71242
    A5        2.61534   0.00002   0.00051  -0.00111  -0.00101   2.61433
    A6        2.85269  -0.00067   0.00022  -0.00025  -0.00007   2.85263
```

A7	2.71088	0.00029	0.00004	0.00176	0.00156	2.71244
A8	2.85266	-0.00067	0.00023	-0.00027	-0.00008	2.85258
A9	2.06906	0.00205	0.00450	0.00244	0.00716	2.07622
A10	2.10481	-0.00722	-0.00645	-0.01320	-0.01989	2.08492
A11	2.10909	0.00518	0.00199	0.01122	0.01294	2.12203
A12	2.06912	0.00201	0.00449	0.00236	0.00706	2.07617
A13	2.10927	0.00518	0.00199	0.01122	0.01294	2.12221
A14	2.10457	-0.00717	-0.00642	-0.01311	-0.01978	2.08479
A15	2.16702	0.00286	0.00245	0.01420	0.01665	2.18366
A16	1.99444	0.00248	0.02229	-0.01646	0.00583	2.00027
A17	2.16766	0.00282	0.00228	0.01398	0.01626	2.18392
A18	1.99521	0.00236	0.02219	-0.01717	0.00502	2.00023
A19	2.00998	-0.00204	0.00601	-0.02133	-0.01531	1.99467
A20	1.92321	0.00014	-0.00438	0.01273	0.00835	1.93156
A21	1.94296	-0.00002	0.00038	-0.00199	-0.00161	1.94136
A22	1.87966	0.00094	-0.00276	0.00787	0.00512	1.88478
A23	1.82852	0.00079	0.00070	0.00182	0.00251	1.83103
A24	1.87231	0.00039	-0.00020	0.00187	0.00167	1.87398
A25	2.00941	-0.00204	0.00602	-0.02135	-0.01533	1.99409
A26	1.92309	0.00016	-0.00438	0.01288	0.00851	1.93160
A27	1.94352	-0.00004	0.00036	-0.00203	-0.00167	1.94184
A28	1.87973	0.00093	-0.00276	0.00785	0.00509	1.88482
A29	1.82861	0.00078	0.00069	0.00177	0.00245	1.83107
A30	1.87231	0.00039	-0.00018	0.00185	0.00167	1.87398
A31	2.90768	-0.00063	-0.00065	0.00720	0.00668	2.91436
A32	3.14046	-0.00166	-0.00484	-0.01002	-0.01457	3.12589
A33	2.90766	-0.00062	-0.00064	0.00727	0.00677	2.91443
A34	3.14045	-0.00166	-0.00488	-0.01001	-0.01460	3.12585
A35	4.16146	0.00534	0.02474	-0.00226	0.02247	4.18394
A36	4.16287	0.00518	0.02447	-0.00319	0.02128	4.18415
A37	3.15761	-0.00029	-0.00130	-0.00494	-0.00604	3.15157
A38	3.10881	0.00186	0.00377	0.06713	0.07102	3.17982
A39	3.15749	-0.00028	-0.00128	-0.00477	-0.00585	3.15164
A40	3.10921	0.00184	0.00376	0.06638	0.07026	3.17947
A41	3.64759	0.00023	0.01204	-0.03029	-0.01825	3.62934
A42	3.64594	0.00012	0.01189	-0.03146	-0.01957	3.62637
D1	0.00417	0.00032	-0.00018	0.01079	0.01074	0.01491
D2	-0.01374	0.00051	0.00097	0.02090	0.02204	0.00831
D3	-0.00838	0.00005	0.00127	0.00676	0.00806	-0.00032
D4	0.00413	0.00032	-0.00017	0.01074	0.01069	0.01482
D5	0.01121	-0.00018	-0.00019	0.00030	0.00003	0.01125
D6	-0.00829	0.00005	0.00127	0.00662	0.00793	-0.00036
D7	0.04272	-0.00113	-0.00572	-0.05175	-0.05715	-0.01443
D8	-3.13650	0.00067	0.00034	0.01365	0.01344	-3.12307
D9	0.01110	-0.00018	-0.00019	0.00022	-0.00005	0.01105
D10	0.04290	-0.00112	-0.00569	-0.05194	-0.05732	-0.01442
D11	-3.13586	0.00067	0.00030	0.01317	0.01291	-3.12295
D12	-0.02257	-0.00023	0.00294	0.00726	0.01037	-0.01220

D13	-3.14155	-0.00062	-0.00104	-0.01603	-0.01721	3.12443
D14	-3.14136	-0.00062	-0.00111	-0.01582	-0.01706	3.12477
D15	0.02285	-0.00101	-0.00509	-0.03911	-0.04464	-0.02179
D16	2.89780	-0.00502	-0.02875	-0.19236	-0.22111	2.67669
D17	-0.26707	-0.00450	-0.02459	-0.16860	-0.19319	-0.46026
D18	-0.26591	-0.00449	-0.02429	-0.16813	-0.19241	-0.45832
D19	2.89876	-0.00501	-0.02838	-0.19210	-0.22048	2.67828
D20	-1.74087	0.00068	0.00001	0.00839	0.00840	-1.73247
D21	0.38925	0.00054	-0.00278	0.01327	0.01049	0.39974
D22	2.46437	0.00111	-0.00560	0.02260	0.01700	2.48137
D23	-1.74554	0.00067	-0.00002	0.00832	0.00830	-1.73723
D24	0.38416	0.00054	-0.00281	0.01327	0.01047	0.39463
D25	2.45957	0.00112	-0.00561	0.02266	0.01704	2.47661

Item	Value	Threshold	Converged?
Maximum Force	0.008557	0.000450	NO
RMS Force	0.002856	0.000300	NO
Maximum Displacement	0.536084	0.001800	NO
RMS Displacement	0.202918	0.001200	NO

Predicted change in Energy=-3.289251D-03
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 21:48:46 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.025835	0.670076	-0.012853
2	6	0	3.343018	1.693818	-0.030612
3	6	0	4.025855	-0.669695	0.013989
4	6	0	2.141346	2.282602	-0.027525
5	6	0	3.343092	-1.693472	0.031580
6	6	0	0.912594	2.315296	-0.008414
7	6	0	2.141424	-2.282285	0.028254
8	6	0	-0.380213	1.968287	0.026675
9	6	0	0.912690	-2.315027	0.008947
10	6	0	-1.464650	1.390480	0.047929
11	6	0	-0.380136	-1.967999	-0.026245
12	6	0	-2.681647	0.717538	0.020773
13	6	0	-1.464584	-1.390263	-0.047491
14	6	0	-2.681661	-0.717309	-0.020798
15	6	0	-3.884618	1.457260	0.029067
16	6	0	-3.884432	-1.457175	-0.029149
17	7	0	-3.707689	2.916403	0.036155
18	7	0	-3.708642	-2.916498	-0.037303

19	1	0	-3.132476	3.279393	-0.744406
20	1	0	-4.608675	3.387441	0.007898
21	1	0	-3.131609	-3.279678	0.741758
22	1	0	-4.609885	-3.386890	-0.006539
23	1	0	-3.226258	3.227678	0.885382
24	1	0	-4.820039	1.121608	-0.381793
25	1	0	-4.820416	-1.121240	0.380072
26	1	0	-3.229711	-3.228270	-0.887778

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.230692	0.000000			
3	C	1.340040	2.460579	0.000000		
4	C	2.480273	1.338168	3.502736	0.000000	
5	C	2.460583	3.387861	1.230688	4.154137	0.000000
6	C	3.521227	2.508722	4.313127	1.229335	4.688191
7	C	3.502731	4.154117	2.480268	4.565228	1.338177
8	C	4.593493	3.733774	5.135421	2.541651	5.222213
9	C	4.313118	4.688166	3.521212	4.759109	2.508724
10	C	5.537879	4.817869	5.864394	3.715479	5.711866
11	C	5.135386	5.222145	4.593470	4.942214	3.733783
12	C	6.707735	6.103471	6.849456	5.070801	6.489266
13	C	5.864375	5.711819	5.537862	5.147142	4.817876
14	C	6.849482	6.489252	6.707775	5.679869	6.103547
15	C	7.949634	7.231753	8.191444	6.082486	7.884599
16	C	8.191324	7.884466	7.949505	7.091964	7.231641
17	N	8.053308	7.156231	8.524569	5.883618	8.424041
18	N	8.525623	8.425021	8.054390	7.826436	7.157338
19	H	7.654092	6.704892	8.210491	5.414860	8.201495
20	H	9.052031	8.130146	9.540204	6.839935	9.436463
21	H	8.209689	8.200793	7.653165	7.702909	6.703891
22	H	9.541209	9.437312	9.053153	8.816048	8.131357
23	H	7.742158	6.807875	8.279009	5.526096	8.252457
24	H	8.865071	8.190621	9.034116	7.066421	8.644783
25	H	9.034343	8.644933	8.865349	7.760052	8.190956
26	H	8.282846	8.256056	7.746143	7.743256	6.811943

		6	7	8	9	10
6	C	0.000000				
7	C	4.759108	0.000000			
8	C	1.339028	4.942269	0.000000		
9	C	4.630355	1.229322	4.474225	0.000000	
10	C	2.551421	5.147170	1.228950	4.402731	0.000000
11	C	4.474157	2.541654	3.936642	1.339054	3.530021
12	C	3.933479	5.679877	2.619353	4.702749	1.390924
13	C	4.402689	3.715472	3.530045	2.551431	2.782379
14	C	4.702714	5.070868	3.537138	3.933567	2.434874
15	C	4.873487	7.092064	3.541470	6.102845	2.420962

16	C	6.102740	6.082355	4.900660	4.873371	3.737703
17	N	4.659434	7.825505	3.459929	6.979720	2.712895
18	N	6.980568	5.884708	5.911317	4.660538	4.857244
19	H	4.223003	7.703459	3.144601	6.944670	2.641483
20	H	5.624427	8.815330	4.460296	7.937481	3.724829
21	H	6.944211	5.413756	5.968472	4.221838	5.007047
22	H	7.938054	6.841165	6.824160	5.625653	5.720029
23	H	4.331444	7.739920	3.228531	6.972847	2.679531
24	H	5.867486	7.759935	4.538256	6.695321	3.393463
25	H	6.695379	7.066754	5.420837	5.867824	4.204785
26	H	6.975894	5.530198	5.996672	4.335622	5.032279

		11	12	13	14	15
11	C	0.000000				
12	C	3.537128	0.000000			
13	C	1.228926	2.434898	0.000000		
14	C	2.619404	1.435449	1.390992	0.000000	
15	C	4.900699	1.412231	3.737755	2.485627	0.000000
16	C	3.541334	2.485671	2.420843	1.412137	2.915017
17	N	5.910489	2.426521	4.856530	3.776220	1.469848
18	N	3.461030	3.776812	2.713908	2.427220	4.377800
19	H	5.968773	2.711429	5.007319	4.086621	2.117581
20	H	6.823668	3.292716	5.719688	4.534664	2.061627
21	H	3.143395	4.086565	2.640412	2.711029	4.849075
22	H	4.461437	4.534884	3.725737	3.293161	4.898272
23	H	5.993875	2.710157	5.029824	4.084198	2.073908
24	H	5.420777	2.213154	4.204799	2.843342	1.075398
25	H	4.538522	2.843331	3.393640	2.213172	2.765426
26	H	3.232739	4.085981	2.683287	2.712368	4.819098

		16	17	18	19	20
16	C	0.000000				
17	N	4.377635	0.000000			
18	N	1.469895	5.833364	0.000000		
19	H	4.848929	1.035330	6.262670	0.000000	
20	H	4.898592	1.017080	6.368026	1.660362	0.000000
21	H	2.117205	6.262680	1.035279	6.725332	6.868096
22	H	2.061696	6.367675	1.017081	6.867788	6.774346
23	H	4.818445	1.024625	6.231769	1.633304	1.645169
24	H	2.765834	2.152509	4.202401	2.763223	2.308795
25	H	1.075351	4.202261	2.152486	4.845531	4.528967
26	H	2.074290	6.232104	1.024639	6.509969	6.816994

		21	22	23	24	25
21	H	0.000000				
22	H	1.660345	0.000000			
23	H	6.509629	6.816338	0.000000		
24	H	4.846078	4.528965	2.929404	0.000000	
25	H	2.764370	2.308021	4.659374	2.368713	0.000000
26	H	1.633295	1.645182	6.695026	4.659034	2.928714

		26

Supporting Information file

26 H 0.000000
Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=3 Diff= 6.00D-02
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.528858	-0.669506	0.016305
2	6	0	3.846131	-1.693226	0.038308
3	6	0	4.528762	0.670139	-0.016194
4	6	0	2.644511	-2.282125	0.037567
5	6	0	3.845910	1.693771	-0.038188
6	6	0	1.415765	-2.315009	0.018451
7	6	0	2.644189	2.282485	-0.037488
8	6	0	0.122931	-1.968268	-0.018254
9	6	0	1.415450	2.315198	-0.018463
10	6	0	-0.961555	-1.390652	-0.042073
11	6	0	0.122651	1.968207	0.018044
12	6	0	-2.178616	-0.717711	-0.017901
13	6	0	-0.961748	1.390468	0.041604
14	6	0	-2.178762	0.717299	0.017611
15	6	0	-3.381519	-1.457569	-0.023212
16	6	0	-3.381600	1.457086	0.022697
17	7	0	-3.204459	-2.916713	-0.024117
18	7	0	-3.205941	2.916446	0.024709
19	1	0	-2.629305	-3.276353	0.758037
20	1	0	-4.105407	-3.387708	0.006024
21	1	0	-2.628849	3.276384	-0.755811
22	1	0	-4.107222	3.386623	-0.008145
23	1	0	-2.722902	-3.231529	-0.871966
24	1	0	-4.317019	-1.120268	0.386118
25	1	0	-4.317506	1.119342	-0.385211
26	1	0	-2.727137	3.231850	0.873916

Rotational constants (GHZ): 0.5975940 0.2713967 0.1870729
Leave Link 202 at Fri Sep 25 21:48:46 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.

606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1009.3425429762 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0154409629 Hartrees.
Nuclear repulsion after empirical dispersion term = 1009.3271020133 Hartrees.
Leave Link 301 at Fri Sep 25 21:48:46 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23225 LenP2D= 51892.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.89D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Fri Sep 25 21:48:47 2026, MaxMem= 805306368 cpu: 5.6 elap: 0.9
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 21:48:47 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 0.000000 -0.000000
Rot= 0.999999 -0.001396 -0.000005 -0.000118 Ang= -0.16 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.

Supporting Information file

HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.993240664379
Leave Link 401 at Fri Sep 25 21:48:54 2026, MaxMem= 805306368 cpu: 42.5 elap: 7.1
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.308773491207
DIIS: error= 1.49D-02 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.308773491207 IErMin= 1 ErrMin= 1.49D-02
ErrMax= 1.49D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-01 BMatP= 1.64D-01
IDIUse=3 WtCom= 8.51D-01 WtEn= 1.49D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Recover alternate guess density for next cycle.
RMSDP=8.67D-03 MaxDP=3.85D-01 OVMax= 0.00D+00

Cycle 2 Pass 0 IDiag 1:
RMSU= 8.31D-03 CP: 1.18D+00
E= -723.075182168679 Delta-E= 0.233591322528 Rises=F Damp=F
Switch densities from cycles 1 and 2 for lowest energy.
DIIS: error= 6.04D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -723.308773491207 IErMin= 1 ErrMin= 1.49D-02
ErrMax= 6.04D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.67D+00 BMatP= 1.64D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.910D+00 0.898D-01
Coeff: 0.910D+00 0.898D-01
Gap= 0.154 Goal= None Shift= 0.000
RMSDP=1.16D-02 MaxDP=4.09D-01 DE= 2.34D-01 OVMax= 3.55D-01

Cycle 3 Pass 0 IDiag 1:
RMSU= 7.45D-03 CP: 1.55D+00 5.87D-01
E= -723.403845238752 Delta-E= -0.328663070073 Rises=F Damp=F
DIIS: error= 1.83D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.403845238752 IErMin= 3 ErrMin= 1.83D-03
ErrMax= 1.83D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.78D-03 BMatP= 1.64D-01
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.331D-01 0.116D-01 0.102D+01
Coeff: -0.331D-01 0.116D-01 0.102D+01
Gap= 0.163 Goal= None Shift= 0.000
RMSDP=1.07D-02 MaxDP=3.81D-01 DE=-3.29D-01 OVMax= 4.61D-02

Cycle 4 Pass 0 IDiag 1:
RMSU= 4.58D-03 CP: 9.81D-01 3.22D-01 2.70D-01
E= -723.406536320163 Delta-E= -0.002691081412 Rises=F Damp=F
DIIS: error= 5.83D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.406536320163 IErMin= 3 ErrMin= 1.83D-03
ErrMax= 5.83D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.20D-03 BMatP= 2.78D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.262D-01 0.352D-02 0.565D+00 0.458D+00
Coeff: -0.262D-01 0.352D-02 0.565D+00 0.458D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=7.13D+02 MaxDP=2.86D+04 DE=-2.69D-03 OVMax= 9.77D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 5 Pass 1 IDiag 1:
E= -723.406339649332 Delta-E= 0.000196670831 Rises=F Damp=F
DIIS: error= 2.49D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.406339649332 IErMin= 1 ErrMin= 2.49D-03
ErrMax= 2.49D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.31D-03 BMatP= 2.31D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.100D+01
Coeff: 0.100D+01
Gap= 0.188 Goal= None Shift= 0.000
GapD= 0.188 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=4.67D-03 MaxDP=1.41D-01 DE= 1.97D-04 OVMax= 4.94D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 4.63D-03 CP: 9.55D-01
E= -723.403983977156 Delta-E= 0.002355672176 Rises=F Damp=F
DIIS: error= 4.47D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -723.406339649332 IErMin= 1 ErrMin= 2.49D-03
ErrMax= 4.47D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.22D-03 BMatP= 2.31D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.579D+00 0.421D+00
Coeff: 0.579D+00 0.421D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=3.29D-04 MaxDP=1.18D-02 DE= 2.36D-03 OVMax= 3.10D-02

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.81D-04 CP: 9.62D-01 1.03D+00
E= -723.408970009977 Delta-E= -0.004986032820 Rises=F Damp=F
DIIS: error= 9.36D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.408970009977 IErMin= 3 ErrMin= 9.36D-04
ErrMax= 9.36D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.47D-04 BMatP= 2.31D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.230D+00 0.208D+00 0.562D+00
Coeff: 0.230D+00 0.208D+00 0.562D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.42D-04 MaxDP=6.57D-03 DE=-4.99D-03 OVMax= 4.81D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.01D-04 CP: 9.57D-01 1.04D+00 9.94D-01
E= -723.409141897577 Delta-E= -0.000171887600 Rises=F Damp=F
DIIS: error= 3.04D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.409141897577 IErMin= 4 ErrMin= 3.04D-04
ErrMax= 3.04D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.16D-05 BMatP= 1.47D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.403D-01-0.916D-02 0.267D+00 0.782D+00
Coeff: -0.403D-01-0.916D-02 0.267D+00 0.782D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.34D-04 MaxDP=5.68D-03 DE=-1.72D-04 OVMax= 4.04D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.98D-05 CP: 9.53D-01 1.06D+00 1.09D+00 1.75D+00
E= -723.409185137100 Delta-E= -0.000043239523 Rises=F Damp=F
DIIS: error= 1.11D-04 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.409185137100 IErMin= 5 ErrMin= 1.11D-04
ErrMax= 1.11D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.77D-06 BMatP= 2.16D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.254D-01-0.157D-01 0.319D-01 0.208D+00 0.801D+00
Coeff: -0.254D-01-0.157D-01 0.319D-01 0.208D+00 0.801D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.02D-04 MaxDP=3.91D-03 DE=-4.32D-05 OVMax= 2.25D-03

Cycle 10 Pass 1 IDiag 1:
RMSU= 3.99D-05 CP: 9.47D-01 1.05D+00 1.07D+00 2.09D+00 1.59D+00
E= -723.409193145944 Delta-E= -0.000008008844 Rises=F Damp=F
DIIS: error= 6.66D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -723.409193145944 IErMin= 6 ErrMin= 6.66D-05
ErrMax= 6.66D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.06D-06 BMatP= 1.77D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.183D-02-0.607D-02-0.102D+00-0.224D+00 0.511D+00 0.819D+00
Coeff: 0.183D-02-0.607D-02-0.102D+00-0.224D+00 0.511D+00 0.819D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.11D-04 MaxDP=4.22D-03 DE=-8.01D-06 OVMax= 2.38D-03

Cycle 11 Pass 1 IDiag 1:
RMSU= 6.04D-06 CP: 9.42D-01 1.04D+00 1.03D+00 2.38D+00 2.24D+00
CP: 2.17D+00
E= -723.409198123373 Delta-E= -0.000004977429 Rises=F Damp=F
DIIS: error= 2.75D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.409198123373 IErMin= 7 ErrMin= 2.75D-05
ErrMax= 2.75D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.21D-07 BMatP= 1.06D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.622D-02-0.111D-03-0.593D-01-0.160D+00 0.110D+00 0.430D+00
Coeff-Com: 0.674D+00
Coeff: 0.622D-02-0.111D-03-0.593D-01-0.160D+00 0.110D+00 0.430D+00
Coeff: 0.674D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=4.77D-05 MaxDP=1.78D-03 DE=-4.98D-06 OVMax= 9.52D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.66D-06 CP: 9.39D-01 1.04D+00 1.01D+00 2.47D+00 2.51D+00
CP: 2.70D+00 1.38D+00
E= -723.409199046635 Delta-E= -0.000000923261 Rises=F Damp=F
DIIS: error= 1.33D-05 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.409199046635 IErMin= 8 ErrMin= 1.33D-05
ErrMax= 1.33D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.17D-08 BMatP= 2.21D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.108D-02 0.164D-02 0.124D-01 0.161D-01-0.109D+00-0.115D+00
Coeff-Com: 0.175D+00 0.102D+01
Coeff: 0.108D-02 0.164D-02 0.124D-01 0.161D-01-0.109D+00-0.115D+00
Coeff: 0.175D+00 0.102D+01
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=3.44D-05 MaxDP=1.33D-03 DE=-9.23D-07 OVMax= 6.50D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 5.24D-06 CP: 9.38D-01 1.04D+00 9.92D-01 2.52D+00 2.69D+00
CP: 3.00D+00 1.80D+00 1.72D+00
E= -723.409199289323 Delta-E= -0.000000242689 Rises=F Damp=F
DIIS: error= 5.01D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.409199289323 IErMin= 9 ErrMin= 5.01D-06
ErrMax= 5.01D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.20D-09 BMatP= 3.17D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.103D-02 0.872D-03 0.200D-01 0.450D-01-0.736D-01-0.154D+00
Coeff-Com: -0.884D-01 0.461D+00 0.790D+00

Coeff: -0.103D-02 0.872D-03 0.200D-01 0.450D-01-0.736D-01-0.154D+00
Coeff: -0.884D-01 0.461D+00 0.790D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.02D-05 MaxDP=4.46D-04 DE=-2.43D-07 OVMax= 2.36D-04

Cycle 14 Pass 1 IDiag 1:
RMSU= 1.41D-06 CP: 9.37D-01 1.04D+00 9.87D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.96D+00 2.08D+00 1.93D+00
E= -723.409199322281 Delta-E= -0.000000032958 Rises=F Damp=F
DIIS: error= 1.39D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.409199322281 IErMin=10 ErrMin= 1.39D-06
ErrMax= 1.39D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.62D-10 BMatP= 8.20D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.259D-03 0.906D-04 0.283D-02 0.664D-02-0.521D-02-0.195D-01
Coeff-Com: -0.301D-01 0.202D-01 0.119D+00 0.906D+00
Coeff: -0.259D-03 0.906D-04 0.283D-02 0.664D-02-0.521D-02-0.195D-01
Coeff: -0.301D-01 0.202D-01 0.119D+00 0.906D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=7.67D-07 MaxDP=3.37D-05 DE=-3.30D-08 OVMax= 4.09D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 4.26D-07 CP: 9.37D-01 1.04D+00 9.87D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.97D+00 2.10D+00 1.98D+00 8.35D-01
E= -723.409199324602 Delta-E= -0.000000002321 Rises=F Damp=F
DIIS: error= 1.02D-06 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.409199324602 IErMin=11 ErrMin= 1.02D-06
ErrMax= 1.02D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.11D-10 BMatP= 4.62D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.171D-03-0.203D-03-0.446D-02-0.100D-01 0.194D-01 0.353D-01
Coeff-Com: 0.937D-02-0.123D+00-0.184D+00 0.525D+00 0.732D+00
Coeff: 0.171D-03-0.203D-03-0.446D-02-0.100D-01 0.194D-01 0.353D-01
Coeff: 0.937D-02-0.123D+00-0.184D+00 0.525D+00 0.732D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=4.69D-07 MaxDP=1.83D-05 DE=-2.32D-09 OVMax= 2.24D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 6.81D-08 CP: 9.37D-01 1.04D+00 9.88D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.98D+00 2.10D+00 1.97D+00 7.15D-01
CP: 1.66D+00
E= -723.409199325620 Delta-E= -0.000000001019 Rises=F Damp=F
DIIS: error= 5.20D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.409199325620 IErMin=12 ErrMin= 5.20D-07
ErrMax= 5.20D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.71D-11 BMatP= 3.11D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.137D-03-0.117D-03-0.275D-02-0.624D-02 0.106D-01 0.209D-01
Coeff-Com: 0.103D-01-0.611D-01-0.120D+00 0.880D-01 0.329D+00 0.730D+00
Coeff: 0.137D-03-0.117D-03-0.275D-02-0.624D-02 0.106D-01 0.209D-01
Coeff: 0.103D-01-0.611D-01-0.120D+00 0.880D-01 0.329D+00 0.730D+00

Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.84D-07 MaxDP=7.19D-06 DE=-1.02D-09 OVMax= 1.03D-05

Cycle 17 Pass 1 IDiag 1:
RMSU= 4.76D-08 CP: 9.37D-01 1.04D+00 9.88D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.98D+00 2.09D+00 1.96D+00 6.75D-01
CP: 1.89D+00 1.64D+00
E= -723.409199325890 Delta-E= -0.000000000269 Rises=F Damp=F
DIIS: error= 3.89D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.409199325890 IErMin=13 ErrMin= 3.89D-07
ErrMax= 3.89D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.30D-11 BMatP= 5.71D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.290D-04 0.435D-04 0.940D-03 0.208D-02-0.426D-02-0.760D-02
Coeff-Com: -0.120D-02 0.303D-01 0.320D-01-0.140D+00-0.205D+00 0.125D+00
Coeff-Com: 0.117D+01
Coeff: -0.290D-04 0.435D-04 0.940D-03 0.208D-02-0.426D-02-0.760D-02
Coeff: -0.120D-02 0.303D-01 0.320D-01-0.140D+00-0.205D+00 0.125D+00
Coeff: 0.117D+01
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.73D-07 MaxDP=7.46D-06 DE=-2.69D-10 OVMax= 1.16D-05

Cycle 18 Pass 1 IDiag 1:
RMSU= 2.31D-08 CP: 9.37D-01 1.04D+00 9.88D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.97D+00 2.07D+00 1.95D+00 6.47D-01
CP: 2.00D+00 2.45D+00 2.24D+00
E= -723.409199326023 Delta-E= -0.000000000133 Rises=F Damp=F
DIIS: error= 1.91D-07 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.409199326023 IErMin=14 ErrMin= 1.91D-07
ErrMax= 1.91D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.32D-12 BMatP= 1.30D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.440D-04 0.457D-04 0.935D-03 0.214D-02-0.378D-02-0.716D-02
Coeff-Com: -0.326D-02 0.228D-01 0.377D-01-0.361D-01-0.142D+00-0.232D+00
Coeff-Com: 0.244D+00 0.112D+01
Coeff: -0.440D-04 0.457D-04 0.935D-03 0.214D-02-0.378D-02-0.716D-02
Coeff: -0.326D-02 0.228D-01 0.377D-01-0.361D-01-0.142D+00-0.232D+00
Coeff: 0.244D+00 0.112D+01
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=8.90D-08 MaxDP=3.80D-06 DE=-1.33D-10 OVMax= 7.31D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.82D-08 CP: 9.37D-01 1.04D+00 9.88D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.97D+00 2.07D+00 1.95D+00 6.28D-01
CP: 2.02D+00 2.85D+00 2.92D+00 1.96D+00
E= -723.409199326061 Delta-E= -0.000000000038 Rises=F Damp=F
DIIS: error= 6.01D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.409199326061 IErMin=15 ErrMin= 6.01D-08
ErrMax= 6.01D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.13D-13 BMatP= 3.32D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.713D-07-0.741D-06-0.449D-04-0.873D-04 0.231D-03 0.430D-03
Coeff-Com: -0.170D-03-0.216D-02-0.125D-02 0.192D-01 0.112D-01-0.554D-01
Coeff-Com: -0.129D+00 0.104D+00 0.105D+01
Coeff: -0.713D-07-0.741D-06-0.449D-04-0.873D-04 0.231D-03 0.430D-03
Coeff: -0.170D-03-0.216D-02-0.125D-02 0.192D-01 0.112D-01-0.554D-01
Coeff: -0.129D+00 0.104D+00 0.105D+01
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=3.08D-08 MaxDP=1.34D-06 DE=-3.75D-11 OVMax= 2.29D-06

Cycle 20 Pass 1 IDiag 1:
RMSU= 7.14D-09 CP: 9.37D-01 1.04D+00 9.88D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.97D+00 2.07D+00 1.95D+00 6.19D-01
CP: 2.02D+00 2.89D+00 3.00D+00 2.42D+00 1.65D+00
E= -723.409199326074 Delta-E= -0.000000000014 Rises=F Damp=F
DIIS: error= 1.67D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.409199326074 IErMin=16 ErrMin= 1.67D-08
ErrMax= 1.67D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 7.67D-14 BMatP= 3.13D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.629D-05-0.743D-05-0.149D-03-0.343D-03 0.628D-03 0.118D-02
Coeff-Com: 0.422D-03-0.406D-02-0.594D-02 0.135D-01 0.244D-01 0.130D-01
Coeff-Com: -0.770D-01-0.128D+00 0.381D+00 0.781D+00
Coeff: 0.629D-05-0.743D-05-0.149D-03-0.343D-03 0.628D-03 0.118D-02
Coeff: 0.422D-03-0.406D-02-0.594D-02 0.135D-01 0.244D-01 0.130D-01
Coeff: -0.770D-01-0.128D+00 0.381D+00 0.781D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.61D-08 MaxDP=6.76D-07 DE=-1.36D-11 OVMax= 4.25D-07

Cycle 21 Pass 1 IDiag 1:
RMSU= 2.86D-09 CP: 9.37D-01 1.04D+00 9.88D-01 2.53D+00 2.76D+00
CP: 3.00D+00 1.97D+00 2.07D+00 1.95D+00 6.19D-01
CP: 2.01D+00 2.87D+00 3.00D+00 2.52D+00 1.86D+00
CP: 1.34D+00
E= -723.409199326069 Delta-E= 0.000000000005 Rises=F Damp=F
DIIS: error= 6.77D-09 at cycle 17 NSaved= 17.
NSaved=17 IEnMin=16 EnMin= -723.409199326074 IErMin=17 ErrMin= 6.77D-09
ErrMax= 6.77D-09 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.67D-15 BMatP= 7.67D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.943D-07-0.195D-06 0.630D-05 0.101D-04-0.324D-04-0.603D-04
Coeff-Com: 0.506D-04 0.328D-03 0.440D-04-0.306D-02-0.207D-02 0.956D-02
Coeff-Com: 0.247D-01-0.244D-01-0.190D+00 0.514D-01 0.113D+01
Coeff: 0.943D-07-0.195D-06 0.630D-05 0.101D-04-0.324D-04-0.603D-04
Coeff: 0.506D-04 0.328D-03 0.440D-04-0.306D-02-0.207D-02 0.956D-02
Coeff: 0.247D-01-0.244D-01-0.190D+00 0.514D-01 0.113D+01
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=2.49D-08 MaxDP=9.71D-07 DE= 5.46D-12 OVMax= 2.90D-07

Cycle 22 Pass 1 IDiag 1:
RMSU= 1.39D-09 CP: 9.37D-01 1.04D+00 9.88D-01 2.53D+00 2.76D+00

Supporting Information file

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               CP:  3.00D+00  1.97D+00  2.07D+00  1.95D+00  6.22D-01
               CP:  2.00D+00  2.86D+00  3.00D+00  2.51D+00  1.93D+00
               CP:  1.49D+00  2.18D+00
 E= -723.409199326055     Delta-E=        0.000000000013 Rises=F Damp=F
 DIIS: error= 3.03D-09 at cycle  18 NSaved=  18.
 NSaved=18 IEnMin=16 EnMin= -723.409199326074     IErMin=18 ErrMin= 3.03D-09
 ErrMax= 3.03D-09  0.00D+00 EMaxC= 1.00D+00 BMatC= 4.06D-15 BMatP= 9.67D-15
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Large coefficients: NSaved= 18 BigCof=    0.00 CofMax=   10.00 Det=-7.21D-15
 Inversion failed.  Reducing to 17 matrices.
 Large coefficients: NSaved= 17 BigCof=    0.00 CofMax=   10.00 Det=-7.31D-15
 Inversion failed.  Reducing to 16 matrices.
 Large coefficients: NSaved= 16 BigCof=    0.00 CofMax=   10.00 Det=-7.34D-15
 Inversion failed.  Reducing to 15 matrices.
 Coeff-Com: -0.920D-06-0.534D-05-0.675D-05 0.265D-04 0.108D-03-0.655D-04
 Coeff-Com: -0.130D-02-0.114D-02 0.349D-02 0.125D-01-0.329D-02-0.109D+00
 Coeff-Com: -0.456D-01 0.495D+00 0.649D+00
 Coeff:     -0.920D-06-0.534D-05-0.675D-05 0.265D-04 0.108D-03-0.655D-04
 Coeff:     -0.130D-02-0.114D-02 0.349D-02 0.125D-01-0.329D-02-0.109D+00
 Coeff:     -0.456D-01 0.495D+00 0.649D+00
 Gap=     0.173 Goal=   None    Shift=    0.000
 RMSDP=7.33D-09 MaxDP=3.10D-07 DE= 1.34D-11 OVMax= 8.04D-08

 SCF Done:  E(RwB97XD) =  -723.409199326     A.U. after   22 cycles
            NFock= 22  Conv=0.73D-08     -V/T= 2.0047
 KE= 7.199896089050D+02 PE=-3.699968332520D+03 EE= 1.247242422276D+03
 Leave Link  502 at Fri Sep 25 22:12:32 2026, MaxMem=    805306368 cpu:             8503.6 elap:
1417.6
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23225 LenP2D=   51892.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 Leave Link  701 at Fri Sep 25 22:12:32 2026, MaxMem=    805306368 cpu:               2.9 elap:
0.5
 (Enter /home/user/gauss16/g16/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link  702 at Fri Sep 25 22:12:32 2026, MaxMem=    805306368 cpu:               0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l703.exe)
 Integral derivatives from FoFJK, PRISM(SPDF).
 Compute integral first derivatives, UseDBF=F ICtDFT=          0.
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
```

Supporting Information file

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 22:24:02 2026, MaxMem= 805306368 cpu: 4137.3 elap: 689.7
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-5.35700094D+00 2.00202253D-03 2.01375428D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000716221	-0.002869336	0.000327990
2	6	-0.001747485	0.002323741	-0.000096091
3	6	0.000709389	0.002871586	-0.000329527
4	6	0.002236288	-0.001224860	0.000074514
5	6	-0.001741732	-0.002327496	0.000096674
6	6	-0.002449223	0.000402388	0.000693920
7	6	0.002234246	0.001227457	-0.000075833
8	6	0.001320435	0.000328643	0.000815288
9	6	-0.002449439	-0.000401020	-0.000687426
10	6	-0.000919373	-0.000666779	-0.001964254
11	6	0.001312733	-0.000331370	-0.000810538
12	6	-0.001218800	0.003577939	-0.002951060
13	6	-0.000926252	0.000653960	0.001938512
14	6	-0.001182592	-0.003689879	0.002960848
15	6	0.000476736	-0.005070582	0.009088866
16	6	0.000409939	0.005100072	-0.009063982
17	7	0.002676204	0.004111316	-0.003850082
18	7	0.002775431	-0.004021619	0.003837458
19	1	-0.001321273	-0.001230702	0.001838972
20	1	0.000760911	-0.001952427	0.000108451
21	1	-0.001322130	0.001214899	-0.001823810
22	1	0.000762565	0.001964389	-0.000108879
23	1	-0.000375669	-0.002039087	-0.001602581
24	1	-0.000172730	-0.000185510	-0.002329431
25	1	-0.000190756	0.000196818	0.002312617
26	1	-0.000373644	0.002037459	0.001599385

Cartesian Forces: Max 0.009088866 RMS 0.002438849
Leave Link 716 at Fri Sep 25 22:24:02 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Supporting Information file

Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.008026733 RMS 0.002056480
Search for a local minimum.
Step number 8 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .20565D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 6 7 8
DE= -1.71D-03 DEPred=-3.29D-03 R= 5.20D-01
TightC=F SS= 1.41D+00 RLast= 4.48D-01 DXNew= 2.4000D+00 1.3437D+00
Trust test= 5.20D-01 RLast= 4.48D-01 DXMaxT set to 1.43D+00
ITU= 1 1 1 1 0 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00442	0.00984	0.01598	0.01660	0.01759
Eigenvalues ---	0.01969	0.02405	0.02731	0.02800	0.02879
Eigenvalues ---	0.03101	0.03306	0.03787	0.03880	0.04439
Eigenvalues ---	0.04461	0.04469	0.04902	0.05026	0.05026
Eigenvalues ---	0.08330	0.08687	0.09933	0.10982	0.11276
Eigenvalues ---	0.11507	0.11550	0.14707	0.14861	0.15274
Eigenvalues ---	0.15999	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16478	0.21640	0.24928	0.24957	0.24984
Eigenvalues ---	0.24993	0.25000	0.25000	0.25000	0.25358
Eigenvalues ---	0.29164	0.30923	0.37230	0.37902	0.40644
Eigenvalues ---	0.44926	0.45828	0.47062	0.47311	0.47688
Eigenvalues ---	0.47688	0.47688	0.47708	0.49811	0.52502
Eigenvalues ---	0.54796	0.55036	0.55378	0.55659	0.55665
Eigenvalues ---	0.93679	0.93775	0.95021	0.95588	0.97674
Eigenvalues ---	0.98165	1.36034			

RFO step: Lambda=-1.38574661D-03 EMin= 4.42026953D-03
Quartic linear search produced a step of -0.31485.
Iteration 1 RMS(Cart)= 0.12125351 RMS(Int)= 0.00321081
Iteration 2 RMS(Cart)= 0.00724115 RMS(Int)= 0.00022257
Iteration 3 RMS(Cart)= 0.00002350 RMS(Int)= 0.00022246
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00022246
ITry= 1 IFail=0 DXMaxC= 4.36D-01 DCOld= 1.00D+10 DXMaxT= 1.43D+00 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.32567	0.00182	-0.00065	0.00279	0.00203	2.32770
R2	2.53231	-0.00117	0.00123	-0.00436	-0.00326	2.52905
R3	2.52877	-0.00120	0.00111	-0.00418	-0.00313	2.52564
R4	2.32566	0.00182	-0.00065	0.00279	0.00203	2.32769
R5	2.32311	0.00122	-0.00065	0.00239	0.00174	2.32484
R6	2.52879	-0.00120	0.00111	-0.00418	-0.00313	2.52566
R7	2.53040	-0.00127	0.00091	-0.00385	-0.00291	2.52749
R8	2.32308	0.00122	-0.00066	0.00240	0.00174	2.32482
R9	2.32238	0.00010	-0.00058	0.00166	0.00114	2.32352

R10	2.53044	-0.00127	0.00091	-0.00386	-0.00291	2.52753
R11	2.62847	-0.00102	0.00223	-0.00557	-0.00327	2.62519
R12	2.32233	0.00009	-0.00059	0.00167	0.00114	2.32348
R13	2.71261	-0.00334	-0.00364	0.00385	0.00034	2.71295
R14	2.66873	-0.00506	0.00349	-0.00954	-0.00605	2.66268
R15	2.62859	-0.00103	0.00224	-0.00559	-0.00328	2.62531
R16	2.66855	-0.00514	0.00342	-0.00954	-0.00612	2.66243
R17	2.77761	-0.00091	-0.01010	0.01807	0.00797	2.78558
R18	2.03221	0.00110	0.00049	0.00088	0.00137	2.03358
R19	2.77770	-0.00099	-0.01010	0.01802	0.00793	2.78563
R20	2.03212	0.00111	0.00050	0.00088	0.00138	2.03350
R21	1.95649	-0.00255	0.00104	-0.00569	-0.00465	1.95184
R22	1.92200	-0.00158	0.00044	-0.00229	-0.00185	1.92015
R23	1.93626	-0.00212	-0.00034	-0.00230	-0.00263	1.93362
R24	1.95639	-0.00254	0.00104	-0.00567	-0.00463	1.95176
R25	1.92200	-0.00159	0.00044	-0.00229	-0.00185	1.92015
R26	1.93629	-0.00212	-0.00033	-0.00231	-0.00264	1.93365
A1	2.55345	0.00078	-0.00007	0.00246	0.00148	2.55493
A2	2.61436	-0.00003	0.00031	-0.00026	-0.00069	2.61367
A3	2.55347	0.00079	-0.00008	0.00249	0.00150	2.55498
A4	2.71242	0.00022	-0.00049	0.00213	0.00120	2.71362
A5	2.61433	-0.00004	0.00032	-0.00029	-0.00071	2.61361
A6	2.85263	-0.00118	0.00002	-0.00218	-0.00232	2.85031
A7	2.71244	0.00022	-0.00049	0.00214	0.00121	2.71365
A8	2.85258	-0.00118	0.00003	-0.00219	-0.00233	2.85025
A9	2.07622	0.00180	-0.00225	0.00620	0.00436	2.08058
A10	2.08492	0.00268	0.00626	-0.00055	0.00542	2.09034
A11	2.12203	-0.00448	-0.00408	-0.00559	-0.00994	2.11209
A12	2.07617	0.00184	-0.00222	0.00624	0.00443	2.08060
A13	2.12221	-0.00450	-0.00407	-0.00563	-0.00998	2.11223
A14	2.08479	0.00266	0.00623	-0.00053	0.00540	2.09019
A15	2.18366	0.00075	-0.00524	0.00718	0.00194	2.18561
A16	2.00027	0.00002	-0.00183	-0.01462	-0.01645	1.98382
A17	2.18392	0.00083	-0.00512	0.00764	0.00252	2.18645
A18	2.00023	0.00012	-0.00158	-0.01439	-0.01597	1.98425
A19	1.99467	0.00017	0.00482	-0.01162	-0.00681	1.98786
A20	1.93156	-0.00132	-0.00263	0.00213	-0.00050	1.93106
A21	1.94136	-0.00163	0.00051	-0.00655	-0.00605	1.93530
A22	1.88478	0.00098	-0.00161	0.00871	0.00709	1.89187
A23	1.83103	0.00060	-0.00079	0.00227	0.00146	1.83249
A24	1.87398	0.00144	-0.00053	0.00639	0.00586	1.87984
A25	1.99409	0.00019	0.00483	-0.01154	-0.00673	1.98736
A26	1.93160	-0.00134	-0.00268	0.00212	-0.00056	1.93104
A27	1.94184	-0.00163	0.00053	-0.00657	-0.00605	1.93579
A28	1.88482	0.00098	-0.00160	0.00868	0.00707	1.89189
A29	1.83107	0.00061	-0.00077	0.00226	0.00147	1.83254
A30	1.87398	0.00144	-0.00052	0.00637	0.00585	1.87983
A31	2.91436	-0.00087	-0.00210	0.00192	-0.00003	2.91433

A32	3.12589	-0.00069	0.00459	-0.00945	-0.00445	3.12144
A33	2.91443	-0.00087	-0.00213	0.00187	-0.00011	2.91432
A34	3.12585	-0.00069	0.00460	-0.00936	-0.00435	3.12151
A35	4.18394	0.00077	-0.00708	-0.00744	-0.01451	4.16942
A36	4.18415	0.00094	-0.00670	-0.00675	-0.01345	4.17070
A37	3.15157	-0.00092	0.00190	-0.01555	-0.01350	3.13807
A38	3.17982	-0.00361	-0.02236	-0.06301	-0.08532	3.09450
A39	3.15164	-0.00092	0.00184	-0.01551	-0.01353	3.13811
A40	3.17947	-0.00360	-0.02212	-0.06310	-0.08518	3.09429
A41	3.62934	0.00794	0.00575	0.04804	0.05378	3.68312
A42	3.62637	0.00803	0.00616	0.04850	0.05466	3.68103
D1	0.01491	-0.00104	-0.00338	-0.01402	-0.01734	-0.00243
D2	0.00831	-0.00140	-0.00694	-0.02786	-0.03470	-0.02640
D3	-0.00032	-0.00053	-0.00254	-0.01352	-0.01606	-0.01638
D4	0.01482	-0.00104	-0.00337	-0.01399	-0.01729	-0.00247
D5	0.01125	-0.00003	-0.00001	-0.00220	-0.00228	0.00897
D6	-0.00036	-0.00052	-0.00250	-0.01349	-0.01598	-0.01634
D7	-0.01443	0.00166	0.01799	0.04401	0.06208	0.04765
D8	-3.12307	-0.00124	-0.00423	-0.01603	-0.02052	3.13960
D9	0.01105	-0.00002	0.00002	-0.00218	-0.00224	0.00882
D10	-0.01442	0.00166	0.01805	0.04393	0.06206	0.04764
D11	-3.12295	-0.00124	-0.00407	-0.01618	-0.02051	3.13973
D12	-0.01220	0.00022	-0.00326	-0.00984	-0.01317	-0.02537
D13	3.12443	0.00073	0.00542	0.00625	0.01157	3.13600
D14	3.12477	0.00072	0.00537	0.00622	0.01150	3.13627
D15	-0.02179	0.00123	0.01405	0.02230	0.03625	0.01446
D16	2.67669	0.00254	0.06962	-0.04766	0.02188	2.69857
D17	-0.46026	0.00205	0.06083	-0.06382	-0.00292	-0.46318
D18	-0.45832	0.00205	0.06058	-0.06338	-0.00273	-0.46105
D19	2.67828	0.00256	0.06942	-0.04720	0.02215	2.70043
D20	-1.73247	0.00016	-0.00265	0.00956	0.00692	-1.72555
D21	0.39974	0.00056	-0.00330	0.01420	0.01091	0.41065
D22	2.48137	0.00044	-0.00535	0.01936	0.01399	2.49537
D23	-1.73723	0.00017	-0.00261	0.00955	0.00695	-1.73029
D24	0.39463	0.00056	-0.00330	0.01420	0.01091	0.40555
D25	2.47661	0.00043	-0.00537	0.01933	0.01395	2.49056

Item	Value	Threshold	Converged?
Maximum Force	0.008027	0.000450	NO
RMS Force	0.002056	0.000300	NO
Maximum Displacement	0.436453	0.001800	NO
RMS Displacement	0.123436	0.001200	NO

Predicted change in Energy=-1.206558D-03
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 22:24:02 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Supporting Information file

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.023769	0.665491	0.067823
2	6	0	3.342004	1.687062	0.161825
3	6	0	4.023692	-0.666055	-0.066611
4	6	0	2.142342	2.274724	0.203436
5	6	0	3.341854	-1.687556	-0.160790
6	6	0	0.912883	2.312159	0.179877
7	6	0	2.142104	-2.275041	-0.202679
8	6	0	-0.378263	1.969438	0.113826
9	6	0	0.912647	-2.312324	-0.179421
10	6	0	-1.462898	1.395480	0.036751
11	6	0	-0.378475	-1.969372	-0.113626
12	6	0	-2.675389	0.717952	0.010767
13	6	0	-1.462996	-1.395226	-0.036713
14	6	0	-2.675462	-0.717510	-0.011196
15	6	0	-3.882918	1.443791	0.030530
16	6	0	-3.882854	-1.443324	-0.031101
17	7	0	-3.710518	2.905130	-0.056856
18	7	0	-3.710073	-2.904651	0.056125
19	1	0	-3.143363	3.212007	-0.863688
20	1	0	-4.612781	3.370086	-0.103744
21	1	0	-3.140820	-3.210814	0.861699
22	1	0	-4.612168	-3.369653	0.105711
23	1	0	-3.217769	3.264086	0.764940
24	1	0	-4.822916	1.095589	-0.360876
25	1	0	-4.823681	-1.095201	0.358259
26	1	0	-3.219436	-3.264188	-0.766695

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.231766	0.000000			
3	C	1.338315	2.460496	0.000000		
4	C	2.479474	1.336513	3.501512	0.000000	
5	C	2.460509	3.390004	1.231763	4.155858	0.000000
6	C	3.521602	2.508326	4.313658	1.230254	4.691873
7	C	3.501509	4.155825	2.479461	4.567855	1.336523
8	C	4.591327	3.731277	5.133770	2.540606	5.223820
9	C	4.313652	4.691834	3.521581	4.764424	2.508332
10	C	5.535103	4.815365	5.862020	3.714648	5.712248
11	C	5.133729	5.223729	4.591288	4.946453	3.731285
12	C	6.699607	6.096803	6.840991	5.066675	6.482524
13	C	5.861917	5.712087	5.535010	5.150210	4.815333
14	C	6.840952	6.482422	6.699581	5.675453	6.096840

15	C	7.944988	7.230208	8.183848	6.084744	7.876501
16	C	8.183616	7.876236	7.944739	7.083916	7.229998
17	N	8.052994	7.160277	8.518889	5.892464	8.416622
18	N	8.518119	8.415865	8.052174	7.816546	7.159472
19	H	7.662913	6.740706	8.187880	5.473201	8.158298
20	H	9.051755	8.135213	9.533126	6.850246	9.426517
21	H	8.184578	8.155122	7.659491	7.644360	6.737274
22	H	9.532220	9.425622	9.050813	8.802951	8.134306
23	H	7.725189	6.773579	8.281078	5.479500	8.270695
24	H	8.867503	8.202986	9.025102	7.086863	8.628407
25	H	9.025617	8.628904	8.867959	7.739886	8.203430
26	H	8.282681	8.272213	7.726792	7.769772	6.775205

		6	7	8	9	10
6	C	0.000000				
7	C	4.764424	0.000000			
8	C	1.337490	4.946517	0.000000		
9	C	4.638420	1.230242	4.481733	0.000000	
10	C	2.550514	5.150349	1.229553	4.408827	0.000000
11	C	4.481658	2.540607	3.945372	1.337513	3.538476
12	C	3.930114	5.675545	2.617943	4.700292	1.389192
13	C	4.408675	3.714615	3.538400	2.550512	2.791673
14	C	4.700173	5.066706	3.537293	3.930173	2.436665
15	C	4.876072	7.084137	3.544834	6.095074	2.420510
16	C	6.094855	6.084514	4.893884	4.875857	3.730897
17	N	4.667279	7.817201	3.465339	6.972123	2.709170
18	N	6.971524	5.891635	5.904323	4.666462	4.851938
19	H	4.283911	7.647273	3.185167	6.887501	2.633348
20	H	5.633171	8.803734	4.465455	7.926277	3.720292
21	H	6.884811	5.469722	5.918281	4.280398	4.971308
22	H	7.925571	6.849340	6.814096	5.632301	5.712193
23	H	4.279107	7.768299	3.187923	7.003464	2.664868
24	H	5.888281	7.739359	4.554547	6.674090	3.396729
25	H	6.674586	7.087231	5.404951	5.888629	4.195441
26	H	7.004834	5.481116	6.019836	4.280776	5.044151

		11	12	13	14	15
11	C	0.000000				
12	C	3.537372	0.000000			
13	C	1.229530	2.436734	0.000000		
14	C	2.617977	1.435629	1.389253	0.000000	
15	C	4.894036	1.409028	3.731027	2.476068	0.000000
16	C	3.544603	2.476052	2.420342	1.408899	2.887773
17	N	5.904787	2.420705	4.852301	3.767884	1.474066
18	N	3.464550	3.767742	2.708568	2.420442	4.351952
19	H	5.920632	2.684023	4.973340	4.048058	2.114983
20	H	6.814636	3.286399	5.712604	4.524402	2.064302
21	H	3.181664	4.046716	2.630323	2.682363	4.786115
22	H	4.464644	4.524228	3.719668	3.286086	4.868953
23	H	6.018518	2.710305	5.042923	4.092626	2.072500

```
  24  H    5.404459   2.211922   4.195033   2.832166   1.076123
  25  H    4.554856   2.832566   3.397090   2.212237   2.727439
  26  H    3.189687   4.093638   2.666641   2.711505   4.820876
                16         17         18         19         20
  16  C    0.000000
  17  N    4.351944   0.000000
  18  N    1.474089   5.810880   0.000000
  19  H    4.786664   1.032867   6.211338   0.000000
  20  H    4.868982   1.016101   6.341354   1.661834   0.000000
  21  H    2.114646   6.210723   1.032828   6.650533   6.812268
  22  H    2.064306   6.341318   1.016101   6.812882   6.742993
  23  H    4.820345   1.023230   6.228812   1.631158   1.646787
  24  H    2.727370   2.145763   4.173036   2.748262   2.298611
  25  H    1.076080   4.173021   2.146047   4.782119   4.494076
  26  H    2.072865   6.229408   1.023242   6.477368   6.811352
                21         22         23         24         25
  21  H    0.000000
  22  H    1.661810   0.000000
  23  H    6.476080   6.810685   0.000000
  24  H    4.782180   4.494497   2.923413   0.000000
  25  H    2.749780   2.298184   4.663446   2.305800   0.000000
  26  H    1.631164   1.646790   6.705541   4.662992   2.922949
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 3.80D-02
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.526107   -0.667801   -0.046470
    2          6           0        3.844224   -1.691716   -0.108769
    3          6           0        4.526182    0.667279    0.046520
    4          6           0        2.644494   -2.280241   -0.132252
    5          6           0        3.844461    1.691298    0.108821
    6          6           0        1.415027   -2.316775   -0.107700
    7          6           0        2.644780    2.279948    0.132279
    8          6           0        0.123916   -1.972009   -0.052498
    9          6           0        1.415330    2.316640    0.107715
   10          6           0       -0.960656   -1.395800    0.006564
   11          6           0        0.124174    1.971967    0.052444
   12          6           0       -2.173065   -0.717643    0.011324
```

13	6	0	-0.960410	1.395841	-0.006730
14	6	0	-2.172959	0.717808	-0.011331
15	6	0	-3.380683	-1.443598	0.013972
16	6	0	-3.380261	1.444038	-0.014146
17	7	0	-3.208478	-2.901537	0.146750
18	7	0	-3.207285	2.901928	-0.146720
19	1	0	-2.641463	-3.183262	0.962801
20	1	0	-4.110806	-3.364701	0.207947
21	1	0	-2.637893	3.182839	-0.961345
22	1	0	-4.109315	3.365274	-0.210848
23	1	0	-2.715672	-3.285918	-0.663432
24	1	0	-4.320686	-1.083286	0.394246
25	1	0	-4.321084	1.084098	-0.392622
26	1	0	-2.716705	3.286800	0.664593

Rotational constants (GHZ): 0.5991511 0.2713079 0.1874171

Leave Link 202 at Fri Sep 25 22:24:02 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0

(Enter /home/user/gauss16/g16/l301.exe)

Standard basis: def2TZVP (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 696 symmetry adapted cartesian basis functions of A symmetry.

There are 606 symmetry adapted basis functions of A symmetry.

606 basis functions, 982 primitive gaussians, 696 cartesian basis functions

59 alpha electrons 59 beta electrons

nuclear repulsion energy 1009.9196058499 Hartrees.

IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000

ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000

IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121

HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000

NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D2 Dispersion energy= -0.0154324651 Hartrees.

Nuclear repulsion after empirical dispersion term = 1009.9041733848 Hartrees.

Leave Link 301 at Fri Sep 25 22:24:02 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0

(Enter /home/user/gauss16/g16/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51901.

Supporting Information file

LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.90D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Fri Sep 25 22:24:03 2026, MaxMem= 805306368 cpu: 5.7 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 22:24:03 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 -0.000000 0.000000
Rot= 1.000000 0.000636 0.000001 0.000086 Ang= 0.07 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.991308166509
Leave Link 401 at Fri Sep 25 22:24:18 2026, MaxMem= 805306368 cpu: 87.7 elap: 14.6
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.

Supporting Information file

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.349200167599
DIIS: error= 1.74D-02 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.349200167599 IErMin= 1 ErrMin= 1.74D-02
ErrMax= 1.74D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-01 BMatP= 1.44D-01
IDIUse=3 WtCom= 8.26D-01 WtEn= 1.74D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Recover alternate guess density for next cycle.
RMSDP=6.74D-03 MaxDP=2.58D-01 OVMax= 0.00D+00

Cycle 2 Pass 0 IDiag 1:
RMSU= 5.65D-03 CP: 1.26D+00
E= -723.081198616885 Delta-E= 0.268001550715 Rises=F Damp=F
Switch densities from cycles 1 and 2 for lowest energy.
DIIS: error= 5.88D-02 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -723.349200167599 IErMin= 1 ErrMin= 1.74D-02
ErrMax= 5.88D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.67D+00 BMatP= 1.44D-01
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.921D+00 0.792D-01
Coeff: 0.921D+00 0.792D-01
Gap= 0.161 Goal= None Shift= 0.000
RMSDP=5.54D-03 MaxDP=1.71D-01 DE= 2.68D-01 OVMax= 3.33D-01

Cycle 3 Pass 0 IDiag 1:
RMSU= 5.06D-03 CP: 1.11D+00 2.82D-01
E= -723.406222654296 Delta-E= -0.325024037411 Rises=F Damp=F
DIIS: error= 2.68D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.406222654296 IErMin= 3 ErrMin= 2.68D-03
ErrMax= 2.68D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.73D-03 BMatP= 1.44D-01
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.113D-01 0.117D-01 0.100D+01
Coeff: -0.113D-01 0.117D-01 0.100D+01
Gap= 0.161 Goal= None Shift= 0.000
RMSDP=8.06D-03 MaxDP=2.34D-01 DE=-3.25D-01 OVMax= 5.19D-02

Cycle 4 Pass 0 IDiag 1:
RMSU= 7.02D-03 CP: 1.38D+00 4.43D-01 8.70D-01
E= -723.404410644180 Delta-E= 0.001812010116 Rises=F Damp=F
DIIS: error= 3.86D-03 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 3 EnMin= -723.406222654296 IErMin= 3 ErrMin= 2.68D-03
ErrMax= 3.86D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.56D-03 BMatP= 2.73D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.180D-01 0.416D-02 0.622D+00 0.392D+00
Coeff: -0.180D-01 0.416D-02 0.622D+00 0.392D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=2.66D+01 MaxDP=1.09D+03 DE= 1.81D-03 OVMax= 2.36D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 5 Pass 1 IDiag 1:
E= -723.404080310363 Delta-E= 0.000330333817 Rises=F Damp=F
DIIS: error= 3.86D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.404080310363 IErMin= 1 ErrMin= 3.86D-03
ErrMax= 3.86D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.26D-03 BMatP= 5.26D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.100D+01
Coeff: 0.100D+01
Gap= 0.197 Goal= None Shift= 0.000
GapD= 0.197 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=9.21D-03 MaxDP=3.22D-01 DE= 3.30D-04 OVMax= 8.29D-02

Cycle 6 Pass 1 IDiag 1:
RMSU= 5.21D-03 CP: 6.45D-01
E= -723.391668453501 Delta-E= 0.012411856862 Rises=F Damp=F
DIIS: error= 7.60D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -723.404080310363 IErMin= 1 ErrMin= 3.86D-03
ErrMax= 7.60D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.61D-02 BMatP= 5.26D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.639D+00 0.361D+00
Coeff: 0.639D+00 0.361D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=9.00D-04 MaxDP=3.04D-02 DE= 1.24D-02 OVMax= 4.90D-02

Cycle 7 Pass 1 IDiag 1:
RMSU= 6.41D-04 CP: 6.74D-01 1.02D+00
E= -723.410094779917 Delta-E= -0.018426326416 Rises=F Damp=F
DIIS: error= 4.04D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.410094779917 IErMin= 3 ErrMin= 4.04D-04
ErrMax= 4.04D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.10D-04 BMatP= 5.26D-03
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.249D+00 0.152D+00 0.599D+00
Coeff: 0.249D+00 0.152D+00 0.599D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.81D-04 MaxDP=8.65D-03 DE=-1.84D-02 OVMax= 2.89D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.17D-04 CP: 6.68D-01 1.03D+00 1.05D+00
E= -723.410193551946 Delta-E= -0.000098772029 Rises=F Damp=F
DIIS: error= 1.61D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.410193551946 IErMin= 4 ErrMin= 1.61D-04

ErrMax= 1.61D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.21D-05 BMatP= 1.10D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.210D-01-0.794D-02 0.230D+00 0.799D+00
Coeff: -0.210D-01-0.794D-02 0.230D+00 0.799D+00
Gap= 0.173 Goal= None Shift= 0.000
RMSDP=1.24D-04 MaxDP=6.07D-03 DE=-9.88D-05 OVMax= 1.92D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.79D-05 CP: 6.69D-01 1.04D+00 1.15D+00 1.66D+00
E= -723.410211539512 Delta-E= -0.000017987566 Rises=F Damp=F
DIIS: error= 9.10D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.410211539512 IErMin= 5 ErrMin= 9.10D-05
ErrMax= 9.10D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.62D-06 BMatP= 1.21D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.203D-01-0.101D-01 0.782D-01 0.382D+00 0.571D+00
Coeff: -0.203D-01-0.101D-01 0.782D-01 0.382D+00 0.571D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=4.58D-05 MaxDP=2.27D-03 DE=-1.80D-05 OVMax= 9.66D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.15D-05 CP: 6.70D-01 1.04D+00 1.17D+00 1.83D+00 1.29D+00
E= -723.410214721608 Delta-E= -0.000003182096 Rises=F Damp=F
DIIS: error= 5.38D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.410214721608 IErMin= 6 ErrMin= 5.38D-05
ErrMax= 5.38D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.89D-07 BMatP= 1.62D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.167D-02-0.209D-02-0.614D-01-0.140D+00 0.267D+00 0.938D+00
Coeff: -0.167D-02-0.209D-02-0.614D-01-0.140D+00 0.267D+00 0.938D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=7.84D-05 MaxDP=3.47D-03 DE=-3.18D-06 OVMax= 1.11D-03

Cycle 11 Pass 1 IDiag 1:
RMSU= 7.39D-06 CP: 6.73D-01 1.04D+00 1.22D+00 2.01D+00 1.75D+00
CP: 2.37D+00
E= -723.410216699438 Delta-E= -0.000001977831 Rises=F Damp=F
DIIS: error= 2.01D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.410216699438 IErMin= 7 ErrMin= 2.01D-05
ErrMax= 2.01D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.07D-07 BMatP= 3.89D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.396D-02 0.116D-02-0.514D-01-0.159D+00 0.141D-01 0.479D+00
Coeff-Com: 0.712D+00
Coeff: 0.396D-02 0.116D-02-0.514D-01-0.159D+00 0.141D-01 0.479D+00
Coeff: 0.712D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=3.65D-05 MaxDP=1.46D-03 DE=-1.98D-06 OVMax= 6.10D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.07D-06 CP: 6.75D-01 1.04D+00 1.24D+00 2.07D+00 1.97D+00

CP: 3.00D+00 1.54D+00
E= -723.410217170032 Delta-E= -0.000000470593 Rises=F Damp=F
DIIS: error= 9.64D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.410217170032 IErMin= 8 ErrMin= 9.64D-06
ErrMax= 9.64D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.65D-08 BMatP= 1.07D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.153D-02 0.700D-03-0.320D-02-0.196D-01-0.465D-01-0.466D-01
Coeff-Com: 0.194D+00 0.920D+00
Coeff: 0.153D-02 0.700D-03-0.320D-02-0.196D-01-0.465D-01-0.466D-01
Coeff: 0.194D+00 0.920D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.93D-05 MaxDP=6.77D-04 DE=-4.71D-07 OVMax= 3.07D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 3.75D-06 CP: 6.75D-01 1.04D+00 1.25D+00 2.07D+00 2.06D+00
CP: 3.00D+00 1.90D+00 2.40D+00
E= -723.410217287011 Delta-E= -0.000000116979 Rises=F Damp=F
DIIS: error= 5.24D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.410217287011 IErMin= 9 ErrMin= 5.24D-06
ErrMax= 5.24D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.40D-09 BMatP= 1.65D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.629D-03-0.153D-04 0.175D-01 0.484D-01-0.282D-01-0.197D+00
Coeff-Com: -0.173D+00 0.482D+00 0.852D+00
Coeff: -0.629D-03-0.153D-04 0.175D-01 0.484D-01-0.282D-01-0.197D+00
Coeff: -0.173D+00 0.482D+00 0.852D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.21D-05 MaxDP=4.23D-04 DE=-1.17D-07 OVMax= 2.13D-04

Cycle 14 Pass 1 IDiag 1:
RMSU= 9.87D-07 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.12D+00
CP: 3.00D+00 2.11D+00 3.00D+00 1.58D+00
E= -723.410217322242 Delta-E= -0.000000035231 Rises=F Damp=F
DIIS: error= 2.35D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.410217322242 IErMin=10 ErrMin= 2.35D-06
ErrMax= 2.35D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.54D-09 BMatP= 6.40D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.556D-03-0.101D-03 0.957D-02 0.277D-01-0.771D-02-0.919D-01
Coeff-Com: -0.121D+00 0.106D+00 0.453D+00 0.625D+00
Coeff: -0.556D-03-0.101D-03 0.957D-02 0.277D-01-0.771D-02-0.919D-01
Coeff: -0.121D+00 0.106D+00 0.453D+00 0.625D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=2.46D-06 MaxDP=8.72D-05 DE=-3.52D-08 OVMax= 5.27D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.87D-07 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.13D+00
CP: 3.00D+00 2.14D+00 3.00D+00 1.67D+00 1.46D+00
E= -723.410217326638 Delta-E= -0.000000004396 Rises=F Damp=F
DIIS: error= 1.45D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -723.410217326638 IErMin=11 ErrMin= 1.45D-06
ErrMax= 1.45D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.10D-10 BMatP= 1.54D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.621D-04-0.216D-04-0.292D-02-0.796D-02 0.552D-02 0.377D-01
Coeff-Com: 0.219D-01-0.123D+00-0.129D+00 0.142D+00 0.106D+01
Coeff: 0.621D-04-0.216D-04-0.292D-02-0.796D-02 0.552D-02 0.377D-01
Coeff: 0.219D-01-0.123D+00-0.129D+00 0.142D+00 0.106D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=6.54D-07 MaxDP=2.46D-05 DE=-4.40D-09 OVMax= 3.76D-05

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.92D-07 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.14D+00
CP: 3.00D+00 2.14D+00 3.00D+00 1.69D+00 1.63D+00
CP: 2.00D+00
E= -723.410217328189 Delta-E= -0.000000001550 Rises=F Damp=F
DIIS: error= 7.32D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.410217328189 IErMin=12 ErrMin= 7.32D-07
ErrMax= 7.32D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.02D-11 BMatP= 2.10D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.125D-03 0.692D-06-0.276D-02-0.764D-02 0.321D-02 0.294D-01
Coeff-Com: 0.303D-01-0.612D-01-0.113D+00-0.711D-01 0.255D+00 0.938D+00
Coeff: 0.125D-03 0.692D-06-0.276D-02-0.764D-02 0.321D-02 0.294D-01
Coeff: 0.303D-01-0.612D-01-0.113D+00-0.711D-01 0.255D+00 0.938D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=2.04D-07 MaxDP=6.60D-06 DE=-1.55D-09 OVMax= 1.70D-05

Cycle 17 Pass 1 IDiag 1:
RMSU= 7.80D-08 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.13D+00
CP: 3.00D+00 2.13D+00 3.00D+00 1.68D+00 1.63D+00
CP: 2.47D+00 1.55D+00
E= -723.410217328536 Delta-E= -0.000000000347 Rises=F Damp=F
DIIS: error= 4.21D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.410217328536 IErMin=13 ErrMin= 4.21D-07
ErrMax= 4.21D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.54D-11 BMatP= 4.02D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.691D-05-0.362D-05 0.136D-03 0.491D-03-0.640D-03-0.322D-02
Coeff-Com: 0.560D-03 0.119D-01 0.161D-01-0.435D-01-0.248D+00 0.258D+00
Coeff-Com: 0.101D+01
Coeff: 0.691D-05-0.362D-05 0.136D-03 0.491D-03-0.640D-03-0.322D-02
Coeff: 0.560D-03 0.119D-01 0.161D-01-0.435D-01-0.248D+00 0.258D+00
Coeff: 0.101D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.91D-07 MaxDP=1.01D-05 DE=-3.47D-10 OVMax= 1.09D-05

Cycle 18 Pass 1 IDiag 1:
RMSU= 2.89D-08 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.13D+00
CP: 3.00D+00 2.13D+00 3.00D+00 1.68D+00 1.63D+00
CP: 2.70D+00 1.83D+00 2.13D+00

E= -723.410217328658 Delta-E= -0.000000000122 Rises=F Damp=F
DIIS: error= 1.67D-07 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.410217328658 IErMin=14 ErrMin= 1.67D-07
ErrMax= 1.67D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.44D-12 BMatP= 1.54D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.348D-04-0.215D-06 0.768D-03 0.221D-02-0.110D-02-0.794D-02
Coeff-Com: -0.875D-02 0.166D-01 0.372D-01 0.224D-01-0.108D+00-0.200D+00
Coeff-Com: -0.474D-01 0.129D+01
Coeff: -0.348D-04-0.215D-06 0.768D-03 0.221D-02-0.110D-02-0.794D-02
Coeff: -0.875D-02 0.166D-01 0.372D-01 0.224D-01-0.108D+00-0.200D+00
Coeff: -0.474D-01 0.129D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.40D-07 MaxDP=5.84D-06 DE=-1.22D-10 OVMax= 8.18D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.88D-08 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.13D+00
CP: 3.00D+00 2.12D+00 3.00D+00 1.68D+00 1.63D+00
CP: 2.79D+00 1.98D+00 2.95D+00 1.92D+00
E= -723.410217328695 Delta-E= -0.000000000037 Rises=F Damp=F
DIIS: error= 4.57D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.410217328695 IErMin=15 ErrMin= 4.57D-08
ErrMax= 4.57D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.27D-13 BMatP= 2.44D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.608D-05 0.817D-06 0.860D-04 0.251D-03-0.948D-04-0.495D-03
Coeff-Com: -0.151D-02-0.481D-04 0.442D-02 0.119D-01 0.176D-01-0.577D-01
Coeff-Com: -0.202D+00 0.301D+00 0.926D+00
Coeff: -0.608D-05 0.817D-06 0.860D-04 0.251D-03-0.948D-04-0.495D-03
Coeff: -0.151D-02-0.481D-04 0.442D-02 0.119D-01 0.176D-01-0.577D-01
Coeff: -0.202D+00 0.301D+00 0.926D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=2.91D-08 MaxDP=9.61D-07 DE=-3.73D-11 OVMax= 2.23D-06

Cycle 20 Pass 1 IDiag 1:
RMSU= 7.93D-09 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.13D+00
CP: 3.00D+00 2.12D+00 3.00D+00 1.68D+00 1.63D+00
CP: 2.79D+00 2.00D+00 3.00D+00 2.17D+00 1.68D+00
E= -723.410217328703 Delta-E= -0.000000000008 Rises=F Damp=F
DIIS: error= 2.17D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.410217328703 IErMin=16 ErrMin= 2.17D-08
ErrMax= 2.17D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.06D-13 BMatP= 4.27D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.412D-05-0.106D-06-0.108D-03-0.313D-03 0.177D-03 0.123D-02
Coeff-Com: 0.101D-02-0.325D-02-0.487D-02 0.388D-03 0.252D-01 0.183D-01
Coeff-Com: -0.801D-01-0.136D+00 0.325D+00 0.853D+00
Coeff: 0.412D-05-0.106D-06-0.108D-03-0.313D-03 0.177D-03 0.123D-02
Coeff: 0.101D-02-0.325D-02-0.487D-02 0.388D-03 0.252D-01 0.183D-01
Coeff: -0.801D-01-0.136D+00 0.325D+00 0.853D+00
Gap= 0.174 Goal= None Shift= 0.000

Supporting Information file

RMSDP=1.56D-08 MaxDP=6.49D-07 DE=-7.96D-12 OVMax= 9.54D-07

Cycle 21 Pass 1 IDiag 1:
RMSU= 3.07D-09 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.13D+00
CP: 3.00D+00 2.12D+00 3.00D+00 1.68D+00 1.63D+00
CP: 2.79D+00 2.00D+00 3.00D+00 2.25D+00 2.04D+00
CP: 1.60D+00
E= -723.410217328695 Delta-E= 0.000000000008 Rises=F Damp=F
DIIS: error= 5.23D-09 at cycle 17 NSaved= 17.
NSaved=17 IEnMin=16 EnMin= -723.410217328703 IErMin=17 ErrMin= 5.23D-09
ErrMax= 5.23D-09 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.07D-14 BMatP= 1.06D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.213D-05-0.200D-06-0.447D-04-0.131D-03 0.724D-04 0.449D-03
Coeff-Com: 0.503D-03-0.999D-03-0.196D-02-0.157D-02 0.442D-02 0.145D-01
Coeff-Com: 0.287D-02-0.708D-01-0.407D-01 0.206D+00 0.888D+00
Coeff: 0.213D-05-0.200D-06-0.447D-04-0.131D-03 0.724D-04 0.449D-03
Coeff: 0.503D-03-0.999D-03-0.196D-02-0.157D-02 0.442D-02 0.145D-01
Coeff: 0.287D-02-0.708D-01-0.407D-01 0.206D+00 0.888D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.31D-08 MaxDP=6.02D-07 DE= 7.50D-12 OVMax= 2.55D-07

Cycle 22 Pass 1 IDiag 1:
RMSU= 1.80D-09 CP: 6.76D-01 1.04D+00 1.26D+00 2.07D+00 2.13D+00
CP: 3.00D+00 2.12D+00 3.00D+00 1.68D+00 1.64D+00
CP: 2.79D+00 2.00D+00 3.00D+00 2.24D+00 2.15D+00
CP: 1.78D+00 2.00D+00
E= -723.410217328698 Delta-E= -0.000000000002 Rises=F Damp=F
DIIS: error= 4.13D-09 at cycle 18 NSaved= 18.
NSaved=18 IEnMin=16 EnMin= -723.410217328703 IErMin=18 ErrMin= 4.13D-09
ErrMax= 4.13D-09 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.55D-15 BMatP= 1.07D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.484D-06-0.786D-07-0.586D-05-0.178D-04 0.903D-05 0.351D-04
Coeff-Com: 0.990D-04 0.293D-04-0.200D-03-0.980D-03-0.230D-02 0.519D-02
Coeff-Com: 0.167D-01-0.127D-01-0.877D-01-0.532D-01 0.511D+00 0.624D+00
Coeff: 0.484D-06-0.786D-07-0.586D-05-0.178D-04 0.903D-05 0.351D-04
Coeff: 0.990D-04 0.293D-04-0.200D-03-0.980D-03-0.230D-02 0.519D-02
Coeff: 0.167D-01-0.127D-01-0.877D-01-0.532D-01 0.511D+00 0.624D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=7.43D-09 MaxDP=3.31D-07 DE=-2.05D-12 OVMax= 9.24D-08

SCF Done: E(RwB97XD) = -723.410217329 A.U. after 22 cycles
NFock= 22 Conv=0.74D-08 -V/T= 2.0047
KE= 7.200275161677D+02 PE=-3.701117253608D+03 EE= 1.247775346727D+03
Leave Link 502 at Fri Sep 25 22:50:30 2026, MaxMem= 805306368 cpu: 9424.9 elap: 1571.7
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.

Supporting Information file

R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51901.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 22:50:30 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 22:50:30 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 23:01:37 2026, MaxMem= 805306368 cpu: 4000.9 elap: 666.9
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-5.34726245D+00 1.65587940D-03 8.36714255D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000281048	-0.001537953	0.000341722
2	6	-0.000649215	0.001335652	-0.000676067
3	6	0.000269606	0.001541517	-0.000341611
4	6	0.000902304	-0.000885649	0.000148272
5	6	-0.000641902	-0.001343471	0.000675585
6	6	-0.001038220	0.000748849	-0.001032729
7	6	0.000899926	0.000892925	-0.000149605
8	6	0.000337200	-0.000237376	0.000125385
9	6	-0.001036893	-0.000754040	0.001037342
10	6	0.000326333	-0.000187362	0.002342115
11	6	0.000341407	0.000243112	-0.000122379
12	6	-0.000764038	0.001369339	-0.001537883
13	6	0.000326020	0.000194824	-0.002352929
14	6	-0.000791430	-0.001321221	0.001541549
15	6	-0.001760310	-0.000828674	0.006690955
16	6	-0.001689337	0.000765684	-0.006684147
17	7	0.002541332	0.001568220	-0.002114447

```
    18        7        0.002468693  -0.001555625   0.002099631
    19        1       -0.000774788  -0.000326934   0.000599372
    20        1        0.000432905  -0.001269086   0.000284142
    21        1       -0.000768996   0.000324760  -0.000592704
    22        1        0.000428810   0.001258640  -0.000285492
    23        1       -0.000411039  -0.001237025  -0.000954746
    24        1        0.000586518  -0.000904947  -0.002756212
    25        1        0.000591258   0.000905452   0.002758410
    26        1       -0.000407192   0.001240388   0.000956466
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.006690955 RMS     0.001568881
 Leave Link  716 at Fri Sep 25 23:01:37 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.005392881 RMS     0.001354760
 Search for a local minimum.
 Step number   9 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .13548D-02 SwitMx=.10000D-02 MixMth= 1
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    6    7    8    9
 DE= -1.02D-03 DEPred=-1.21D-03 R= 8.44D-01
 TightC=F SS=  1.41D+00  RLast= 1.93D-01 DXNew= 2.4000D+00 5.7777D-01
 Trust test= 8.44D-01 RLast= 1.93D-01 DXMaxT set to 1.43D+00
 ITU=  1  1  1  1  1  0  0  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.00442   0.01074   0.01449   0.01660   0.01756
    Eigenvalues ---    0.01925   0.02403   0.02727   0.02800   0.03104
    Eigenvalues ---    0.03117   0.03594   0.03720   0.04070   0.04399
    Eigenvalues ---    0.04439   0.04468   0.05026   0.05026   0.05948
    Eigenvalues ---    0.08526   0.08730   0.09945   0.11288   0.11318
    Eigenvalues ---    0.11581   0.11636   0.14716   0.15234   0.15862
    Eigenvalues ---    0.16000   0.16000   0.16000   0.16000   0.16019
    Eigenvalues ---    0.16614   0.21077   0.24345   0.24961   0.24967
    Eigenvalues ---    0.24987   0.24999   0.25000   0.25000   0.25036
    Eigenvalues ---    0.28360   0.32405   0.37230   0.38698   0.40644
    Eigenvalues ---    0.44969   0.45830   0.46268   0.47300   0.47688
    Eigenvalues ---    0.47688   0.47688   0.47747   0.49170   0.50115
    Eigenvalues ---    0.54799   0.55014   0.55369   0.55659   0.55666
    Eigenvalues ---    0.93416   0.93685   0.95022   0.95520   0.97675
    Eigenvalues ---    0.98202   1.36034
 RFO step:  Lambda=-1.94374357D-03 EMin= 4.42019555D-03
 Quartic linear search produced a step of -0.12085.
```

Supporting Information file

Iteration 1 RMS(Cart)= 0.04797710 RMS(Int)= 0.00118032
Iteration 2 RMS(Cart)= 0.00397277 RMS(Int)= 0.00009864
Iteration 3 RMS(Cart)= 0.00000428 RMS(Int)= 0.00009861
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00009861
ITry= 1 IFail=0 DXMaxC= 1.42D-01 DCOld= 1.00D+10 DXMaxT= 1.43D+00 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.32770	0.00092	-0.00025	0.00506	0.00478	2.33248
R2	2.52905	-0.00058	0.00039	-0.00812	-0.00777	2.52128
R3	2.52564	-0.00049	0.00038	-0.00764	-0.00728	2.51836
R4	2.32769	0.00092	-0.00025	0.00507	0.00478	2.33248
R5	2.32484	0.00055	-0.00021	0.00438	0.00417	2.32901
R6	2.52566	-0.00049	0.00038	-0.00764	-0.00728	2.51838
R7	2.52749	-0.00048	0.00035	-0.00695	-0.00659	2.52090
R8	2.32482	0.00055	-0.00021	0.00439	0.00418	2.32900
R9	2.32352	-0.00021	-0.00014	0.00308	0.00296	2.32648
R10	2.52753	-0.00048	0.00035	-0.00697	-0.00660	2.52093
R11	2.62519	0.00006	0.00040	-0.00768	-0.00726	2.61794
R12	2.32348	-0.00020	-0.00014	0.00310	0.00298	2.32646
R13	2.71295	-0.00180	-0.00004	0.00457	0.00457	2.71752
R14	2.66268	-0.00205	0.00073	-0.01165	-0.01092	2.65175
R15	2.62531	0.00006	0.00040	-0.00770	-0.00728	2.61803
R16	2.66243	-0.00202	0.00074	-0.01163	-0.01089	2.65154
R17	2.78558	-0.00092	-0.00096	0.02706	0.02610	2.81168
R18	2.03358	0.00078	-0.00017	0.00317	0.00300	2.03658
R19	2.78563	-0.00093	-0.00096	0.02697	0.02602	2.81164
R20	2.03350	0.00077	-0.00017	0.00315	0.00298	2.03648
R21	1.95184	-0.00099	0.00056	-0.00971	-0.00915	1.94269
R22	1.92015	-0.00098	0.00022	-0.00390	-0.00368	1.91647
R23	1.93362	-0.00140	0.00032	-0.00527	-0.00495	1.92867
R24	1.95176	-0.00098	0.00056	-0.00966	-0.00910	1.94266
R25	1.92015	-0.00097	0.00022	-0.00390	-0.00367	1.91648
R26	1.93365	-0.00140	0.00032	-0.00529	-0.00497	1.92868
A1	2.55493	0.00054	-0.00018	0.00424	0.00374	2.55867
A2	2.61367	-0.00009	0.00008	-0.00147	-0.00166	2.61201
A3	2.55498	0.00055	-0.00018	0.00432	0.00381	2.55879
A4	2.71362	0.00029	-0.00015	0.00371	0.00340	2.71702
A5	2.61361	-0.00009	0.00009	-0.00154	-0.00172	2.61189
A6	2.85031	-0.00096	0.00028	-0.00600	-0.00578	2.84452
A7	2.71365	0.00030	-0.00015	0.00376	0.00345	2.71709
A8	2.85025	-0.00095	0.00028	-0.00601	-0.00579	2.84446
A9	2.08058	0.00080	-0.00053	0.00849	0.00812	2.08870
A10	2.09034	0.00145	-0.00065	0.00936	0.00862	2.09897
A11	2.11209	-0.00225	0.00120	-0.01803	-0.01691	2.09518
A12	2.08060	0.00078	-0.00054	0.00851	0.00814	2.08874
A13	2.11223	-0.00225	0.00121	-0.01811	-0.01698	2.09524
A14	2.09019	0.00147	-0.00065	0.00941	0.00868	2.09887

A15	2.18561	-0.00071	-0.00023	-0.00088	-0.00112	2.18449
A16	1.98382	0.00120	0.00199	-0.03483	-0.03285	1.95097
A17	2.18645	-0.00076	-0.00031	-0.00042	-0.00073	2.18572
A18	1.98425	0.00116	0.00193	-0.03469	-0.03276	1.95150
A19	1.98786	0.00041	0.00082	-0.01774	-0.01700	1.97086
A20	1.93106	-0.00114	0.00006	0.00029	0.00034	1.93139
A21	1.93530	-0.00084	0.00073	-0.01316	-0.01251	1.92279
A22	1.89187	0.00048	-0.00086	0.01616	0.01529	1.90716
A23	1.83249	0.00047	-0.00018	0.00456	0.00423	1.83673
A24	1.87984	0.00074	-0.00071	0.01210	0.01138	1.89122
A25	1.98736	0.00041	0.00081	-0.01764	-0.01691	1.97045
A26	1.93104	-0.00112	0.00007	0.00031	0.00037	1.93140
A27	1.93579	-0.00085	0.00073	-0.01319	-0.01255	1.92325
A28	1.89189	0.00048	-0.00085	0.01611	0.01524	1.90713
A29	1.83254	0.00047	-0.00018	0.00454	0.00421	1.83675
A30	1.87983	0.00074	-0.00071	0.01207	0.01135	1.89118
A31	2.91433	-0.00026	0.00000	0.00288	0.00293	2.91727
A32	3.12144	-0.00021	0.00054	-0.01088	-0.01020	3.11124
A33	2.91432	-0.00025	0.00001	0.00291	0.00297	2.91729
A34	3.12151	-0.00022	0.00053	-0.01095	-0.01029	3.11121
A35	4.16942	0.00049	0.00175	-0.03572	-0.03396	4.13546
A36	4.17070	0.00040	0.00163	-0.03511	-0.03348	4.13722
A37	3.13807	0.00219	0.00163	0.01252	0.01413	3.15220
A38	3.09450	0.00373	0.01031	0.03906	0.04925	3.14375
A39	3.13811	0.00219	0.00163	0.01253	0.01414	3.15225
A40	3.09429	0.00375	0.01029	0.03939	0.04956	3.14385
A41	3.68312	0.00539	-0.00650	0.12096	0.11446	3.79758
A42	3.68103	0.00531	-0.00661	0.12077	0.11416	3.79520
D1	-0.00243	0.00166	0.00210	0.01354	0.01560	0.01317
D2	-0.02640	0.00187	0.00419	0.01975	0.02391	-0.00249
D3	-0.01638	0.00057	0.00194	0.00198	0.00389	-0.01249
D4	-0.00247	0.00166	0.00209	0.01362	0.01568	0.01321
D5	0.00897	0.00002	0.00028	-0.00053	-0.00027	0.00869
D6	-0.01634	0.00057	0.00193	0.00211	0.00401	-0.01233
D7	0.04765	-0.00156	-0.00750	-0.02392	-0.03164	0.01601
D8	3.13960	0.00117	0.00248	-0.00774	-0.00508	3.13452
D9	0.00882	0.00003	0.00027	-0.00044	-0.00020	0.00862
D10	0.04764	-0.00156	-0.00750	-0.02381	-0.03153	0.01611
D11	3.13973	0.00117	0.00248	-0.00758	-0.00492	3.13481
D12	-0.02537	0.00012	0.00159	0.00598	0.00744	-0.01793
D13	3.13600	0.00033	-0.00140	0.01684	0.01543	-3.13175
D14	3.13627	0.00033	-0.00139	0.01665	0.01525	-3.13167
D15	0.01446	0.00053	-0.00438	0.02750	0.02325	0.03770
D16	2.69857	0.00078	-0.00264	-0.02333	-0.02591	2.67266
D17	-0.46318	0.00057	0.00035	-0.03407	-0.03378	-0.49696
D18	-0.46105	0.00056	0.00033	-0.03418	-0.03391	-0.49496
D19	2.70043	0.00078	-0.00268	-0.02325	-0.02586	2.67457
D20	-1.72555	0.00051	-0.00084	0.01984	0.01911	-1.70644

D21	0.41065	0.00058	-0.00132	0.02838	0.02706	0.43770
D22	2.49537	0.00022	-0.00169	0.03518	0.03339	2.52875
D23	-1.73029	0.00051	-0.00084	0.01983	0.01910	-1.71119
D24	0.40555	0.00058	-0.00132	0.02840	0.02708	0.43262
D25	2.49056	0.00023	-0.00169	0.03516	0.03337	2.52393

Item	Value	Threshold	Converged?
Maximum Force	0.005393	0.000450	NO
RMS Force	0.001355	0.000300	NO
Maximum Displacement	0.142155	0.001800	NO
RMS Displacement	0.047978	0.001200	NO

Predicted change in Energy=-1.045378D-03
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 23:01:37 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.015804	0.665767	0.038824
2	6	0	3.336448	1.694636	0.097055
3	6	0	4.015697	-0.666240	-0.037719
4	6	0	2.141389	2.282959	0.138173
5	6	0	3.336300	-1.695074	-0.096038
6	6	0	0.909647	2.324264	0.145839
7	6	0	2.141142	-2.283206	-0.137333
8	6	0	-0.378379	1.977287	0.133286
9	6	0	0.909404	-2.324398	-0.145281
10	6	0	-1.466052	1.401974	0.092748
11	6	0	-0.378587	-1.977214	-0.133056
12	6	0	-2.669712	0.718003	0.041907
13	6	0	-1.466179	-1.401764	-0.092736
14	6	0	-2.669786	-0.717595	-0.041995
15	6	0	-3.884158	1.418108	0.105755
16	6	0	-3.884163	-1.417597	-0.105844
17	7	0	-3.710612	2.888919	-0.036968
18	7	0	-3.710268	-2.888430	0.036028
19	1	0	-3.128530	3.146955	-0.844083
20	1	0	-4.610835	3.349788	-0.112512
21	1	0	-3.126167	-3.146290	0.841720
22	1	0	-4.610290	-3.349301	0.113960
23	1	0	-3.223518	3.266351	0.776622
24	1	0	-4.816947	1.082580	-0.317080
25	1	0	-4.817877	-1.082335	0.315014
26	1	0	-3.225258	-3.266067	-0.778715

Supporting Information file

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.234296	0.000000			
3	C	1.334205	2.460341	0.000000		
4	C	2.477622	1.332659	3.498820	0.000000	
5	C	2.460383	3.395205	1.234293	4.160218	0.000000
6	C	3.522823	2.507624	4.315595	1.232459	4.701301
7	C	3.498833	4.160158	2.477591	4.574469	1.332669
8	C	4.586704	3.725741	5.130827	2.538246	5.228543
9	C	4.315635	4.701265	3.522799	4.777643	2.507648
10	C	5.531333	4.811410	5.860384	3.713735	5.717510
11	C	5.130844	5.228472	4.586662	4.957108	3.725769
12	C	6.685721	6.085294	6.827676	5.060144	6.474113
13	C	5.860387	5.717424	5.531274	5.161885	4.811429
14	C	6.827689	6.474028	6.685682	5.673024	6.085348
15	C	7.935988	7.225904	8.171463	6.087384	7.865598
16	C	8.171341	7.865391	7.935803	7.075376	7.225799
17	N	8.040252	7.148799	8.504999	5.885897	8.406869
18	N	8.504382	8.406213	8.039534	7.809968	7.148123
19	H	7.614284	6.692601	8.138222	5.429859	8.111648
20	H	9.035804	8.120514	9.515835	6.840577	9.413174
21	H	8.135365	8.108913	7.611194	7.597294	6.689461
22	H	9.515036	9.412344	9.034903	8.792503	8.119658
23	H	7.727558	6.779767	8.278566	5.491530	8.270941
24	H	8.849739	8.186816	9.008441	7.075776	8.616243
25	H	9.009221	8.616965	8.850401	7.732262	8.187491
26	H	8.280137	8.272335	7.729140	7.773885	6.781453

		6	7	8	9	10
6	C	0.000000				
7	C	4.777609	0.000000			
8	C	1.334002	4.957118	0.000000		
9	C	4.657769	1.232452	4.498942	0.000000	
10	C	2.548996	5.161911	1.231122	4.425527	0.000000
11	C	4.498894	2.538243	3.963461	1.334019	3.557032
12	C	3.924626	5.673067	2.616172	4.701203	1.385352
13	C	4.425467	3.713717	3.557019	2.549002	2.809867
14	C	4.701120	5.060164	3.541703	3.924677	2.441250
15	C	4.878862	7.075525	3.550201	6.086674	2.418195
16	C	6.086500	6.087246	4.885995	4.878742	3.719769
17	N	4.658223	7.810504	3.458878	6.966703	2.695530
18	N	6.966194	5.885180	5.897979	4.657508	4.842240
19	H	4.238353	7.599709	3.144312	6.835856	2.585816
20	H	5.620868	8.793203	4.456215	7.916469	3.704831
21	H	6.833667	5.426601	5.856898	4.235034	4.899351
22	H	7.915810	6.839702	6.803086	5.620022	5.697481
23	H	4.285844	7.772545	3.189103	7.013374	2.651843

24	H	5.877920	7.731482	4.550188	6.665441	3.390939
25	H	6.666189	7.076345	5.394762	5.878464	4.178029
26	H	7.014560	5.493235	6.035663	4.287588	5.064075

		11	12	13	14	15
11	C	0.000000				
12	C	3.541760	0.000000			
13	C	1.231108	2.441318	0.000000		
14	C	2.616205	1.438047	1.385400	0.000000	
15	C	4.886131	1.403247	3.719906	2.461250	0.000000
16	C	3.550067	2.461200	2.418071	1.403136	2.843588
17	N	5.898379	2.408853	4.842577	3.753703	1.487876
18	N	3.458179	3.753552	2.694938	2.408572	4.310611
19	H	5.858742	2.625890	4.900896	3.973479	2.112363
20	H	6.803624	3.273850	5.697938	4.507354	2.075352
21	H	3.141039	3.972507	2.583048	2.624461	4.685074
22	H	4.455440	4.507105	3.704194	3.273492	4.822398
23	H	6.034577	2.709351	5.063133	4.104701	2.074249
24	H	5.394001	2.207353	4.177313	2.815422	1.077712
25	H	4.550701	2.816100	3.391486	2.207892	2.677281
26	H	3.190855	4.105468	2.653404	2.710354	4.812269

		16	17	18	19	20
16	C	0.000000				
17	N	4.310562	0.000000			
18	N	1.487857	5.777810	0.000000		
19	H	4.685201	1.028025	6.126899	0.000000	
20	H	4.822453	1.014154	6.304637	1.665402	0.000000
21	H	2.112064	6.126778	1.028011	6.515126	6.731554
22	H	2.075344	6.304568	1.014157	6.731626	6.702916
23	H	4.811919	1.020610	6.218258	1.627871	1.649900
24	H	2.676863	2.136656	4.137432	2.718478	2.285730
25	H	1.077657	4.137727	2.136963	4.699393	4.457506
26	H	2.074549	6.218489	1.020613	6.414085	6.792142

		21	22	23	24	25
21	H	0.000000				
22	H	1.665373	0.000000			
23	H	6.413710	6.791841	0.000000		
24	H	4.699457	4.457586	2.916171	0.000000	
25	H	2.720149	2.285311	4.654689	2.255306	0.000000
26	H	1.627875	1.649881	6.715025	4.653742	2.915710

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=0 Diff= 1.98D-04
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Supporting Information file

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.519573	-0.667077	-0.017587
2	6	0	3.840114	-1.697184	-0.044042
3	6	0	4.519601	0.666661	0.017711
4	6	0	2.644997	-2.286374	-0.067081
5	6	0	3.840307	1.696876	0.044091
6	6	0	1.413251	-2.327769	-0.073612
7	6	0	2.645207	2.286129	0.067029
8	6	0	0.125261	-1.980436	-0.071953
9	6	0	1.413473	2.327674	0.073552
10	6	0	-0.962355	-1.404031	-0.049363
11	6	0	0.125446	1.980412	0.071920
12	6	0	-2.165948	-0.718690	-0.019850
13	6	0	-0.962203	1.404103	0.049292
14	6	0	-2.165878	0.718816	0.019598
15	6	0	-3.380462	-1.420309	-0.062153
16	6	0	-3.380187	1.420585	0.061616
17	7	0	-3.207090	-2.886019	0.126025
18	7	0	-3.206118	2.886307	-0.125670
19	1	0	-2.625129	-3.119022	0.940806
20	1	0	-4.107371	-3.344237	0.215684
21	1	0	-2.621895	3.119056	-0.938885
22	1	0	-4.106080	3.344639	-0.217930
23	1	0	-2.719942	-3.288490	-0.675441
24	1	0	-4.313263	-1.071764	0.349988
25	1	0	-4.313888	1.072560	-0.348780
26	1	0	-2.721161	3.288918	0.677057

Rotational constants (GHZ): 0.6008072 0.2719285 0.1877635
Leave Link 202 at Fri Sep 25 23:01:37 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.9012801119 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0154256099 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.8858545020 Hartrees.
Leave Link 301 at Fri Sep 25 23:01:37 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23232 LenP2D= 51961.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.84D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Fri Sep 25 23:01:38 2026, MaxMem= 805306368 cpu: 5.7 elap: 0.9
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 23:01:38 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 0.000000 -0.000000
Rot= 1.000000 0.000434 -0.000000 -0.000009 Ang= 0.05 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.987022763042

Supporting Information file

```
 Leave Link  401 at Fri Sep 25 23:01:46 2026, MaxMem=    805306368 cpu:                44.3 elap:
7.4
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
       NFxFlg=          0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=          0 NGrid=          0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.393491341425
 DIIS: error= 8.81D-03 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -723.393491341425     IErMin= 1 ErrMin= 8.81D-03
 ErrMax= 8.81D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.67D-02 BMatP= 3.67D-02
 IDIUse=3 WtCom= 9.12D-01 WtEn= 8.81D-02
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=     0.691 Goal=   None    Shift=    0.000
 GapD=    0.691 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
 RMSDP=4.26D-03 MaxDP=1.42D-01             OVMax= 4.57D-02

 Cycle   2  Pass 0  IDiag  1:
 RMSU=  3.86D-03    CP:  8.83D-01
 E= -723.410341981608     Delta-E=       -0.016850640183 Rises=F Damp=F
 DIIS: error= 7.89D-04 at cycle   2 NSaved=   2.
 NSaved= 2 IEnMin= 2 EnMin= -723.410341981608     IErMin= 2 ErrMin= 7.89D-04
 ErrMax= 7.89D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.51D-04 BMatP= 3.67D-02
 IDIUse=3 WtCom= 9.92D-01 WtEn= 7.89D-03
 Coeff-Com: -0.274D-01 0.103D+01
 Coeff-En:   0.000D+00 0.100D+01
 Coeff:     -0.272D-01 0.103D+01
 Gap=     0.174 Goal=   None    Shift=    0.000
 RMSDP=3.43D-02 MaxDP=1.43D+00 DE=-1.69D-02 OVMax= 1.28D-02

 Cycle   3  Pass 0  IDiag  1:
```

RMSU= 2.05D-02 CP: 2.67D+00 1.72D+00
E= -723.410829239485 Delta-E= -0.000487257877 Rises=F Damp=F
DIIS: error= 1.38D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.410829239485 IErMin= 2 ErrMin= 7.89D-04
ErrMax= 1.38D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.34D-04 BMatP= 3.51D-04
IDIUse=3 WtCom= 2.12D-01 WtEn= 7.88D-01
Coeff-Com: -0.219D-01 0.614D+00 0.408D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.465D-02 0.130D+00 0.874D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=3.74D+02 MaxDP=1.32D+04 DE=-4.87D-04 OVMax= 9.92D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.410435400394 Delta-E= 0.000393839091 Rises=F Damp=F
DIIS: error= 1.51D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.410435400394 IErMin= 1 ErrMin= 1.51D-03
ErrMax= 1.51D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.22D-04 BMatP= 5.22D-04
IDIUse=3 WtCom= 9.85D-01 WtEn= 1.51D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.176 Goal= None Shift= 0.000
GapD= 0.176 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=3.53D-02 MaxDP=1.44D+00 DE= 3.94D-04 OVMax= 1.30D-02

Cycle 5 Pass 1 IDiag 1:
RMSU= 6.76D-03 CP: 2.51D-01
E= -723.410106355867 Delta-E= 0.000329044527 Rises=F Damp=F
DIIS: error= 2.34D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 1 EnMin= -723.410435400394 IErMin= 1 ErrMin= 1.51D-03
ErrMax= 2.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.10D-04 BMatP= 5.22D-04
IDIUse=3 WtCom= 1.71D-01 WtEn= 8.29D-01
Coeff-Com: 0.546D+00 0.454D+00
Coeff-En: 0.626D+00 0.374D+00
Coeff: 0.613D+00 0.387D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=6.17D-04 MaxDP=2.68D-02 DE= 3.29D-04 OVMax= 8.63D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.46D-04 CP: 2.38D-01 1.01D+00
E= -723.410943363024 Delta-E= -0.000837007157 Rises=F Damp=F
DIIS: error= 2.89D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.410943363024 IErMin= 3 ErrMin= 2.89D-04
ErrMax= 2.89D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.00D-05 BMatP= 5.22D-04
IDIUse=3 WtCom= 9.97D-01 WtEn= 2.89D-03
Coeff-Com: 0.222D-01 0.803D-01 0.898D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.221D-01 0.800D-01 0.898D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=1.02D-03 MaxDP=4.14D-02 DE=-8.37D-04 OVMax= 2.72D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.34D-04 CP: 2.17D-01 1.02D+00 2.18D+00
E= -723.410952979780 Delta-E= -0.000009616756 Rises=F Damp=F
DIIS: error= 1.04D-04 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.410952979780 IErMin= 4 ErrMin= 1.04D-04
ErrMax= 1.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.90D-06 BMatP= 1.00D-05
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.04D-03
Coeff-Com: -0.183D-01 0.172D-01 0.495D+00 0.506D+00
Coeff-En: 0.000D+00 0.000D+00 0.242D+00 0.758D+00
Coeff: -0.183D-01 0.171D-01 0.495D+00 0.506D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.30D-04 MaxDP=5.30D-03 DE=-9.62D-06 OVMax= 1.55D-03

Cycle 8 Pass 1 IDiag 1:
RMSU= 1.25D-05 CP: 2.14D-01 1.02D+00 2.35D+00 1.12D+00
E= -723.410961294695 Delta-E= -0.000008314915 Rises=F Damp=F
DIIS: error= 4.43D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.410961294695 IErMin= 5 ErrMin= 4.43D-05
ErrMax= 4.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.03D-07 BMatP= 6.90D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.746D-02 0.871D-03 0.116D+00 0.166D+00 0.725D+00
Coeff: -0.746D-02 0.871D-03 0.116D+00 0.166D+00 0.725D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=3.60D-05 MaxDP=1.50D-03 DE=-8.31D-06 OVMax= 5.03D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 6.54D-06 CP: 2.14D-01 1.02D+00 2.40D+00 1.16D+00 1.12D+00
E= -723.410962194325 Delta-E= -0.000000899630 Rises=F Damp=F
DIIS: error= 2.88D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.410962194325 IErMin= 6 ErrMin= 2.88D-05
ErrMax= 2.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.76D-07 BMatP= 3.03D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.483D-02-0.930D-02-0.195D+00-0.166D+00 0.514D+00 0.852D+00
Coeff: 0.483D-02-0.930D-02-0.195D+00-0.166D+00 0.514D+00 0.852D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=2.81D-05 MaxDP=1.16D-03 DE=-9.00D-07 OVMax= 8.67D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.62D-06 CP: 2.13D-01 1.02D+00 2.45D+00 1.20D+00 1.39D+00
CP: 1.95D+00
E= -723.410963008756 Delta-E= -0.000000814430 Rises=F Damp=F
DIIS: error= 1.39D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.410963008756 IErMin= 7 ErrMin= 1.39D-05

ErrMax= 1.39D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-08 BMatP= 1.76D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.194D-02-0.207D-02-0.544D-01-0.585D-01-0.119D-01 0.223D+00
Coeff-Com: 0.902D+00
Coeff: 0.194D-02-0.207D-02-0.544D-01-0.585D-01-0.119D-01 0.223D+00
Coeff: 0.902D+00
Gap=   0.174 Goal=   None   Shift=   0.000
RMSDP=1.18D-05 MaxDP=4.81D-04 DE=-8.14D-07 OVMax= 3.92D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 2.25D-06   CP: 2.13D-01 1.02D+00 2.43D+00 1.18D+00 1.47D+00
               CP: 2.16D+00 1.52D+00
E= -723.410963175517   Delta-E=   -0.000000166761 Rises=F Damp=F
DIIS: error= 8.25D-06 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -723.410963175517   IErMin= 8 ErrMin= 8.25D-06
ErrMax= 8.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-08 BMatP= 2.15D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.146D-02 0.373D-02 0.713D-01 0.523D-01-0.295D+00-0.285D+00
Coeff-Com: 0.506D+00 0.948D+00
Coeff: -0.146D-02 0.373D-02 0.713D-01 0.523D-01-0.295D+00-0.285D+00
Coeff: 0.506D+00 0.948D+00
Gap=   0.174 Goal=   None   Shift=   0.000
RMSDP=1.27D-05 MaxDP=5.24D-04 DE=-1.67D-07 OVMax= 3.45D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 5.91D-07   CP: 2.13D-01 1.02D+00 2.42D+00 1.17D+00 1.52D+00
               CP: 2.31D+00 2.01D+00 2.09D+00
E= -723.410963260707   Delta-E=   -0.000000085190 Rises=F Damp=F
DIIS: error= 3.41D-06 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.410963260707   IErMin= 9 ErrMin= 3.41D-06
ErrMax= 3.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-09 BMatP= 1.21D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.112D-02 0.224D-02 0.460D-01 0.373D-01-0.142D+00-0.172D+00
Coeff-Com: 0.696D-01 0.386D+00 0.774D+00
Coeff: -0.112D-02 0.224D-02 0.460D-01 0.373D-01-0.142D+00-0.172D+00
Coeff: 0.696D-01 0.386D+00 0.774D+00
Gap=   0.174 Goal=   None   Shift=   0.000
RMSDP=1.08D-06 MaxDP=4.92D-05 DE=-8.52D-08 OVMax= 1.14D-04

Cycle 13 Pass 1 IDiag 1:
RMSU= 4.91D-07   CP: 2.13D-01 1.02D+00 2.42D+00 1.17D+00 1.54D+00
               CP: 2.30D+00 2.10D+00 2.33D+00 1.33D+00
E= -723.410963272988   Delta-E=   -0.000000012282 Rises=F Damp=F
DIIS: error= 1.49D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.410963272988   IErMin=10 ErrMin= 1.49D-06
ErrMax= 1.49D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.71D-10 BMatP= 2.02D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.223D-04-0.240D-03-0.276D-02-0.742D-03 0.321D-01 0.228D-01

Coeff-Com: -0.119D+00-0.171D+00 0.385D+00 0.854D+00
Coeff: -0.223D-04-0.240D-03-0.276D-02-0.742D-03 0.321D-01 0.228D-01
Coeff: -0.119D+00-0.171D+00 0.385D+00 0.854D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=4.02D-06 MaxDP=1.52D-04 DE=-1.23D-08 OVMax= 6.01D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 1.46D-07 CP: 2.13D-01 1.02D+00 2.42D+00 1.18D+00 1.56D+00
CP: 2.27D+00 2.09D+00 2.28D+00 1.55D+00 2.08D+00
E= -723.410963276314 Delta-E= -0.000000003326 Rises=F Damp=F
DIIS: error= 7.17D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.410963276314 IErMin=11 ErrMin= 7.17D-07
ErrMax= 7.17D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-10 BMatP= 6.71D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.204D-03-0.507D-03-0.963D-02-0.739D-02 0.365D-01 0.413D-01
Coeff-Com: -0.531D-01-0.147D+00-0.139D-01 0.315D+00 0.839D+00
Coeff: 0.204D-03-0.507D-03-0.963D-02-0.739D-02 0.365D-01 0.413D-01
Coeff: -0.531D-01-0.147D+00-0.139D-01 0.315D+00 0.839D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.84D-06 MaxDP=7.24D-05 DE=-3.33D-09 OVMax= 2.36D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 8.91D-08 CP: 2.13D-01 1.02D+00 2.43D+00 1.18D+00 1.57D+00
CP: 2.27D+00 2.07D+00 2.20D+00 1.64D+00 2.60D+00
CP: 1.62D+00
E= -723.410963276897 Delta-E= -0.000000000583 Rises=F Damp=F
DIIS: error= 2.52D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.410963276897 IErMin=12 ErrMin= 2.52D-07
ErrMax= 2.52D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-11 BMatP= 1.08D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.775D-04-0.129D-03-0.290D-02-0.257D-02 0.640D-02 0.109D-01
Coeff-Com: 0.651D-02-0.214D-01-0.802D-01-0.501D-01 0.279D+00 0.854D+00
Coeff: 0.775D-04-0.129D-03-0.290D-02-0.257D-02 0.640D-02 0.109D-01
Coeff: 0.651D-02-0.214D-01-0.802D-01-0.501D-01 0.279D+00 0.854D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=5.22D-07 MaxDP=2.08D-05 DE=-5.83D-10 OVMax= 9.55D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 3.13D-08 CP: 2.13D-01 1.02D+00 2.43D+00 1.18D+00 1.57D+00
CP: 2.27D+00 2.06D+00 2.13D+00 1.64D+00 2.81D+00
CP: 2.07D+00 1.83D+00
E= -723.410963276999 Delta-E= -0.000000000102 Rises=F Damp=F
DIIS: error= 1.30D-07 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.410963276999 IErMin=13 ErrMin= 1.30D-07
ErrMax= 1.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.05D-12 BMatP= 1.83D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.273D-04 0.833D-04 0.147D-02 0.101D-02-0.656D-02-0.646D-02
Coeff-Com: 0.133D-01 0.262D-01-0.124D-01-0.778D-01-0.137D+00 0.181D+00

Coeff-Com: 0.102D+01
Coeff: -0.273D-04 0.833D-04 0.147D-02 0.101D-02-0.656D-02-0.646D-02
Coeff: 0.133D-01 0.262D-01-0.124D-01-0.778D-01-0.137D+00 0.181D+00
Coeff: 0.102D+01
Gap=   0.174 Goal=   None   Shift=   0.000
RMSDP=1.21D-07 MaxDP=3.99D-06 DE=-1.02D-10 OVMax= 5.56D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 1.76D-08   CP: 2.13D-01 1.02D+00 2.43D+00 1.18D+00 1.56D+00
               CP: 2.27D+00 2.05D+00 2.10D+00 1.65D+00 2.87D+00
               CP: 2.33D+00 2.44D+00 1.76D+00
E= -723.410963277022   Delta-E=   -0.000000000023 Rises=F Damp=F
DIIS: error= 5.51D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.410963277022   IErMin=14 ErrMin= 5.51D-08
ErrMax= 5.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.36D-13 BMatP= 3.05D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.125D-04 0.238D-04 0.506D-03 0.424D-03-0.137D-02-0.185D-02
Coeff-Com: 0.331D-03 0.452D-02 0.104D-01 0.215D-02-0.541D-01-0.107D+00
Coeff-Com: 0.103D+00 0.104D+01
Coeff: -0.125D-04 0.238D-04 0.506D-03 0.424D-03-0.137D-02-0.185D-02
Coeff: 0.331D-03 0.452D-02 0.104D-01 0.215D-02-0.541D-01-0.107D+00
Coeff: 0.103D+00 0.104D+01
Gap=   0.174 Goal=   None   Shift=   0.000
RMSDP=4.27D-08 MaxDP=1.60D-06 DE=-2.25D-11 OVMax= 2.30D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 8.23D-09   CP: 2.13D-01 1.02D+00 2.43D+00 1.18D+00 1.56D+00
               CP: 2.27D+00 2.05D+00 2.09D+00 1.65D+00 2.88D+00
               CP: 2.41D+00 2.65D+00 2.00D+00 1.61D+00
E= -723.410963277021   Delta-E=   0.000000000001 Rises=F Damp=F
DIIS: error= 2.82D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=14 EnMin= -723.410963277022   IErMin=15 ErrMin= 2.82D-08
ErrMax= 2.82D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.91D-14 BMatP= 4.36D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.549D-05-0.168D-04-0.312D-03-0.212D-03 0.144D-02 0.138D-02
Coeff-Com: -0.326D-02-0.615D-02 0.448D-02 0.199D-01 0.247D-01-0.584D-01
Coeff-Com: -0.226D+00 0.124D+00 0.112D+01
Coeff: 0.549D-05-0.168D-04-0.312D-03-0.212D-03 0.144D-02 0.138D-02
Coeff: -0.326D-02-0.615D-02 0.448D-02 0.199D-01 0.247D-01-0.584D-01
Coeff: -0.226D+00 0.124D+00 0.112D+01
Gap=   0.174 Goal=   None   Shift=   0.000
RMSDP=5.12D-08 MaxDP=1.99D-06 DE= 1.14D-12 OVMax= 1.17D-06

Cycle 19 Pass 1 IDiag 1:
RMSU= 2.69D-09   CP: 2.13D-01 1.02D+00 2.43D+00 1.18D+00 1.56D+00
               CP: 2.27D+00 2.05D+00 2.08D+00 1.65D+00 2.89D+00
               CP: 2.45D+00 2.73D+00 2.09D+00 1.92D+00 1.74D+00
E= -723.410963277033   Delta-E=   -0.000000000012 Rises=F Damp=F

DIIS: error= 1.04D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.410963277033 IErMin=16 ErrMin= 1.04D-08
ErrMax= 1.04D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-14 BMatP= 8.91D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.298D-05-0.799D-05-0.147D-03-0.110D-03 0.586D-03 0.631D-03
Coeff-Com: -0.101D-02-0.241D-02 0.484D-03 0.626D-02 0.126D-01-0.712D-02
Coeff-Com: -0.791D-01-0.652D-01 0.330D+00 0.805D+00
Coeff: 0.298D-05-0.799D-05-0.147D-03-0.110D-03 0.586D-03 0.631D-03
Coeff: -0.101D-02-0.241D-02 0.484D-03 0.626D-02 0.126D-01-0.712D-02
Coeff: -0.791D-01-0.652D-01 0.330D+00 0.805D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.57D-08 MaxDP=5.87D-07 DE=-1.21D-11 OVMax= 2.48D-07

Cycle 20 Pass 1 IDiag 1:
RMSU= 9.22D-10 CP: 2.13D-01 1.02D+00 2.43D+00 1.18D+00 1.56D+00
CP: 2.27D+00 2.05D+00 2.08D+00 1.65D+00 2.89D+00
CP: 2.46D+00 2.73D+00 2.09D+00 1.94D+00 1.87D+00
CP: 1.37D+00
E= -723.410963277035 Delta-E= -0.000000000002 Rises=F Damp=F
DIIS: error= 5.86D-09 at cycle 17 NSaved= 17.
NSaved=17 IEnMin=17 EnMin= -723.410963277035 IErMin=17 ErrMin= 5.86D-09
ErrMax= 5.86D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.83D-15 BMatP= 1.45D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.101D-06 0.829D-06 0.162D-04 0.733D-05-0.123D-03-0.758D-04
Coeff-Com: 0.433D-03 0.492D-03-0.986D-03-0.241D-02-0.128D-02 0.129D-01
Coeff-Com: 0.249D-01-0.628D-01-0.156D+00 0.390D+00 0.795D+00
Coeff: -0.101D-06 0.829D-06 0.162D-04 0.733D-05-0.123D-03-0.758D-04
Coeff: 0.433D-03 0.492D-03-0.986D-03-0.241D-02-0.128D-02 0.129D-01
Coeff: 0.249D-01-0.628D-01-0.156D+00 0.390D+00 0.795D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=6.72D-09 MaxDP=2.62D-07 DE=-1.59D-12 OVMax= 1.24D-07

SCF Done: E(RwB97XD) = -723.410963277 A.U. after 20 cycles
NFock= 20 Conv=0.67D-08 -V/T= 2.0046
KE= 7.200829101582D+02 PE=-3.703045371235D+03 EE= 1.248665643298D+03
Leave Link 502 at Fri Sep 25 23:25:02 2026, MaxMem= 805306368 cpu: 8374.4 elap: 1396.1
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23232 LenP2D= 51961.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 23:25:03 2026, MaxMem= 805306368 cpu: 2.9 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.

Supporting Information file

Leave Link 702 at Fri Sep 25 23:25:03 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 25 23:36:47 2026, MaxMem= 805306368 cpu: 4228.2 elap: 704.9
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-5.26758412D+00 1.75051793D-03 1.67806618D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000797766	0.001911838	0.000218821
2	6	0.002115020	-0.001241072	0.000002004
3	6	-0.000811714	-0.001910684	-0.000217870
4	6	-0.002596226	-0.000000865	-0.000040371
5	6	0.002125279	0.001235122	-0.000000450
6	6	0.002695564	0.001078452	0.000308382
7	6	-0.002608928	0.000009490	0.000035722
8	6	-0.002933655	-0.001484194	-0.000184980
9	6	0.002711887	-0.001087220	-0.000308793
10	6	0.003357015	0.000853892	-0.001115970
11	6	-0.002952514	0.001501145	0.000186783
12	6	0.001568182	-0.004273162	-0.000665894
13	6	0.003379983	-0.000860885	0.001123175
14	6	0.001485192	0.004339221	0.000659657
15	6	-0.006453434	0.009107643	0.004075320
16	6	-0.006354321	-0.009173960	-0.004088091
17	7	0.002093485	-0.004426626	0.001189668
18	7	0.002013143	0.004416445	-0.001185829
19	1	-0.000135843	0.001289378	-0.001546411
20	1	-0.000330357	-0.000078957	0.000324489
21	1	-0.000130440	-0.001285395	0.001543726
22	1	-0.000333798	0.000070415	-0.000321601
23	1	-0.000329488	0.000333755	0.000083423
24	1	0.001765753	-0.002507454	-0.002926220
25	1	0.001781543	0.002515843	0.002937610

```
    26        1          -0.000323561   -0.000332163   -0.000086300
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.009173960 RMS     0.002583326
 Leave Link  716 at Fri Sep 25 23:36:48 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.004843355 RMS     0.001378661
 Search for a local minimum.
 Step number  10 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .13787D-02 SwitMx=.10000D-02 MixMth= 1
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    6    7    8    9   10
 DE= -7.46D-04 DEPred=-1.05D-03 R= 7.14D-01
 TightC=F SS=  1.41D+00  RLast= 2.31D-01 DXNew= 2.4000D+00 6.9256D-01
 Trust test= 7.14D-01 RLast= 2.31D-01 DXMaxT set to 1.43D+00
 ITU=  1  1  1  1  1  1  0  0  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.00442   0.00951   0.01098   0.01660   0.01750
    Eigenvalues ---    0.01861   0.02398   0.02719   0.02805   0.03108
    Eigenvalues ---    0.03140   0.03616   0.03788   0.04267   0.04409
    Eigenvalues ---    0.04439   0.04467   0.05026   0.05026   0.06906
    Eigenvalues ---    0.08681   0.09489   0.09970   0.11401   0.11421
    Eigenvalues ---    0.11655   0.11816   0.14708   0.15246   0.15789
    Eigenvalues ---    0.16000   0.16000   0.16000   0.16000   0.16079
    Eigenvalues ---    0.19017   0.21680   0.24461   0.24994   0.24996
    Eigenvalues ---    0.24996   0.24999   0.25000   0.25000   0.25391
    Eigenvalues ---    0.28953   0.32452   0.37230   0.38998   0.40644
    Eigenvalues ---    0.44873   0.45835   0.46899   0.47489   0.47688
    Eigenvalues ---    0.47688   0.47688   0.47795   0.50063   0.54803
    Eigenvalues ---    0.54895   0.55162   0.55659   0.55664   0.57255
    Eigenvalues ---    0.93697   0.93807   0.95021   0.95687   0.97675
    Eigenvalues ---    0.98469   1.36034
 RFO step:  Lambda=-6.37080351D-04 EMin= 4.41908697D-03
 Quartic linear search produced a step of -0.20712.
 Iteration  1 RMS(Cart)=  0.03020619 RMS(Int)=  0.00059869
 Iteration  2 RMS(Cart)=  0.00085772 RMS(Int)=  0.00002634
 Iteration  3 RMS(Cart)=  0.00000048 RMS(Int)=  0.00002634
  ITry=  1 IFail=0 DXMaxC= 1.34D-01 DCOld= 1.00D+10 DXMaxT= 1.43D+00 DXLimC=
3.00D+00 Rises=F
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                          (Linear)    (Quad)   (Total)
    R1        2.33248  -0.00123  -0.00099   0.00125   0.00026   2.33274
```

R2	2.52128	0.00097	0.00161	-0.00211	-0.00049	2.52079
R3	2.51836	0.00131	0.00151	-0.00151	-0.00000	2.51836
R4	2.33248	-0.00124	-0.00099	0.00124	0.00026	2.33274
R5	2.32901	-0.00127	-0.00086	0.00080	-0.00007	2.32894
R6	2.51838	0.00131	0.00151	-0.00151	-0.00000	2.51838
R7	2.52090	0.00157	0.00137	-0.00095	0.00041	2.52131
R8	2.32900	-0.00128	-0.00086	0.00080	-0.00007	2.32893
R9	2.32648	-0.00167	-0.00061	-0.00030	-0.00092	2.32556
R10	2.52093	0.00158	0.00137	-0.00095	0.00042	2.52135
R11	2.61794	0.00163	0.00150	-0.00088	0.00062	2.61855
R12	2.32646	-0.00168	-0.00062	-0.00031	-0.00093	2.32553
R13	2.71752	-0.00043	-0.00095	-0.00022	-0.00118	2.71634
R14	2.65175	0.00484	0.00226	0.00251	0.00477	2.65652
R15	2.61803	0.00164	0.00151	-0.00089	0.00062	2.61865
R16	2.65154	0.00484	0.00226	0.00252	0.00477	2.65632
R17	2.81168	-0.00270	-0.00541	0.00568	0.00028	2.81196
R18	2.03658	0.00040	-0.00062	0.00242	0.00179	2.03837
R19	2.81164	-0.00270	-0.00539	0.00565	0.00026	2.81190
R20	2.03648	0.00039	-0.00062	0.00238	0.00176	2.03824
R21	1.94269	0.00146	0.00190	-0.00302	-0.00113	1.94156
R22	1.91647	0.00023	0.00076	-0.00201	-0.00125	1.91522
R23	1.92867	0.00003	0.00103	-0.00301	-0.00198	1.92669
R24	1.94266	0.00146	0.00189	-0.00300	-0.00112	1.94154
R25	1.91648	0.00024	0.00076	-0.00200	-0.00124	1.91524
R26	1.92868	0.00004	0.00103	-0.00301	-0.00198	1.92670
A1	2.55867	-0.00007	-0.00077	0.00209	0.00136	2.56003
A2	2.61201	-0.00041	0.00034	-0.00194	-0.00155	2.61046
A3	2.55879	-0.00006	-0.00079	0.00215	0.00141	2.56020
A4	2.71702	0.00040	-0.00070	0.00238	0.00170	2.71872
A5	2.61189	-0.00041	0.00036	-0.00198	-0.00158	2.61031
A6	2.84452	-0.00039	0.00120	-0.00517	-0.00395	2.84057
A7	2.71709	0.00040	-0.00071	0.00242	0.00174	2.71883
A8	2.84446	-0.00039	0.00120	-0.00517	-0.00395	2.84051
A9	2.08870	-0.00102	-0.00168	0.00052	-0.00120	2.08750
A10	2.09897	0.00032	-0.00179	0.00569	0.00389	2.10286
A11	2.09518	0.00072	0.00350	-0.00591	-0.00243	2.09275
A12	2.08874	-0.00105	-0.00169	0.00046	-0.00127	2.08747
A13	2.09524	0.00074	0.00352	-0.00591	-0.00241	2.09283
A14	2.09887	0.00033	-0.00180	0.00575	0.00393	2.10280
A15	2.18449	-0.00408	0.00023	-0.01964	-0.01941	2.16508
A16	1.95097	0.00295	0.00680	-0.00232	0.00449	1.95546
A17	2.18572	-0.00415	0.00015	-0.01997	-0.01982	2.16590
A18	1.95150	0.00290	0.00679	-0.00271	0.00408	1.95557
A19	1.97086	0.00150	0.00352	-0.00078	0.00275	1.97361
A20	1.93139	-0.00105	-0.00007	-0.00728	-0.00736	1.92404
A21	1.92279	0.00043	0.00259	-0.00419	-0.00159	1.92120
A22	1.90716	-0.00064	-0.00317	0.00436	0.00120	1.90836
A23	1.83673	0.00018	-0.00088	0.00540	0.00456	1.84128

A24	1.89122	-0.00043	-0.00236	0.00335	0.00098	1.89220
A25	1.97045	0.00150	0.00350	-0.00076	0.00276	1.97321
A26	1.93140	-0.00104	-0.00008	-0.00721	-0.00729	1.92412
A27	1.92325	0.00042	0.00260	-0.00424	-0.00164	1.92161
A28	1.90713	-0.00064	-0.00316	0.00434	0.00119	1.90831
A29	1.83675	0.00017	-0.00087	0.00538	0.00453	1.84128
A30	1.89118	-0.00043	-0.00235	0.00335	0.00099	1.89216
A31	2.91727	0.00063	-0.00061	0.00170	0.00109	2.91835
A32	3.11124	0.00087	0.00211	0.00054	0.00264	3.11388
A33	2.91729	0.00064	-0.00061	0.00182	0.00121	2.91850
A34	3.11121	0.00086	0.00213	0.00034	0.00246	3.11367
A35	4.13546	-0.00113	0.00703	-0.02196	-0.01493	4.12054
A36	4.13722	-0.00125	0.00694	-0.02268	-0.01574	4.12147
A37	3.15220	-0.00057	-0.00293	-0.00191	-0.00488	3.14732
A38	3.14375	-0.00087	-0.01020	-0.00736	-0.01751	3.12624
A39	3.15225	-0.00057	-0.00293	-0.00194	-0.00491	3.14734
A40	3.14385	-0.00087	-0.01026	-0.00735	-0.01756	3.12629
A41	3.79758	-0.00001	-0.02371	0.06372	0.04002	3.83760
A42	3.79520	-0.00009	-0.02365	0.06244	0.03880	3.83400
D1	0.01317	-0.00036	-0.00323	0.00062	-0.00260	0.01056
D2	-0.00249	-0.00051	-0.00495	-0.00357	-0.00853	-0.01102
D3	-0.01249	-0.00013	-0.00081	-0.00261	-0.00339	-0.01588
D4	0.01321	-0.00036	-0.00325	0.00061	-0.00263	0.01058
D5	0.00869	-0.00002	0.00006	-0.00081	-0.00071	0.00798
D6	-0.01233	-0.00013	-0.00083	-0.00264	-0.00345	-0.01578
D7	0.01601	0.00011	0.00655	-0.00558	0.00105	0.01706
D8	3.13452	-0.00004	0.00105	0.00124	0.00231	3.13683
D9	0.00862	-0.00002	0.00004	-0.00079	-0.00071	0.00791
D10	0.01611	0.00011	0.00653	-0.00561	0.00101	0.01712
D11	3.13481	-0.00004	0.00102	0.00123	0.00227	3.13708
D12	-0.01793	0.00030	-0.00154	0.01248	0.01101	-0.00692
D13	-3.13175	-0.00029	-0.00320	-0.00018	-0.00333	-3.13508
D14	-3.13167	-0.00028	-0.00316	-0.00016	-0.00327	-3.13494
D15	0.03770	-0.00087	-0.00481	-0.01282	-0.01762	0.02008
D16	2.67266	-0.00156	0.00537	-0.07075	-0.06542	2.60725
D17	-0.49696	-0.00100	0.00700	-0.05812	-0.05108	-0.54804
D18	-0.49496	-0.00100	0.00702	-0.05812	-0.05105	-0.54601
D19	2.67457	-0.00157	0.00536	-0.07076	-0.06544	2.60913
D20	-1.70644	0.00126	-0.00396	0.02266	0.01868	-1.68776
D21	0.43770	0.00073	-0.00560	0.02234	0.01673	0.45443
D22	2.52875	-0.00020	-0.00692	0.01915	0.01226	2.54102
D23	-1.71119	0.00125	-0.00396	0.02262	0.01864	-1.69255
D24	0.43262	0.00073	-0.00561	0.02235	0.01673	0.44936
D25	2.52393	-0.00019	-0.00691	0.01917	0.01229	2.53621

Item	Value	Threshold	Converged?
Maximum Force	0.004843	0.000450	NO
RMS Force	0.001379	0.000300	NO
Maximum Displacement	0.133979	0.001800	NO

Supporting Information file

RMS Displacement 0.030315 0.001200 NO
Predicted change in Energy=-3.721498D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Sep 25 23:36:48 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.010040	0.665584	0.048459
2	6	0	3.331942	1.694680	0.118955
3	6	0	4.010036	-0.664901	-0.047547
4	6	0	2.136699	2.282496	0.161889
5	6	0	3.332103	-1.694099	-0.118083
6	6	0	0.905048	2.326131	0.160798
7	6	0	2.136859	-2.281933	-0.161088
8	6	0	-0.382323	1.976942	0.130986
9	6	0	0.905222	-2.325719	-0.160135
10	6	0	-1.468679	1.401117	0.078834
11	6	0	-0.382192	-1.976598	-0.130469
12	6	0	-2.673460	0.717771	0.038321
13	6	0	-1.468653	-1.401000	-0.078430
14	6	0	-2.673480	-0.717629	-0.037960
15	6	0	-3.891978	1.417026	0.087800
16	6	0	-3.891863	-1.416909	-0.087309
17	7	0	-3.704446	2.887533	-0.041245
18	7	0	-3.705832	-2.887735	0.039920
19	1	0	-3.091087	3.148253	-0.823181
20	1	0	-4.601140	3.347098	-0.150355
21	1	0	-3.090938	-3.149535	0.820277
22	1	0	-4.602783	-3.346358	0.150950
23	1	0	-3.252549	3.257408	0.794510
24	1	0	-4.800506	1.081627	-0.387166
25	1	0	-4.801179	-1.081409	0.385913
26	1	0	-3.256348	-3.257761	-0.797073

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.234433	0.000000			
3	C	1.333944	2.460722	0.000000		
4	C	2.477232	1.332658	3.498628	0.000000	
5	C	2.460780	3.397059	1.234430	4.161813	0.000000
6	C	3.522927	2.508047	4.316321	1.232425	4.704320

7	C	3.498653	4.161742	2.477192	4.575842	1.332669
8	C	4.584683	3.724994	5.128744	2.537674	5.228340
9	C	4.316399	4.704303	3.522906	4.780782	2.508080
10	C	5.527955	4.809755	5.856681	3.712476	5.715474
11	C	5.128824	5.228316	4.584658	4.956830	3.725043
12	C	6.683712	6.084876	6.825560	5.059770	6.473668
13	C	5.856872	5.715584	5.528004	5.159889	4.809859
14	C	6.825700	6.473712	6.683731	5.672610	6.084977
15	C	7.937764	7.229321	8.172794	6.090934	7.868217
16	C	8.172838	7.868156	7.937701	7.077517	7.229347
17	N	8.028599	7.138580	8.493118	5.875909	8.397040
18	N	8.494752	8.398513	8.030146	7.802649	7.140186
19	H	7.572939	6.652503	8.097388	5.389772	8.074832
20	H	9.021223	8.107824	9.500476	6.828569	9.399524
21	H	8.097822	8.075374	7.573002	7.567604	6.652389
22	H	9.501942	9.400689	9.022764	8.780930	8.109547
23	H	7.747215	6.801030	8.296909	5.513135	8.289022
24	H	8.831115	8.171212	8.988401	7.061753	8.597464
25	H	8.989074	8.598000	8.831697	7.713637	8.171884
26	H	8.301081	8.292849	7.751455	7.790957	6.805421

		6	7	8	9	10
6	C	0.000000				
7	C	4.780714	0.000000			
8	C	1.334220	4.956773	0.000000		
9	C	4.662908	1.232415	4.500601	0.000000	
10	C	2.548911	5.159682	1.230635	4.425135	0.000000
11	C	4.500589	2.537673	3.962175	1.334241	3.554324
12	C	3.925244	5.672491	2.615991	4.702040	1.385678
13	C	4.425290	3.712491	3.554498	2.548934	2.806526
14	C	4.702110	5.059799	3.540996	3.925301	2.440137
15	C	4.882956	7.077508	3.554300	6.089560	2.423368
16	C	6.089520	6.090911	4.886998	4.882956	3.720309
17	N	4.647949	7.801191	3.448963	6.959969	2.687472
18	N	6.961265	5.877451	5.892290	4.649484	4.837418
19	H	4.196807	7.566816	3.101581	6.809881	2.549181
20	H	5.608680	8.779905	4.444649	7.905755	3.694818
21	H	6.810708	5.389404	5.838877	4.196329	4.887730
22	H	7.906544	6.830311	6.793394	5.610401	5.689142
23	H	4.307491	7.787373	3.212173	7.026358	2.672115
24	H	5.865356	7.713085	4.537666	6.649577	3.379394
25	H	6.650040	7.062354	5.380036	5.865960	4.166869
26	H	7.029551	5.517553	6.043462	4.311967	5.066371

		11	12	13	14	15
11	C	0.000000				
12	C	3.540907	0.000000			
13	C	1.230618	2.440160	0.000000		
14	C	2.616020	1.437425	1.385728	0.000000	
15	C	4.887016	1.405771	3.720404	2.461159	0.000000

16	C	3.554280	2.461127	2.423278	1.405662	2.839340
17	N	5.891104	2.403566	4.836493	3.749679	1.488023
18	N	3.450476	3.750395	2.688746	2.404407	4.309049
19	H	5.837984	2.612248	4.886987	3.966864	2.113873
20	H	6.792765	3.265717	5.688767	4.500056	2.069977
21	H	3.101130	3.967593	2.548894	2.612472	4.693790
22	H	4.446215	4.500235	3.695918	3.266208	4.816540
23	H	6.040642	2.712364	5.064096	4.102346	2.072514
24	H	5.379603	2.199489	4.166533	2.807758	1.078661
25	H	4.538223	2.808034	3.379864	2.199798	2.675387
26	H	3.216600	4.103961	2.675792	2.714454	4.800069

		16	17	18	19	20
16	C	0.000000				
17	N	4.308766	0.000000			
18	N	1.487993	5.775838	0.000000		
19	H	4.692915	1.027428	6.128295	0.000000	
20	H	4.816929	1.013492	6.301660	1.665081	0.000000
21	H	2.113572	6.129013	1.027419	6.508693	6.740109
22	H	2.070012	6.301217	1.013501	6.739000	6.700234
23	H	4.799538	1.019561	6.207870	1.629389	1.649094
24	H	2.675487	2.140632	4.139631	2.717198	2.286522
25	H	1.078590	4.139781	2.140633	4.719784	4.465341
26	H	2.072771	6.207794	1.019566	6.408198	6.771327

		21	22	23	24	25
21	H	0.000000				
22	H	1.665057	0.000000			
23	H	6.409032	6.771043	0.000000		
24	H	4.720516	4.464942	2.920026	0.000000	
25	H	2.718592	2.285730	4.624990	2.297036	0.000000
26	H	1.629385	1.649086	6.706756	4.624147	2.919327

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=3 Diff= 2.04D-03
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.516561	-0.665938	-0.026351
2	6	0	3.838633	-1.696886	-0.063583
3	6	0	4.516337	0.666956	0.026562
4	6	0	2.643487	-2.285976	-0.087591

5	6	0	3.838235	1.697788	0.063701
6	6	0	1.411843	-2.329751	-0.085206
7	6	0	2.642893	2.286513	0.087553
8	6	0	0.124414	-1.979988	-0.066829
9	6	0	1.411250	2.330046	0.085067
10	6	0	-0.962038	-1.402952	-0.033436
11	6	0	0.123894	1.979941	0.066589
12	6	0	-2.166932	-0.718847	-0.015167
13	6	0	-0.962471	1.402785	0.033094
14	6	0	-2.167186	0.718268	0.014639
15	6	0	-3.385334	-1.419534	-0.042114
16	6	0	-3.385684	1.418583	0.041223
17	7	0	-3.197582	-2.885066	0.134454
18	7	0	-3.199873	2.884552	-0.133504
19	1	0	-2.584260	-3.120254	0.924474
20	1	0	-4.094215	-3.341005	0.258288
21	1	0	-2.584942	3.121070	-0.921864
22	1	0	-4.096886	3.339199	-0.259398
23	1	0	-2.745543	-3.281712	-0.688855
24	1	0	-4.293962	-1.069091	0.421667
25	1	0	-4.294900	1.067802	-0.420984
26	1	0	-2.750531	3.281535	0.691123

Rotational constants (GHZ): 0.6008609 0.2722471 0.1879571

Leave Link 202 at Fri Sep 25 23:36:48 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0

(Enter /home/user/gauss16/g16/l301.exe)

Standard basis: def2TZVP (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 696 symmetry adapted cartesian basis functions of A symmetry.

There are 606 symmetry adapted basis functions of A symmetry.

606 basis functions, 982 primitive gaussians, 696 cartesian basis functions

59 alpha electrons 59 beta electrons

nuclear repulsion energy 1011.2041162238 Hartrees.

IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000

ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000

IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121

HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000

NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D2 Dispersion energy= -0.0154316062 Hartrees.

Nuclear repulsion after empirical dispersion term = 1011.1886846176 Hartrees.

Leave Link 301 at Fri Sep 25 23:36:48 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23235 LenP2D= 51987.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.83D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Fri Sep 25 23:36:49 2026, MaxMem= 805306368 cpu: 6.2 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Fri Sep 25 23:36:49 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 0.000000 -0.000000
Rot= 1.000000 -0.000011 -0.000004 -0.000108 Ang= -0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.985418985273
Leave Link 401 at Fri Sep 25 23:37:00 2026, MaxMem= 805306368 cpu: 65.3 elap: 10.9
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Supporting Information file

Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.408701218145
DIIS: error= 3.00D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.408701218145 IErMin= 1 ErrMin= 3.00D-03
ErrMax= 3.00D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.51D-03 BMatP= 4.51D-03
IDIUse=3 WtCom= 9.70D-01 WtEn= 3.00D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.694 Goal= None Shift= 0.000
GapD= 0.694 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=8.49D-03 MaxDP=2.64D-01 OVMax= 1.49D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 6.51D-03 CP: 1.45D+00
E= -723.411451462420 Delta-E= -0.002750244275 Rises=F Damp=F
DIIS: error= 1.44D-03 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.411451462420 IErMin= 2 ErrMin= 1.44D-03
ErrMax= 1.44D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-04 BMatP= 4.51D-03
IDIUse=3 WtCom= 9.86D-01 WtEn= 1.44D-02
Coeff-Com: -0.710D-02 0.101D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.699D-02 0.101D+01
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=1.20D-02 MaxDP=4.38D-01 DE=-2.75D-03 OVMax= 4.54D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 4.94D-03 CP: 7.31D-01 -1.91D-02
E= -723.411505553634 Delta-E= -0.000054091213 Rises=F Damp=F
DIIS: error= 2.85D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.411505553634 IErMin= 2 ErrMin= 1.44D-03
ErrMax= 2.85D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.87D-04 BMatP= 1.70D-04
IDIUse=3 WtCom= 1.58D-01 WtEn= 8.42D-01
Coeff-Com: -0.353D-01 0.642D+00 0.394D+00
Coeff-En: 0.000D+00 0.293D+00 0.707D+00

Coeff: -0.557D-02 0.348D+00 0.658D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=7.19D+02 MaxDP=3.05D+04 DE=-5.41D-05 OVMax= 9.51D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.411368320127 Delta-E= 0.000137233507 Rises=F Damp=F
DIIS: error= 8.68D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.411368320127 IErMin= 1 ErrMin= 8.68D-04
ErrMax= 8.68D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.91D-04 BMatP= 1.91D-04
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.68D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=5.64D-03 MaxDP=1.86D-01 DE= 1.37D-04 OVMax= 3.29D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 5.62D-03 CP: 1.05D+00
E= -723.411470428416 Delta-E= -0.000102108289 Rises=F Damp=F
DIIS: error= 2.28D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.411470428416 IErMin= 2 ErrMin= 2.28D-04
ErrMax= 2.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.21D-05 BMatP= 1.91D-04
IDIUse=3 WtCom= 9.98D-01 WtEn= 2.28D-03
Coeff-Com: 0.195D+00 0.805D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.195D+00 0.805D+00
Gap= 0.174 Goal= None Shift= 0.000
RMSDP=6.58D-04 MaxDP=2.56D-02 DE=-1.02D-04 OVMax= 2.32D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.28D-04 CP: 1.07D+00 1.09D+00
E= -723.411476018100 Delta-E= -0.000005589684 Rises=F Damp=F
DIIS: error= 2.78D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.411476018100 IErMin= 2 ErrMin= 2.28D-04
ErrMax= 2.78D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-05 BMatP= 3.21D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 2.78D-03
Coeff-Com: -0.101D-01 0.472D+00 0.538D+00
Coeff-En: 0.000D+00 0.457D+00 0.543D+00
Coeff: -0.101D-01 0.472D+00 0.538D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=2.33D-04 MaxDP=8.81D-03 DE=-5.59D-06 OVMax= 1.27D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.49D-05 CP: 1.08D+00 1.12D+00 1.36D+00
E= -723.411501212602 Delta-E= -0.000025194502 Rises=F Damp=F
DIIS: error= 8.21D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -723.411501212602 IErMin= 4 ErrMin= 8.21D-05
ErrMax= 8.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-06 BMatP= 2.56D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.126D-01 0.255D+00 0.325D+00 0.433D+00
Coeff: -0.126D-01 0.255D+00 0.325D+00 0.433D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=3.87D-05 MaxDP=1.62D-03 DE=-2.52D-05 OVMax= 3.04D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 5.42D-06 CP: 1.08D+00 1.13D+00 1.42D+00 1.06D+00
E= -723.411502846281 Delta-E= -0.000001633679 Rises=F Damp=F
DIIS: error= 7.98D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.411502846281 IErMin= 5 ErrMin= 7.98D-06
ErrMax= 7.98D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-08 BMatP= 1.48D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.204D-02-0.677D-01-0.756D-01-0.371D-01 0.118D+01
Coeff: 0.204D-02-0.677D-01-0.756D-01-0.371D-01 0.118D+01
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=5.31D-05 MaxDP=2.27D-03 DE=-1.63D-06 OVMax= 2.83D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 4.84D-06 CP: 1.09D+00 1.13D+00 1.51D+00 1.16D+00 2.52D+00
E= -723.411502950000 Delta-E= -0.000000103719 Rises=F Damp=F
DIIS: error= 5.02D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.411502950000 IErMin= 6 ErrMin= 5.02D-06
ErrMax= 5.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.36D-09 BMatP= 1.83D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.240D-02-0.608D-01-0.723D-01-0.668D-01 0.539D+00 0.658D+00
Coeff: 0.240D-02-0.608D-01-0.723D-01-0.668D-01 0.539D+00 0.658D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=7.41D-06 MaxDP=3.32D-04 DE=-1.04D-07 OVMax= 1.27D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 7.67D-07 CP: 1.09D+00 1.13D+00 1.52D+00 1.18D+00 2.85D+00
CP: 1.20D+00
E= -723.411502974498 Delta-E= -0.000000024498 Rises=F Damp=F
DIIS: error= 3.13D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.411502974498 IErMin= 7 ErrMin= 3.13D-06
ErrMax= 3.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.41D-09 BMatP= 7.36D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.428D-03 0.151D-01 0.167D-01 0.351D-02-0.300D+00 0.912D-01
Coeff-Com: 0.117D+01
Coeff: -0.428D-03 0.151D-01 0.167D-01 0.351D-02-0.300D+00 0.912D-01
Coeff: 0.117D+01
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=2.63D-06 MaxDP=1.25D-04 DE=-2.45D-08 OVMax= 1.14D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.49D-07 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 2.98D+00
CP: 1.30D+00 2.45D+00
E= -723.411502986555 Delta-E= -0.000000012057 Rises=F Damp=F
DIIS: error= 2.23D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.411502986555 IErMin= 8 ErrMin= 2.23D-06
ErrMax= 2.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.26D-10 BMatP= 1.41D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.753D-03 0.216D-01 0.250D-01 0.150D-01-0.289D+00-0.667D-01
Coeff-Com: 0.666D+00 0.629D+00
Coeff: -0.753D-03 0.216D-01 0.250D-01 0.150D-01-0.289D+00-0.667D-01
Coeff: 0.666D+00 0.629D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=9.22D-07 MaxDP=4.00D-05 DE=-1.21D-08 OVMax= 4.75D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.61D-07 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 3.00D+00
CP: 1.30D+00 2.99D+00 1.33D+00
E= -723.411502989221 Delta-E= -0.000000002666 Rises=F Damp=F
DIIS: error= 1.07D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.411502989221 IErMin= 9 ErrMin= 1.07D-06
ErrMax= 1.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-10 BMatP= 6.26D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.160D-03 0.357D-02 0.428D-02 0.386D-02-0.979D-02-0.471D-01
Coeff-Com: -0.169D+00 0.260D+00 0.954D+00
Coeff: -0.160D-03 0.357D-02 0.428D-02 0.386D-02-0.979D-02-0.471D-01
Coeff: -0.169D+00 0.260D+00 0.954D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=4.22D-07 MaxDP=1.51D-05 DE=-2.67D-09 OVMax= 2.71D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 2.24D-07 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 2.98D+00
CP: 1.28D+00 3.00D+00 1.57D+00 2.33D+00
E= -723.411502990268 Delta-E= -0.000000001047 Rises=F Damp=F
DIIS: error= 6.25D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.411502990268 IErMin=10 ErrMin= 6.25D-07
ErrMax= 6.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.84D-11 BMatP= 1.46D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.151D-03-0.493D-02-0.563D-02-0.287D-02 0.869D-01-0.210D-02
Coeff-Com: -0.327D+00-0.442D-01 0.564D+00 0.736D+00
Coeff: 0.151D-03-0.493D-02-0.563D-02-0.287D-02 0.869D-01-0.210D-02
Coeff: -0.327D+00-0.442D-01 0.564D+00 0.736D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=3.58D-07 MaxDP=1.40D-05 DE=-1.05D-09 OVMax= 1.56D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 4.89D-08 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 2.97D+00
CP: 1.26D+00 3.00D+00 1.67D+00 3.00D+00 1.33D+00
E= -723.411502990551 Delta-E= -0.000000000283 Rises=F Damp=F

DIIS: error= 2.95D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.411502990551 IErMin=11 ErrMin= 2.95D-07
ErrMax= 2.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.43D-12 BMatP= 5.84D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.900D-04-0.261D-02-0.303D-02-0.201D-02 0.355D-01 0.110D-01
Coeff-Com: -0.949D-01-0.667D-01 0.213D-01 0.284D+00 0.817D+00
Coeff: 0.900D-04-0.261D-02-0.303D-02-0.201D-02 0.355D-01 0.110D-01
Coeff: -0.949D-01-0.667D-01 0.213D-01 0.284D+00 0.817D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=1.48D-07 MaxDP=7.49D-06 DE=-2.83D-10 OVMax= 6.77D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 3.99D-08 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 2.97D+00
CP: 1.26D+00 3.00D+00 1.65D+00 3.00D+00 1.33D+00
CP: 1.96D+00
E= -723.411502990606 Delta-E= -0.000000000055 Rises=F Damp=F
DIIS: error= 1.38D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.411502990606 IErMin=12 ErrMin= 1.38D-07
ErrMax= 1.38D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.02D-12 BMatP= 9.43D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.950D-06 0.175D-03 0.175D-03-0.225D-03-0.952D-02 0.870D-02
Coeff-Com: 0.586D-01-0.240D-01-0.187D+00-0.985D-01 0.490D+00 0.761D+00
Coeff: 0.950D-06 0.175D-03 0.175D-03-0.225D-03-0.952D-02 0.870D-02
Coeff: 0.586D-01-0.240D-01-0.187D+00-0.985D-01 0.490D+00 0.761D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=5.44D-08 MaxDP=2.80D-06 DE=-5.53D-11 OVMax= 3.86D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.95D-08 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 2.96D+00
CP: 1.26D+00 3.00D+00 1.62D+00 3.00D+00 1.28D+00
CP: 2.56D+00 1.55D+00
E= -723.411502990613 Delta-E= -0.000000000007 Rises=F Damp=F
DIIS: error= 5.55D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.411502990613 IErMin=13 ErrMin= 5.55D-08
ErrMax= 5.55D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.97D-13 BMatP= 4.02D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.190D-04 0.625D-03 0.719D-03 0.332D-03-0.113D-01 0.147D-02
Coeff-Com: 0.415D-01 0.484D-02-0.733D-01-0.994D-01 0.794D-02 0.285D+00
Coeff-Com: 0.841D+00
Coeff: -0.190D-04 0.625D-03 0.719D-03 0.332D-03-0.113D-01 0.147D-02
Coeff: 0.415D-01 0.484D-02-0.733D-01-0.994D-01 0.794D-02 0.285D+00
Coeff: 0.841D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=5.21D-08 MaxDP=2.59D-06 DE=-7.05D-12 OVMax= 1.90D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 6.63D-09 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 2.96D+00
CP: 1.25D+00 3.00D+00 1.60D+00 3.00D+00 1.25D+00

CP: 2.71D+00 1.74D+00 1.83D+00
E= -723.411502990612 Delta-E= 0.000000000001 Rises=F Damp=F
DIIS: error= 2.78D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.411502990613 IErMin=14 ErrMin= 2.78D-08
ErrMax= 2.78D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.12D-14 BMatP= 4.97D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.102D-06-0.304D-04-0.288D-04 0.287D-04 0.151D-02-0.970D-03
Coeff-Com: -0.101D-01 0.396D-02 0.305D-01 0.141D-01-0.798D-01-0.117D+00
Coeff-Com: -0.856D-02 0.117D+01
Coeff: -0.102D-06-0.304D-04-0.288D-04 0.287D-04 0.151D-02-0.970D-03
Coeff: -0.101D-01 0.396D-02 0.305D-01 0.141D-01-0.798D-01-0.117D+00
Coeff: -0.856D-02 0.117D+01
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=2.82D-08 MaxDP=1.53D-06 DE= 1.36D-12 OVMax= 9.21D-07

Cycle 18 Pass 1 IDiag 1:
RMSU= 3.77D-09 CP: 1.09D+00 1.13D+00 1.52D+00 1.17D+00 2.96D+00
CP: 1.25D+00 3.00D+00 1.59D+00 3.00D+00 1.24D+00
CP: 2.72D+00 1.79D+00 2.26D+00 1.89D+00
E= -723.411502990624 Delta-E= -0.000000000012 Rises=F Damp=F
DIIS: error= 9.93D-09 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.411502990624 IErMin=15 ErrMin= 9.93D-09
ErrMax= 9.93D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-14 BMatP= 6.12D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.399D-05-0.146D-03-0.166D-03-0.573D-04 0.306D-02-0.632D-03
Coeff-Com: -0.135D-01 0.900D-03 0.294D-01 0.272D-01-0.374D-01-0.112D+00
Coeff-Com: -0.182D+00 0.523D+00 0.762D+00
Coeff: 0.399D-05-0.146D-03-0.166D-03-0.573D-04 0.306D-02-0.632D-03
Coeff: -0.135D-01 0.900D-03 0.294D-01 0.272D-01-0.374D-01-0.112D+00
Coeff: -0.182D+00 0.523D+00 0.762D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=4.79D-09 MaxDP=3.27D-07 DE=-1.21D-11 OVMax= 3.29D-07

SCF Done: E(RwB97XD) = -723.411502991 A.U. after 18 cycles
NFock= 18 Conv=0.48D-08 -V/T= 2.0046
KE= 7.200913423921D+02 PE=-3.703629841633D+03 EE= 1.248938311633D+03
Leave Link 502 at Fri Sep 25 23:58:40 2026, MaxMem= 805306368 cpu: 7798.8 elap: 1300.3
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23235 LenP2D= 51987.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Fri Sep 25 23:58:41 2026, MaxMem= 805306368 cpu: 3.2 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)

Supporting Information file

L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 25 23:58:41 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 00:10:37 2026, MaxMem= 805306368 cpu: 4298.5 elap: 716.5
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-5.14674698D+00 2.70972827D-03 2.84931861D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000967309	0.002524226	0.000415692
2	6	0.002358305	-0.001713400	-0.000288094
3	6	-0.000978918	-0.002525358	-0.000415130
4	6	-0.002884511	0.000238224	0.000030392
5	6	0.002370663	0.001713132	0.000288669
6	6	0.002959677	0.000767147	-0.000153453
7	6	-0.002904185	-0.000234423	-0.000032371
8	6	-0.002360071	-0.000972019	0.000016042
9	6	0.002983261	-0.000771098	0.000153007
10	6	0.002329460	0.000610000	0.000410070
11	6	-0.002402163	0.000983078	-0.000016695
12	6	0.001325690	-0.004741285	-0.002043859
13	6	0.002360703	-0.000658420	-0.000411864
14	6	0.001279488	0.004633540	0.002057774
15	6	-0.003956885	0.007839254	0.004629599
16	6	-0.004008693	-0.007799629	-0.004642741
17	7	0.000034821	-0.004689577	0.000891057
18	7	0.000160428	0.004762675	-0.000876486
19	1	0.000528395	0.001423018	-0.001939093
20	1	-0.000664655	0.000748305	0.000333377
21	1	0.000527395	-0.001427955	0.001938276
22	1	-0.000662208	-0.000729761	-0.000330277
23	1	-0.000074677	0.000601442	0.000170951
24	1	0.001361787	-0.002033126	-0.002458281

```
    25        1           0.001357088    0.002055638    0.002452325
    26        1          -0.000072888   -0.000603628   -0.000178887
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.007839254 RMS     0.002352371
 Leave Link  716 at Sat Sep 26 00:10:37 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.004394061 RMS     0.001224487
 Search for a local minimum.
 Step number  11 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .12245D-02 SwitMx=.10000D-02 MixMth= 1
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    6    8    9   10   11
 DE= -5.40D-04 DEPred=-3.72D-04 R= 1.45D+00
 TightC=F SS=  1.41D+00  RLast= 1.46D-01 DXNew= 2.4000D+00 4.3794D-01
 Trust test= 1.45D+00 RLast= 1.46D-01 DXMaxT set to 1.43D+00
 ITU=  1  1  1  1  1  1  1  0  0  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.00442   0.00667   0.01099   0.01660   0.01747
    Eigenvalues ---    0.02029   0.02395   0.02714   0.02804   0.03112
    Eigenvalues ---    0.03140   0.03617   0.03784   0.04321   0.04438
    Eigenvalues ---    0.04467   0.04474   0.05026   0.05039   0.06881
    Eigenvalues ---    0.08698   0.09902   0.09960   0.11299   0.11413
    Eigenvalues ---    0.11662   0.11676   0.13737   0.15026   0.15449
    Eigenvalues ---    0.16000   0.16000   0.16000   0.16000   0.16080
    Eigenvalues ---    0.16415   0.22395   0.24473   0.24998   0.25000
    Eigenvalues ---    0.25000   0.25000   0.25000   0.25001   0.25108
    Eigenvalues ---    0.28895   0.32495   0.37230   0.38536   0.40646
    Eigenvalues ---    0.45151   0.45835   0.47245   0.47535   0.47688
    Eigenvalues ---    0.47688   0.47688   0.47755   0.49889   0.54587
    Eigenvalues ---    0.54805   0.55208   0.55400   0.55659   0.55670
    Eigenvalues ---    0.93701   0.94150   0.95021   0.95706   0.97676
    Eigenvalues ---    0.98277   1.36035
 RFO step:  Lambda=-7.47003812D-04 EMin= 4.42345181D-03
 Quartic linear search produced a step of  0.70807.
 Iteration  1 RMS(Cart)=  0.02808449 RMS(Int)=  0.00130614
 Iteration  2 RMS(Cart)=  0.00399819 RMS(Int)=  0.00002468
 Iteration  3 RMS(Cart)=  0.00001077 RMS(Int)=  0.00002390
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00002390
  ITry=  1 IFail=0 DXMaxC=  1.17D-01 DCOld=  1.00D+10 DXMaxT=  1.43D+00 DXLimC=
3.00D+00 Rises=F
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
```

Supporting Information file

		(Linear)	(Quad)	(Total)		
R1	2.33274	-0.00163	0.00018	-0.00126	-0.00108	2.33166
R2	2.52079	0.00124	-0.00035	0.00136	0.00101	2.52179
R3	2.51836	0.00143	-0.00000	0.00202	0.00202	2.52037
R4	2.33274	-0.00163	0.00018	-0.00127	-0.00109	2.33165
R5	2.32894	-0.00149	-0.00005	-0.00149	-0.00153	2.32741
R6	2.51838	0.00143	-0.00000	0.00203	0.00203	2.52041
R7	2.52131	0.00156	0.00029	0.00250	0.00279	2.52411
R8	2.32893	-0.00150	-0.00005	-0.00151	-0.00156	2.32737
R9	2.32556	-0.00098	-0.00065	-0.00166	-0.00231	2.32326
R10	2.52135	0.00157	0.00030	0.00252	0.00282	2.52417
R11	2.61855	0.00137	0.00044	0.00134	0.00178	2.62033
R12	2.32553	-0.00101	-0.00066	-0.00171	-0.00236	2.32317
R13	2.71634	-0.00063	-0.00083	-0.00301	-0.00383	2.71251
R14	2.65652	0.00439	0.00338	0.00959	0.01296	2.66949
R15	2.61865	0.00138	0.00044	0.00139	0.00183	2.62048
R16	2.65632	0.00426	0.00338	0.00905	0.01243	2.66874
R17	2.81196	-0.00187	0.00020	-0.00014	0.00006	2.81201
R18	2.03837	0.00057	0.00127	0.00410	0.00537	2.04374
R19	2.81190	-0.00194	0.00018	-0.00025	-0.00007	2.81183
R20	2.03824	0.00057	0.00125	0.00411	0.00536	2.04360
R21	1.94156	0.00215	-0.00080	0.00201	0.00121	1.94277
R22	1.91522	0.00089	-0.00089	0.00020	-0.00069	1.91454
R23	1.92669	0.00033	-0.00140	-0.00169	-0.00309	1.92360
R24	1.94154	0.00215	-0.00079	0.00203	0.00124	1.94278
R25	1.91524	0.00088	-0.00088	0.00016	-0.00071	1.91453
R26	1.92670	0.00033	-0.00140	-0.00167	-0.00307	1.92363
A1	2.56003	-0.00004	0.00096	0.00195	0.00288	2.56291
A2	2.61046	-0.00025	-0.00110	-0.00198	-0.00310	2.60735
A3	2.56020	-0.00004	0.00100	0.00201	0.00297	2.56316
A4	2.71872	0.00035	0.00120	0.00346	0.00464	2.72336
A5	2.61031	-0.00026	-0.00112	-0.00206	-0.00321	2.60710
A6	2.84057	-0.00019	-0.00280	-0.00440	-0.00720	2.83337
A7	2.71883	0.00035	0.00123	0.00346	0.00467	2.72351
A8	2.84051	-0.00019	-0.00280	-0.00446	-0.00726	2.83325
A9	2.08750	-0.00055	-0.00085	0.00090	0.00004	2.08754
A10	2.10286	0.00034	0.00275	0.00156	0.00426	2.10711
A11	2.09275	0.00021	-0.00172	-0.00270	-0.00447	2.08828
A12	2.08747	-0.00050	-0.00090	0.00120	0.00030	2.08777
A13	2.09283	0.00022	-0.00171	-0.00266	-0.00442	2.08842
A14	2.10280	0.00028	0.00278	0.00122	0.00396	2.10676
A15	2.16508	-0.00374	-0.01374	-0.03623	-0.04998	2.11510
A16	1.95546	0.00096	0.00318	-0.00080	0.00238	1.95783
A17	2.16590	-0.00368	-0.01404	-0.03459	-0.04862	2.11728
A18	1.95557	0.00107	0.00289	0.00118	0.00407	1.95964
A19	1.97361	0.00121	0.00195	0.00644	0.00837	1.98199
A20	1.92404	-0.00015	-0.00521	-0.00622	-0.01145	1.91259
A21	1.92120	0.00049	-0.00112	0.00059	-0.00058	1.92063

A22	1.90836	-0.00075	0.00085	-0.00148	-0.00062	1.90773
A23	1.84128	-0.00013	0.00323	0.00431	0.00750	1.84878
A24	1.89220	-0.00074	0.00069	-0.00358	-0.00293	1.88927
A25	1.97321	0.00122	0.00195	0.00661	0.00855	1.98176
A26	1.92412	-0.00018	-0.00516	-0.00647	-0.01165	1.91247
A27	1.92161	0.00049	-0.00116	0.00061	-0.00060	1.92101
A28	1.90831	-0.00074	0.00084	-0.00151	-0.00067	1.90765
A29	1.84128	-0.00013	0.00321	0.00436	0.00753	1.84881
A30	1.89216	-0.00073	0.00070	-0.00351	-0.00286	1.88930
A31	2.91835	0.00024	0.00077	-0.00200	-0.00121	2.91714
A32	3.11388	0.00042	0.00187	0.00184	0.00374	3.11761
A33	2.91850	0.00024	0.00086	-0.00238	-0.00151	2.91699
A34	3.11367	0.00042	0.00174	0.00240	0.00416	3.11784
A35	4.12054	-0.00278	-0.01057	-0.03703	-0.04760	4.07294
A36	4.12147	-0.00261	-0.01115	-0.03341	-0.04456	4.07691
A37	3.14732	0.00041	-0.00345	0.00394	0.00046	3.14778
A38	3.12624	0.00063	-0.01240	0.00823	-0.00412	3.12212
A39	3.14734	0.00041	-0.00348	0.00396	0.00045	3.14779
A40	3.12629	0.00062	-0.01244	0.00763	-0.00477	3.12152
A41	3.83760	-0.00012	0.02833	0.05512	0.08345	3.92105
A42	3.83400	0.00008	0.02747	0.06178	0.08925	3.92325
D1	0.01056	0.00030	-0.00184	0.00420	0.00236	0.01292
D2	-0.01102	0.00024	-0.00604	0.00054	-0.00550	-0.01652
D3	-0.01588	0.00013	-0.00240	0.00080	-0.00159	-0.01747
D4	0.01058	0.00029	-0.00186	0.00416	0.00230	0.01287
D5	0.00798	0.00004	-0.00050	0.00018	-0.00030	0.00769
D6	-0.01578	0.00013	-0.00245	0.00070	-0.00173	-0.01752
D7	0.01706	-0.00019	0.00075	0.00484	0.00564	0.02270
D8	3.13683	0.00017	0.00164	-0.00941	-0.00777	3.12906
D9	0.00791	0.00003	-0.00050	0.00014	-0.00032	0.00759
D10	0.01712	-0.00019	0.00071	0.00447	0.00524	0.02236
D11	3.13708	0.00017	0.00161	-0.01000	-0.00838	3.12870
D12	-0.00692	-0.00009	0.00780	-0.01030	-0.00245	-0.00937
D13	-3.13508	0.00009	-0.00236	0.00986	0.00752	-3.12756
D14	-3.13494	0.00009	-0.00232	0.01009	0.00779	-3.12715
D15	0.02008	0.00027	-0.01248	0.03025	0.01777	0.03785
D16	2.60725	0.00001	-0.04632	-0.02012	-0.06646	2.54079
D17	-0.54804	-0.00018	-0.03617	-0.04070	-0.07686	-0.62490
D18	-0.54601	-0.00016	-0.03615	-0.03865	-0.07478	-0.62079
D19	2.60913	0.00003	-0.04634	-0.01831	-0.06466	2.54447
D20	-1.68776	0.00101	0.01323	0.03467	0.04793	-1.63983
D21	0.45443	0.00078	0.01184	0.03271	0.04451	0.49894
D22	2.54102	0.00008	0.00868	0.02474	0.03343	2.57445
D23	-1.69255	0.00101	0.01320	0.03473	0.04797	-1.64458
D24	0.44936	0.00078	0.01185	0.03267	0.04448	0.49383
D25	2.53621	0.00007	0.00870	0.02463	0.03333	2.56955

Item	Value	Threshold	Converged?
Maximum Force	0.004394	0.000450	NO

Supporting Information file

RMS Force 0.001224 0.000300 NO
Maximum Displacement 0.117046 0.001800 NO
RMS Displacement 0.028278 0.001200 NO
Predicted change in Energy=-5.426726D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 00:10:37 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.003623	0.663405	0.053468
2	6	0	3.329141	1.693828	0.129071
3	6	0	4.003211	-0.666922	-0.051681
4	6	0	2.132995	2.282078	0.174011
5	6	0	3.328352	-1.697055	-0.127761
6	6	0	0.902384	2.331672	0.171519
7	6	0	2.131829	-2.284514	-0.173496
8	6	0	-0.385535	1.979341	0.136586
9	6	0	0.901213	-2.333468	-0.171796
10	6	0	-1.468657	1.400655	0.078016
11	6	0	-0.386533	-1.980302	-0.137608
12	6	0	-2.674321	0.717047	0.035890
13	6	0	-1.469187	-1.400780	-0.079634
14	6	0	-2.674550	-0.716396	-0.038987
15	6	0	-3.901671	1.413925	0.095036
16	6	0	-3.901665	-1.412804	-0.099143
17	7	0	-3.704551	2.882695	-0.039731
18	7	0	-3.699287	-2.880189	0.041686
19	1	0	-3.063620	3.143220	-0.800166
20	1	0	-4.599873	3.333363	-0.187134
21	1	0	-3.056212	-3.134966	0.802265
22	1	0	-4.592829	-3.333135	0.192830
23	1	0	-3.294609	3.259333	0.812478
24	1	0	-4.769501	1.066899	-0.449104
25	1	0	-4.772091	-1.065335	0.440402
26	1	0	-3.289545	-3.259518	-0.809446

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.233862	0.000000			
3	C	1.334476	2.461744	0.000000		
4	C	2.476667	1.333724	3.499320	0.000000	

5	C	2.461830	3.400596	1.233854	4.165746	0.000000
6	C	3.523455	2.509540	4.319318	1.231613	4.712274
7	C	3.499336	4.165610	2.476593	4.579795	1.333742
8	C	4.582936	3.725639	5.128279	2.536936	5.232468
9	C	4.319368	4.712162	3.523378	4.789586	2.509575
10	C	5.521774	4.807017	5.850900	3.709180	5.713969
11	C	5.128271	5.232263	4.582815	4.961150	3.725680
12	C	6.678182	6.083118	6.820005	5.057537	6.471997
13	C	5.850660	5.713502	5.521455	5.157858	4.806920
14	C	6.819853	6.471609	6.677956	5.669983	6.083125
15	C	7.940949	7.236307	8.175488	6.097304	7.874075
16	C	8.174810	7.873233	7.940130	7.081236	7.235659
17	N	8.021838	7.135455	8.485842	5.872255	8.393068
18	N	8.478916	8.386183	8.014720	7.789867	7.128550
19	H	7.538176	6.620544	8.063343	5.356808	8.045973
20	H	9.011477	8.102920	9.488608	6.824012	9.389642
21	H	8.051682	8.033876	7.527012	7.527745	6.610234
22	H	9.481072	9.382538	9.003353	8.761717	8.094729
23	H	7.783260	6.840461	8.331892	5.551716	8.325469
24	H	8.796766	8.143422	8.951232	7.036291	8.562589
25	H	8.952732	8.563869	8.798113	7.678304	8.144879
26	H	8.326118	8.320063	7.776892	7.815396	6.833926

		6	7	8	9	10
6	C	0.000000				
7	C	4.789545	0.000000			
8	C	1.335699	4.961223	0.000000		
9	C	4.677756	1.231591	4.511224	0.000000	
10	C	2.548994	5.158219	1.229415	4.429713	0.000000
11	C	4.511096	2.536923	3.969126	1.335733	3.556452
12	C	3.926605	5.670298	2.615735	4.704595	1.386622
13	C	4.429292	3.709058	3.556160	2.548960	2.805867
14	C	4.704199	5.057506	3.540821	3.926658	2.439215
15	C	4.891528	7.081926	3.561549	6.097692	2.433110
16	C	6.096987	6.096594	4.891359	4.890863	3.723771
17	N	4.644578	7.796235	3.444272	6.959803	2.685057
18	N	6.953829	5.865411	5.882601	4.637787	4.827282
19	H	4.163168	7.539608	3.066636	6.790350	2.520247
20	H	5.604181	8.767926	4.438335	7.897794	3.689198
21	H	6.778824	5.347069	5.807907	4.153601	4.859704
22	H	7.892266	6.815777	6.776938	5.596139	5.672953
23	H	4.345818	7.820013	3.249295	7.060675	2.707069
24	H	5.844237	7.676997	4.516054	6.617884	3.359289
25	H	6.619035	7.037568	5.348293	5.845453	4.138249
26	H	7.056626	5.544940	6.064149	4.338965	5.081381

		11	12	13	14	15
11	C	0.000000				
12	C	3.541153	0.000000			
13	C	1.229369	2.439443	0.000000		

```
  14  C    2.615762   1.435397   1.386698   0.000000
  15  C    4.891942   1.412631   3.724251   2.462124   0.000000
  16  C    3.560856   2.461885   2.432586   1.412238   2.833391
  17  N    5.887917   2.399401   4.831832   3.743575   1.488053
  18  N    3.437482   3.740414   2.678939   2.395537   4.299212
  19  H    5.818612   2.595545   4.869220   3.953150   2.119947
  20  H    6.781572   3.256163   5.676694   4.486575   2.061879
  21  H    3.056763   3.946033   2.510736   2.588987   4.680533
  22  H    4.430832   4.484337   3.683119   3.252823   4.798109
  23  H    6.067401   2.729664   5.083766   4.112893   2.070936
  24  H    5.347231   2.178852   4.137392   2.781574   1.081502
  25  H    4.517121   2.782293   3.360376   2.179736   2.650216
  26  H    3.242721   4.111710   2.702080   2.727507   4.799360
                16         17         18         19         20
  16  C    0.000000
  17  N    4.300430   0.000000
  18  N    1.487955   5.763462   0.000000
  19  H    4.685201   1.028070   6.115083   0.000000
  20  H    4.798056   1.013129   6.282646   1.664943   0.000000
  21  H    2.119710   6.110773   1.028075   6.479464   6.723175
  22  H    2.061704   6.283285   1.013125   6.728127   6.677321
  23  H    4.798796   1.017924   6.200937   1.633235   1.645727
  24  H    2.650384   2.144486   4.118949   2.710053   2.287851
  25  H    1.081426   4.117902   2.145595   4.708483   4.446572
  26  H    2.071128   6.204149   1.017941   6.406728   6.750578
                21         22         23         24         25
  21  H    0.000000
  22  H    1.664895   0.000000
  23  H    6.398750   6.747591   0.000000
  24  H    4.707117   4.450122   2.928082   0.000000
  25  H    2.712666   2.288305   4.585210   2.310335   0.000000
  26  H    1.633270   1.645759   6.717595   4.586719   2.928224
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=2 Diff= 3.78D-03
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.511896   -0.668942   -0.029604
    2          6           0        3.836556   -1.700808   -0.069409
```

3	6	0	4.512588	0.664240	0.029146
4	6	0	2.639923	-2.289264	-0.094075
5	6	0	3.838586	1.696963	0.069165
6	6	0	1.409270	-2.337710	-0.090105
7	6	0	2.642551	2.286660	0.094169
8	6	0	0.121643	-1.983298	-0.067725
9	6	0	1.411977	2.336556	0.090516
10	6	0	-0.961000	-1.402015	-0.029566
11	6	0	0.123940	1.983493	0.068390
12	6	0	-2.166094	-0.716345	-0.011518
13	6	0	-0.959193	1.403210	0.030416
14	6	0	-2.165126	0.718835	0.013388
15	6	0	-3.394022	-1.413833	-0.046604
16	6	0	-3.391664	1.417944	0.049003
17	7	0	-3.198166	-2.877182	0.139277
18	7	0	-3.188022	2.879364	-0.142808
19	1	0	-2.557586	-3.111599	0.908454
20	1	0	-4.093893	-3.321692	0.302106
21	1	0	-2.544601	3.106957	-0.911669
22	1	0	-4.081155	3.327519	-0.309816
23	1	0	-2.788394	-3.283617	-0.699214
24	1	0	-4.261653	-1.047337	0.484943
25	1	0	-4.262289	1.052623	-0.478288
26	1	0	-2.778107	3.287763	0.694679

Rotational constants (GHZ): 0.6008385 0.2725131 0.1881194

Leave Link 202 at Sat Sep 26 00:10:37 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0

(Enter /home/user/gauss16/g16/l301.exe)

Standard basis: def2TZVP (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 696 symmetry adapted cartesian basis functions of A symmetry.

There are 606 symmetry adapted basis functions of A symmetry.

606 basis functions, 982 primitive gaussians, 696 cartesian basis functions

59 alpha electrons 59 beta electrons

nuclear repulsion energy 1011.3556550912 Hartrees.

IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000

ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000

IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121

HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000

NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D2 Dispersion energy= -0.0154258128 Hartrees.

Nuclear repulsion after empirical dispersion term = 1011.3402292783 Hartrees.
Leave Link 301 at Sat Sep 26 00:10:38 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23240 LenP2D= 52000.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.83D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 00:10:38 2026, MaxMem= 805306368 cpu: 5.2 elap: 0.9
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 00:10:39 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000167 0.000012 0.000417 Ang= 0.05 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.982848579443
Leave Link 401 at Sat Sep 26 00:10:48 2026, MaxMem= 805306368 cpu: 53.7 elap: 9.0
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666

Supporting Information file

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.409897917342
DIIS: error= 1.18D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.409897917342 IErMin= 1 ErrMin= 1.18D-03
ErrMax= 1.18D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-03 BMatP= 2.27D-03
IDIUse=3 WtCom= 9.88D-01 WtEn= 1.18D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.698 Goal= None Shift= 0.000
GapD= 0.698 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=8.49D-03 MaxDP=2.67D-01 OVMax= 1.43D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 6.47D-03 CP: 1.44D+00
E= -723.412138905439 Delta-E= -0.002240988097 Rises=F Damp=F
DIIS: error= 8.81D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.412138905439 IErMin= 2 ErrMin= 8.81D-04
ErrMax= 8.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-04 BMatP= 2.27D-03
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.81D-03
Coeff-Com: -0.175D-01 0.102D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.174D-01 0.102D+01
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=9.58D-03 MaxDP=3.36D-01 DE=-2.24D-03 OVMax= 3.99D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 3.79D-03 CP: 8.86D-01 1.62D-01
E= -723.412229744586 Delta-E= -0.000090839147 Rises=F Damp=F
DIIS: error= 3.60D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.412229744586 IErMin= 2 ErrMin= 8.81D-04
ErrMax= 3.60D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.60D-04 BMatP= 1.45D-04
IDIUse=3 WtCom= 1.43D-01 WtEn= 8.57D-01
Coeff-Com: -0.521D-01 0.758D+00 0.295D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.744D-02 0.108D+00 0.899D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=7.91D+02 MaxDP=3.34D+04 DE=-9.08D-05 OVMax= 9.35D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.412037109573 Delta-E= 0.000192635013 Rises=F Damp=F
DIIS: error= 8.75D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.412037109573 IErMin= 1 ErrMin= 8.75D-04
ErrMax= 8.75D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-04 BMatP= 1.83D-04
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.75D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=3.54D-03 MaxDP=1.17D-01 DE= 1.93D-04 OVMax= 5.96D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.33D-03 CP: 8.97D-01
E= -723.412122664706 Delta-E= -0.000085555133 Rises=F Damp=F
DIIS: error= 3.91D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.412122664706 IErMin= 2 ErrMin= 3.91D-04
ErrMax= 3.91D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.48D-05 BMatP= 1.83D-04
IDIUse=3 WtCom= 9.96D-01 WtEn= 3.91D-03
Coeff-Com: 0.199D+00 0.801D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.199D+00 0.801D+00
Gap= 0.175 Goal= None Shift= 0.000
RMSDP=3.10D-04 MaxDP=1.07D-02 DE=-8.56D-05 OVMax= 4.63D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.20D-04 CP: 9.08D-01 1.05D+00
E= -723.412104635669 Delta-E= 0.000018029036 Rises=F Damp=F
DIIS: error= 4.20D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.412122664706 IErMin= 2 ErrMin= 3.91D-04
ErrMax= 4.20D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.08D-05 BMatP= 3.48D-05
IDIUse=3 WtCom= 3.28D-01 WtEn= 6.72D-01
Coeff-Com: -0.122D-01 0.552D+00 0.460D+00
Coeff-En: 0.000D+00 0.571D+00 0.429D+00
Coeff: -0.399D-02 0.565D+00 0.439D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=9.21D-05 MaxDP=3.24D-03 DE= 1.80D-05 OVMax= 3.25D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.21D-05 CP: 9.11D-01 1.07D+00 1.28D+00
E= -723.412166304707 Delta-E= -0.000061669038 Rises=F Damp=F

DIIS: error= 3.33D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.412166304707 IErMin= 4 ErrMin= 3.33D-05
ErrMax= 3.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.55D-07 BMatP= 3.48D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.121D-01 0.258D+00 0.208D+00 0.546D+00
Coeff: -0.121D-01 0.258D+00 0.208D+00 0.546D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=3.50D-05 MaxDP=1.31D-03 DE=-6.17D-05 OVMax= 5.19D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 6.52D-06 CP: 9.13D-01 1.07D+00 1.39D+00 1.18D+00
E= -723.412167374517 Delta-E= -0.000001069810 Rises=F Damp=F
DIIS: error= 2.20D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.412167374517 IErMin= 5 ErrMin= 2.20D-05
ErrMax= 2.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.24D-08 BMatP= 7.55D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.464D-02-0.149D+00-0.121D+00-0.862D-01 0.135D+01
Coeff: 0.464D-02-0.149D+00-0.121D+00-0.862D-01 0.135D+01
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=5.21D-05 MaxDP=2.07D-03 DE=-1.07D-06 OVMax= 8.70D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.84D-06 CP: 9.15D-01 1.08D+00 1.55D+00 1.40D+00 2.88D+00
E= -723.412167972763 Delta-E= -0.000000598247 Rises=F Damp=F
DIIS: error= 1.59D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.412167972763 IErMin= 6 ErrMin= 1.59D-05
ErrMax= 1.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-08 BMatP= 6.24D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.411D-02-0.108D+00-0.869D-01-0.139D+00 0.571D+00 0.758D+00
Coeff: 0.411D-02-0.108D+00-0.869D-01-0.139D+00 0.571D+00 0.758D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.30D-05 MaxDP=5.32D-04 DE=-5.98D-07 OVMax= 3.79D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 3.58D-06 CP: 9.16D-01 1.08D+00 1.59D+00 1.45D+00 3.00D+00
CP: 1.37D+00
E= -723.412168117276 Delta-E= -0.000000144513 Rises=F Damp=F
DIIS: error= 9.61D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.412168117276 IErMin= 7 ErrMin= 9.61D-06
ErrMax= 9.61D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.44D-09 BMatP= 2.26D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.818D-04 0.914D-02 0.824D-02-0.450D-01-0.288D+00 0.389D+00
Coeff-Com: 0.927D+00
Coeff: 0.818D-04 0.914D-02 0.824D-02-0.450D-01-0.288D+00 0.389D+00
Coeff: 0.927D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=5.80D-06 MaxDP=2.48D-04 DE=-1.45D-07 OVMax= 3.29D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.14D-06 CP: 9.16D-01 1.08D+00 1.60D+00 1.47D+00 3.00D+00
CP: 1.67D+00 1.83D+00
E= -723.412168184940 Delta-E= -0.000000067664 Rises=F Damp=F
DIIS: error= 4.86D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.412168184940 IErMin= 8 ErrMin= 4.86D-06
ErrMax= 4.86D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.53D-09 BMatP= 9.44D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.128D-02 0.402D-01 0.328D-01 0.118D-01-0.338D+00-0.542D-02
Coeff-Com: 0.484D+00 0.776D+00
Coeff: -0.128D-02 0.402D-01 0.328D-01 0.118D-01-0.338D+00-0.542D-02
Coeff: 0.484D+00 0.776D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.84D-06 MaxDP=6.16D-05 DE=-6.77D-08 OVMax= 1.44D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.41D-07 CP: 9.16D-01 1.08D+00 1.60D+00 1.46D+00 3.00D+00
CP: 1.77D+00 2.12D+00 1.79D+00
E= -723.412168199264 Delta-E= -0.000000014323 Rises=F Damp=F
DIIS: error= 1.62D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.412168199264 IErMin= 9 ErrMin= 1.62D-06
ErrMax= 1.62D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.01D-10 BMatP= 2.53D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.569D-03 0.154D-01 0.124D-01 0.124D-01-0.698D-01-0.805D-01
Coeff-Com: -0.588D-02 0.330D+00 0.787D+00
Coeff: -0.569D-03 0.154D-01 0.124D-01 0.124D-01-0.698D-01-0.805D-01
Coeff: -0.588D-02 0.330D+00 0.787D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=7.33D-07 MaxDP=2.91D-05 DE=-1.43D-08 OVMax= 4.56D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 2.03D-07 CP: 9.16D-01 1.08D+00 1.60D+00 1.46D+00 3.00D+00
CP: 1.74D+00 2.09D+00 2.10D+00 1.79D+00
E= -723.412168201451 Delta-E= -0.000000002187 Rises=F Damp=F
DIIS: error= 1.34D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.412168201451 IErMin=10 ErrMin= 1.34D-06
ErrMax= 1.34D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.22D-10 BMatP= 5.01D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.121D-03-0.481D-02-0.388D-02-0.356D-03 0.635D-01-0.286D-01
Coeff-Com: -0.138D+00-0.854D-01 0.331D+00 0.867D+00
Coeff: 0.121D-03-0.481D-02-0.388D-02-0.356D-03 0.635D-01-0.286D-01
Coeff: -0.138D+00-0.854D-01 0.331D+00 0.867D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=4.52D-07 MaxDP=1.99D-05 DE=-2.19D-09 OVMax= 2.74D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 1.24D-07 CP: 9.16D-01 1.08D+00 1.60D+00 1.46D+00 3.00D+00
CP: 1.71D+00 2.03D+00 2.21D+00 2.26D+00 1.89D+00

E= -723.412168202096 Delta-E= -0.000000000645 Rises=F Damp=F
DIIS: error= 3.82D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.412168202096 IErMin=11 ErrMin= 3.82D-07
ErrMax= 3.82D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.42D-11 BMatP= 1.22D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.174D-03-0.550D-02-0.439D-02-0.298D-02 0.456D-01-0.982D-03
Coeff-Com: -0.728D-01-0.106D+00 0.289D-01 0.456D+00 0.662D+00
Coeff: 0.174D-03-0.550D-02-0.439D-02-0.298D-02 0.456D-01-0.982D-03
Coeff: -0.728D-01-0.106D+00 0.289D-01 0.456D+00 0.662D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.75D-07 MaxDP=8.04D-06 DE=-6.45D-10 OVMax= 1.02D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 4.18D-08 CP: 9.16D-01 1.08D+00 1.60D+00 1.46D+00 3.00D+00
CP: 1.69D+00 2.01D+00 2.21D+00 2.40D+00 2.32D+00
CP: 1.47D+00
E= -723.412168202212 Delta-E= -0.000000000116 Rises=F Damp=F
DIIS: error= 2.33D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.412168202212 IErMin=12 ErrMin= 2.33D-07
ErrMax= 2.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.49D-12 BMatP= 3.42D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.297D-04-0.731D-03-0.561D-03-0.748D-03 0.175D-02 0.631D-02
Coeff-Com: 0.738D-02-0.146D-01-0.609D-01-0.612D-01 0.204D+00 0.919D+00
Coeff: 0.297D-04-0.731D-03-0.561D-03-0.748D-03 0.175D-02 0.631D-02
Coeff: 0.738D-02-0.146D-01-0.609D-01-0.612D-01 0.204D+00 0.919D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=2.58D-07 MaxDP=1.26D-05 DE=-1.16D-10 OVMax= 3.71D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 3.35D-08 CP: 9.16D-01 1.08D+00 1.59D+00 1.46D+00 3.00D+00
CP: 1.68D+00 1.99D+00 2.18D+00 2.48D+00 2.59D+00
CP: 1.80D+00 1.88D+00
E= -723.412168202225 Delta-E= -0.000000000014 Rises=F Damp=F
DIIS: error= 5.02D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.412168202225 IErMin=13 ErrMin= 5.02D-08
ErrMax= 5.02D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.78D-12 BMatP= 4.49D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.241D-04 0.883D-03 0.720D-03 0.309D-03-0.993D-02 0.354D-02
Coeff-Com: 0.213D-01 0.164D-01-0.405D-01-0.146D+00-0.403D-01 0.522D+00
Coeff-Com: 0.671D+00
Coeff: -0.241D-04 0.883D-03 0.720D-03 0.309D-03-0.993D-02 0.354D-02
Coeff: 0.213D-01 0.164D-01-0.405D-01-0.146D+00-0.403D-01 0.522D+00
Coeff: 0.671D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.12D-07 MaxDP=5.37D-06 DE=-1.36D-11 OVMax= 1.56D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 5.29D-09 CP: 9.16D-01 1.08D+00 1.59D+00 1.46D+00 3.00D+00

```
              CP:  1.68D+00  1.98D+00  2.18D+00  2.51D+00  2.68D+00
              CP:  1.95D+00  2.31D+00  1.44D+00
E= -723.412168202234     Delta-E=       -0.000000000008 Rises=F Damp=F
DIIS: error= 2.95D-08 at cycle  14 NSaved=  14.
NSaved=14 IEnMin=14 EnMin= -723.412168202234     IErMin=14 ErrMin= 2.95D-08
ErrMax= 2.95D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-13 BMatP= 1.78D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.760D-05 0.236D-03 0.190D-03 0.168D-03-0.198D-02-0.187D-03
Coeff-Com:  0.283D-02 0.462D-02 0.130D-02-0.199D-01-0.345D-01-0.934D-02
Coeff-Com:  0.119D+00 0.937D+00
Coeff:     -0.760D-05 0.236D-03 0.190D-03 0.168D-03-0.198D-02-0.187D-03
Coeff:      0.283D-02 0.462D-02 0.130D-02-0.199D-01-0.345D-01-0.934D-02
Coeff:      0.119D+00 0.937D+00
Gap=     0.176 Goal=   None    Shift=    0.000
RMSDP=3.74D-08 MaxDP=1.79D-06 DE=-8.41D-12 OVMax= 4.79D-07

Cycle  18  Pass 1  IDiag  1:
RMSU=  3.96D-09    CP:  9.16D-01  1.08D+00  1.59D+00  1.46D+00  3.00D+00
              CP:  1.68D+00  1.97D+00  2.18D+00  2.52D+00  2.70D+00
              CP:  1.97D+00  2.43D+00  1.60D+00  1.68D+00
E= -723.412168202227     Delta-E=        0.000000000007 Rises=F Damp=F
DIIS: error= 1.36D-08 at cycle  15 NSaved=  15.
NSaved=15 IEnMin=14 EnMin= -723.412168202234     IErMin=15 ErrMin= 1.36D-08
ErrMax= 1.36D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 5.17D-14 BMatP= 1.05D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.248D-05-0.114D-03-0.940D-04 0.216D-04 0.168D-02-0.106D-02
Coeff-Com: -0.418D-02-0.191D-02 0.120D-01 0.276D-01-0.874D-02-0.143D+00
Coeff-Com: -0.111D+00 0.506D+00 0.723D+00
Coeff:      0.248D-05-0.114D-03-0.940D-04 0.216D-04 0.168D-02-0.106D-02
Coeff:     -0.418D-02-0.191D-02 0.120D-01 0.276D-01-0.874D-02-0.143D+00
Coeff:     -0.111D+00 0.506D+00 0.723D+00
Gap=     0.176 Goal=   None    Shift=    0.000
RMSDP=1.64D-08 MaxDP=8.01D-07 DE= 6.82D-12 OVMax= 2.52D-07

Cycle  19  Pass 1  IDiag  1:
RMSU=  1.13D-09    CP:  9.16D-01  1.08D+00  1.59D+00  1.46D+00  3.00D+00
              CP:  1.67D+00  1.97D+00  2.18D+00  2.52D+00  2.71D+00
              CP:  1.97D+00  2.45D+00  1.66D+00  2.09D+00  1.43D+00
E= -723.412168202225     Delta-E=        0.000000000002 Rises=F Damp=F
DIIS: error= 6.53D-09 at cycle  16 NSaved=  16.
NSaved=16 IEnMin=14 EnMin= -723.412168202234     IErMin=16 ErrMin= 6.53D-09
ErrMax= 6.53D-09  0.00D+00 EMaxC= 1.00D-01 BMatC= 6.30D-15 BMatP= 5.17D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.221D-05-0.826D-04-0.667D-04-0.265D-04 0.945D-03-0.380D-03
Coeff-Com: -0.200D-02-0.157D-02 0.435D-02 0.137D-01 0.344D-02-0.532D-01
Coeff-Com: -0.626D-01 0.175D-01 0.267D+00 0.812D+00
Coeff:      0.221D-05-0.826D-04-0.667D-04-0.265D-04 0.945D-03-0.380D-03
Coeff:     -0.200D-02-0.157D-02 0.435D-02 0.137D-01 0.344D-02-0.532D-01
```

Supporting Information file

Coeff: -0.626D-01 0.175D-01 0.267D+00 0.812D+00
Gap= 0.176 Goal= None Shift= 0.000
RMSDP=1.71D-09 MaxDP=6.49D-08 DE= 2.05D-12 OVMax= 1.17D-07

SCF Done: E(RwB97XD) = -723.412168202 A.U. after 19 cycles
NFock= 19 Conv=0.17D-08 -V/T= 2.0046
KE= 7.200933905794D+02 PE=-3.703880163984D+03 EE= 1.249034375924D+03
Leave Link 502 at Sat Sep 26 00:36:57 2026, MaxMem= 805306368 cpu: 9416.6 elap: 1569.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23240 LenP2D= 52000.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 00:36:58 2026, MaxMem= 805306368 cpu: 3.1 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 00:36:58 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 00:50:13 2026, MaxMem= 805306368 cpu: 4769.0 elap: 794.9
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.90194253D+00-1.64208321D-03-6.08474955D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000976279	0.003040961	0.000446924
2	6	0.002161761	-0.002172750	-0.000363843
3	6	-0.001003462	-0.003028610	-0.000449015
4	6	-0.002738378	0.000718650	0.000118327
5	6	0.002177523	0.002147083	0.000366833

6	6	0.002713681	0.000040357	-0.000309970
7	6	-0.002733109	-0.000693015	-0.000125108
8	6	-0.001074907	-0.000128908	-0.000039025
9	6	0.002700885	-0.000070924	0.000327848
10	6	0.000693553	0.000155824	0.000859310
11	6	-0.001010409	0.000152308	0.000055410
12	6	0.000899926	-0.004891375	-0.000165021
13	6	0.000726574	-0.000023835	-0.000881671
14	6	0.000766592	0.005543352	0.000139208
15	6	-0.000400768	0.003810008	0.003021601
16	6	0.000061954	-0.004187257	-0.003028987
17	7	-0.002477879	-0.003649773	-0.000203484
18	7	-0.003165877	0.003291473	0.000130257
19	1	0.000718763	0.001058559	-0.001485867
20	1	-0.000855163	0.001566720	0.000265034
21	1	0.000730356	-0.000996670	0.001469872
22	1	-0.000866837	-0.001661540	-0.000271628
23	1	0.000618051	0.000773609	0.000471768
24	1	0.000823826	-0.000292136	-0.001669366
25	1	0.000886732	0.000273166	0.001765362
26	1	0.000622888	-0.000775276	-0.000444767

Cartesian Forces: Max 0.005543352 RMS 0.001778480
Leave Link 716 at Sat Sep 26 00:50:13 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.004440372 RMS 0.001184744
Search for a local minimum.
Step number 12 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .11847D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 9 10 11 12
DE= -6.65D-04 DEPred=-5.43D-04 R= 1.23D+00
TightC=F SS= 1.41D+00 RLast= 2.39D-01 DXNew= 2.4000D+00 7.1603D-01
Trust test= 1.23D+00 RLast= 2.39D-01 DXMaxT set to 1.43D+00
ITU= 1 1 1 1 1 1 1 1 0 0 1 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.00444 0.00704 0.01118 0.01662 0.01747
Eigenvalues --- 0.01951 0.02391 0.02706 0.02802 0.03119
Eigenvalues --- 0.03136 0.03613 0.03781 0.04301 0.04438
Eigenvalues --- 0.04455 0.04467 0.05026 0.05107 0.07028
Eigenvalues --- 0.08744 0.09625 0.09957 0.10623 0.11396

```
    Eigenvalues ---    0.11561   0.11710   0.12990   0.15106   0.15394
    Eigenvalues ---    0.16000   0.16000   0.16000   0.16002   0.16117
    Eigenvalues ---    0.16527   0.23876   0.24512   0.24994   0.24999
    Eigenvalues ---    0.24999   0.25000   0.25000   0.25013   0.25075
    Eigenvalues ---    0.29002   0.33336   0.37230   0.38162   0.40670
    Eigenvalues ---    0.45121   0.45835   0.47214   0.47667   0.47688
    Eigenvalues ---    0.47688   0.47690   0.47746   0.50126   0.54808
    Eigenvalues ---    0.55092   0.55341   0.55659   0.55668   0.62363
    Eigenvalues ---    0.93710   0.94746   0.95021   0.95904   0.97679
    Eigenvalues ---    0.99360   1.36045
 RFO step:  Lambda=-4.32550530D-04 EMin= 4.44266945D-03
 Quartic linear search produced a step of  0.29910.
 Iteration  1 RMS(Cart)=  0.02099730 RMS(Int)=  0.00043211
 Iteration  2 RMS(Cart)=  0.00128063 RMS(Int)=  0.00001643
 Iteration  3 RMS(Cart)=  0.00000113 RMS(Int)=  0.00001642
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00001642
  ITry=  1 IFail=0 DXMaxC= 7.62D-02 DCOld= 1.00D+10 DXMaxT= 1.43D+00 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)  (Quad)   (Total)
    R1        2.33166  -0.00192  -0.00032  -0.00169  -0.00202   2.32965
    R2        2.52179   0.00142   0.00030   0.00223   0.00253   2.52432
    R3        2.52037   0.00130   0.00060   0.00224   0.00284   2.52322
    R4        2.33165  -0.00191  -0.00033  -0.00168  -0.00201   2.32964
    R5        2.32741  -0.00157  -0.00046  -0.00166  -0.00212   2.32529
    R6        2.52041   0.00130   0.00061   0.00224   0.00285   2.52326
    R7        2.52411   0.00116   0.00084   0.00216   0.00300   2.52710
    R8        2.32737  -0.00155  -0.00047  -0.00164  -0.00211   2.32526
    R9        2.32326   0.00009  -0.00069  -0.00088  -0.00157   2.32169
   R10        2.52417   0.00117   0.00084   0.00218   0.00302   2.52719
   R11        2.62033   0.00080   0.00053   0.00121   0.00175   2.62208
   R12        2.32317   0.00015  -0.00071  -0.00081  -0.00152   2.32165
   R13        2.71251  -0.00134  -0.00115  -0.00479  -0.00594   2.70657
   R14        2.66949   0.00300   0.00388   0.00465   0.00853   2.67801
   R15        2.62048   0.00082   0.00055   0.00125   0.00180   2.62228
   R16        2.66874   0.00352   0.00372   0.00614   0.00985   2.67860
   R17        2.81201  -0.00043   0.00002  -0.00313  -0.00312   2.80890
   R18        2.04374   0.00027   0.00161   0.00166   0.00327   2.04701
   R19        2.81183  -0.00014  -0.00002  -0.00291  -0.00293   2.80890
   R20        2.04360   0.00025   0.00160   0.00159   0.00319   2.04679
   R21        1.94277   0.00181   0.00036   0.00150   0.00186   1.94463
   R22        1.91454   0.00141  -0.00021   0.00095   0.00074   1.91528
   R23        1.92360   0.00093  -0.00093   0.00005  -0.00088   1.92272
   R24        1.94278   0.00179   0.00037   0.00145   0.00182   1.94460
   R25        1.91453   0.00147  -0.00021   0.00109   0.00087   1.91540
   R26        1.92363   0.00091  -0.00092   0.00000  -0.00092   1.92271
    A1        2.56291  -0.00019   0.00086   0.00049   0.00134   2.56425
    A2        2.60735  -0.00002  -0.00093  -0.00072  -0.00166   2.60569
```

A3	2.56316	-0.00017	0.00089	0.00063	0.00151	2.56467
A4	2.72336	0.00006	0.00139	0.00124	0.00262	2.72599
A5	2.60710	-0.00003	-0.00096	-0.00073	-0.00170	2.60540
A6	2.83337	0.00032	-0.00215	-0.00122	-0.00338	2.82999
A7	2.72351	0.00009	0.00140	0.00144	0.00283	2.72634
A8	2.83325	0.00033	-0.00217	-0.00115	-0.00332	2.82992
A9	2.08754	-0.00016	0.00001	0.00138	0.00134	2.08888
A10	2.10711	0.00013	0.00127	-0.00041	0.00081	2.10792
A11	2.08828	0.00003	-0.00134	-0.00051	-0.00190	2.08637
A12	2.08777	-0.00040	0.00009	0.00021	0.00025	2.08802
A13	2.08842	0.00004	-0.00132	-0.00047	-0.00184	2.08658
A14	2.10676	0.00036	0.00118	0.00068	0.00182	2.10858
A15	2.11510	-0.00164	-0.01495	-0.01302	-0.02797	2.08713
A16	1.95783	-0.00188	0.00071	-0.00190	-0.00119	1.95665
A17	2.11728	-0.00210	-0.01454	-0.01927	-0.03382	2.08346
A18	1.95964	-0.00234	0.00122	-0.00824	-0.00702	1.95262
A19	1.98199	0.00051	0.00250	0.00553	0.00802	1.99001
A20	1.91259	0.00109	-0.00343	-0.00095	-0.00438	1.90821
A21	1.92063	0.00031	-0.00017	-0.00025	-0.00045	1.92018
A22	1.90773	-0.00072	-0.00019	-0.00240	-0.00258	1.90515
A23	1.84878	-0.00052	0.00224	0.00037	0.00259	1.85138
A24	1.88927	-0.00080	-0.00088	-0.00263	-0.00353	1.88573
A25	1.98176	0.00042	0.00256	0.00489	0.00743	1.98919
A26	1.91247	0.00121	-0.00349	0.00003	-0.00346	1.90900
A27	1.92101	0.00031	-0.00018	-0.00034	-0.00054	1.92047
A28	1.90765	-0.00072	-0.00020	-0.00230	-0.00250	1.90515
A29	1.84881	-0.00052	0.00225	0.00019	0.00242	1.85123
A30	1.88930	-0.00083	-0.00086	-0.00283	-0.00370	1.88560
A31	2.91714	0.00002	-0.00036	-0.00210	-0.00246	2.91468
A32	3.11761	0.00007	0.00112	0.00173	0.00285	3.12046
A33	2.91699	0.00007	-0.00045	-0.00068	-0.00113	2.91586
A34	3.11784	0.00003	0.00125	-0.00025	0.00099	3.11883
A35	4.07294	-0.00352	-0.01424	-0.01492	-0.02916	4.04378
A36	4.07691	-0.00444	-0.01333	-0.02751	-0.04084	4.03607
A37	3.14778	0.00051	0.00014	-0.00135	-0.00122	3.14656
A38	3.12212	0.00100	-0.00123	0.00492	0.00368	3.12580
A39	3.14779	0.00050	0.00014	-0.00140	-0.00128	3.14651
A40	3.12152	0.00106	-0.00143	0.00843	0.00700	3.12852
A41	3.92105	-0.00154	0.02496	0.02836	0.05332	3.97437
A42	3.92325	-0.00270	0.02669	0.00145	0.02815	3.95139
D1	0.01292	0.00043	0.00070	0.00272	0.00341	0.01633
D2	-0.01652	0.00043	-0.00165	0.00053	-0.00113	-0.01765
D3	-0.01747	0.00016	-0.00047	0.00089	0.00041	-0.01705
D4	0.01287	0.00044	0.00069	0.00292	0.00360	0.01647
D5	0.00769	0.00000	-0.00009	0.00020	0.00011	0.00780
D6	-0.01752	0.00017	-0.00052	0.00130	0.00078	-0.01673
D7	0.02270	-0.00051	0.00169	-0.02142	-0.01973	0.00297
D8	3.12906	0.00034	-0.00232	0.00335	0.00105	3.13010

D9	0.00759	0.00002	-0.00010	0.00051	0.00041	0.00800
D10	0.02236	-0.00051	0.00157	-0.01919	-0.01763	0.00473
D11	3.12870	0.00035	-0.00251	0.00639	0.00391	3.13261
D12	-0.00937	0.00000	-0.00073	0.01843	0.01770	0.00832
D13	-3.12756	0.00001	0.00225	-0.00203	0.00023	-3.12733
D14	-3.12715	-0.00003	0.00233	-0.00380	-0.00147	-3.12861
D15	0.03785	-0.00002	0.00531	-0.02426	-0.01893	0.01892
D16	2.54079	0.00054	-0.01988	-0.00904	-0.02891	2.51188
D17	-0.62490	0.00056	-0.02299	0.01347	-0.00952	-0.63442
D18	-0.62079	0.00043	-0.02237	0.00512	-0.01725	-0.63804
D19	2.54447	0.00045	-0.01934	-0.01556	-0.03490	2.50956
D20	-1.63983	0.00062	0.01433	0.02430	0.03865	-1.60118
D21	0.49894	0.00085	0.01331	0.02435	0.03764	0.53658
D22	2.57445	0.00073	0.01000	0.02039	0.03038	2.60483
D23	-1.64458	0.00060	0.01435	0.02417	0.03854	-1.60604
D24	0.49383	0.00086	0.01330	0.02463	0.03791	0.53174
D25	2.56955	0.00078	0.00997	0.02097	0.03094	2.60049

Item	Value	Threshold	Converged?
Maximum Force	0.004440	0.000450	NO
RMS Force	0.001185	0.000300	NO
Maximum Displacement	0.076240	0.001800	NO
RMS Displacement	0.020697	0.001200	NO

Predicted change in Energy=-2.816262D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 00:50:13 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.003644	0.673275	0.051371
2	6	0	3.329862	1.702904	0.126642
3	6	0	4.004871	-0.658462	-0.052898
4	6	0	2.131467	2.289775	0.174245
5	6	0	3.333431	-1.689695	-0.127072
6	6	0	0.902017	2.340302	0.176351
7	6	0	2.136176	-2.279087	-0.172794
8	6	0	-0.386634	1.984138	0.147104
9	6	0	0.906867	-2.332610	-0.173202
10	6	0	-1.466306	1.400193	0.094776
11	6	0	-0.382627	-1.979468	-0.142397
12	6	0	-2.671415	0.713602	0.054900
13	6	0	-1.464276	-1.399340	-0.088927
14	6	0	-2.670737	-0.715234	-0.043994

15	6	0	-3.904596	1.409124	0.116609
16	6	0	-3.903422	-1.412578	-0.102069
17	7	0	-3.696360	2.871839	-0.046178
18	7	0	-3.719924	-2.881203	0.035275
19	1	0	-3.048680	3.120710	-0.806127
20	1	0	-4.589682	3.321759	-0.209812
21	1	0	-3.074058	-3.153188	0.788800
22	1	0	-4.620041	-3.319158	0.194474
23	1	0	-3.297203	3.263540	0.803802
24	1	0	-4.749831	1.051168	-0.458574
25	1	0	-4.744142	-1.054764	0.479562
26	1	0	-3.329890	-3.265465	-0.822298

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.232795	0.000000			
3	C	1.335814	2.462503	0.000000		
4	C	2.476533	1.335228	3.500477	0.000000	
5	C	2.462652	3.402074	1.232791	4.167936	0.000000
6	C	3.523448	2.510613	4.321208	1.230489	4.716430
7	C	3.500590	4.167829	2.476453	4.582026	1.335250
8	C	4.582802	3.727178	5.129196	2.536727	5.235562
9	C	4.321552	4.716586	3.523474	4.794456	2.510713
10	C	5.518211	4.805817	5.847533	3.706971	5.712626
11	C	5.129714	5.235916	4.582925	4.964611	3.727370
12	C	6.675182	6.082696	6.816669	5.056306	6.470481
13	C	5.849237	5.714381	5.519218	5.158313	4.806637
14	C	6.817948	6.471761	6.675855	5.669115	6.083298
15	C	7.942669	7.240427	8.176999	6.100240	7.877252
16	C	8.178999	7.879018	7.944319	7.085453	7.242200
17	N	8.008325	7.124891	8.471837	5.860968	8.380459
18	N	8.502240	8.409629	8.038707	7.810064	7.155129
19	H	7.514021	6.600456	8.037541	5.337181	8.020751
20	H	8.995996	8.090307	9.472757	6.810751	9.375353
21	H	8.079573	8.064135	7.552705	7.556522	6.636005
22	H	9.504102	9.403545	9.029374	8.777436	8.125039
23	H	7.783187	6.841938	8.332846	5.551127	8.328647
24	H	8.776456	8.127033	8.929289	7.020460	8.541741
25	H	8.927106	8.539252	8.774155	7.652003	8.125167
26	H	8.370047	8.362862	7.822222	7.853674	6.882313

		6	7	8	9	10
6	C	0.000000				
7	C	4.794143	0.000000			
8	C	1.337285	4.964071	0.000000		
9	C	4.685970	1.230474	4.517749	0.000000	
10	C	2.549395	5.156217	1.228585	4.431431	0.000000
11	C	4.518000	2.536743	3.974167	1.337330	3.557067

12	C	3.928144	5.667536	2.615910	4.704842	1.387546
13	C	4.433356	3.707323	3.558785	2.549591	2.805555
14	C	4.706317	5.056545	3.541222	3.928340	2.438225
15	C	4.896345	7.083614	3.564776	6.102028	2.438404
16	C	6.103594	6.101851	4.895667	4.897999	3.726924
17	N	4.634342	7.782452	3.432150	6.949254	2.675584
18	N	6.974694	5.890649	5.898718	4.663863	4.838666
19	H	4.145154	7.512766	3.047447	6.766509	2.505137
20	H	5.592060	8.752601	4.425181	7.885765	3.679765
21	H	6.809017	5.369848	5.833193	4.176909	4.878506
22	H	7.907145	6.845663	6.785936	5.626294	5.676994
23	H	4.345056	7.822791	3.246464	7.067223	2.706837
24	H	5.831671	7.654369	4.502751	6.597698	3.348067
25	H	6.595265	7.018783	5.322906	5.830343	4.113281
26	H	7.094431	5.592198	6.095968	4.386531	5.107087

		11	12	13	14	15
11	C	0.000000				
12	C	3.539789	0.000000			
13	C	1.228565	2.437703	0.000000		
14	C	2.615994	1.432254	1.387649	0.000000	
15	C	4.894273	1.417143	3.726242	2.461929	0.000000
16	C	3.566369	2.462341	2.439217	1.417453	2.830163
17	N	5.875821	2.391383	4.819440	3.730817	1.486404
18	N	3.461538	3.744647	2.701720	2.408008	4.295070
19	H	5.793117	2.584157	4.843095	3.929142	2.124515
20	H	6.768078	3.248431	5.663176	4.472936	2.057685
21	H	3.080349	3.956362	2.537280	2.607650	4.685758
22	H	4.456897	4.481047	3.704709	3.261453	4.782737
23	H	6.072823	2.730320	5.089110	4.116049	2.068821
24	H	5.325148	2.167353	4.115398	2.759471	1.083231
25	H	4.501636	2.757472	3.346556	2.165271	2.628177
26	H	3.286702	4.127474	2.738753	2.746619	4.802459

		16	17	18	19	20
16	C	0.000000				
17	N	4.289782	0.000000			
18	N	1.486404	5.753667	0.000000		
19	H	4.666581	1.029053	6.097663	0.000000	
20	H	4.785029	1.013523	6.268436	1.664542	0.000000
21	H	2.123963	6.114360	1.029037	6.473503	6.724529
22	H	2.058283	6.264147	1.013587	6.703900	6.653281
23	H	4.801477	1.017458	6.207028	1.635248	1.643565
24	H	2.629362	2.143529	4.094892	2.701428	2.289785
25	H	1.083114	4.097860	2.140630	4.686382	4.433176
26	H	2.069024	6.197029	1.017455	6.392384	6.734518

		21	22	23	24	25
21	H	0.000000				
22	H	1.664582	0.000000			
23	H	6.420625	6.741891	0.000000		

```
  24  H    4.694760   4.420754   2.932288   0.000000
  25  H    2.699665   2.285641   4.565798   2.305446   0.000000
  26  H    1.635143   1.643533   6.728534   4.558711   2.929531
            26
  26  H    0.000000
 Stoichiometry    C16H8N2
 Framework group  C1[X(C16H8N2)]
 Deg. of freedom    72
 Full point group                 C1      NOp   1
 RotChk:  IX=3 Diff= 6.55D-03
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        4.514236   -0.657440   -0.026932
     2          6           0        3.844036   -1.691465   -0.064467
     3          6           0        4.510835    0.677209    0.028741
     4          6           0        2.647688   -2.283845   -0.090352
     5          6           0        3.835815    1.708118    0.065459
     6          6           0        1.418421   -2.338691   -0.090306
     7          6           0        2.636519    2.294618    0.089974
     8          6           0        0.128540   -1.986182   -0.073733
     9          6           0        1.407031    2.343844    0.088742
    10          6           0       -0.953153   -1.404476   -0.042445
    11          6           0        0.118772    1.985332    0.071149
    12          6           0       -2.160642   -0.721084   -0.027311
    13          6           0       -0.960856    1.399882    0.039125
    14          6           0       -2.164932    0.710400    0.019453
    15          6           0       -3.391400   -1.422677   -0.063325
    16          6           0       -3.400032    1.405106    0.052390
    17          7           0       -3.178047   -2.877756    0.152599
    18          7           0       -3.221670    2.868381   -0.138423
    19          1           0       -2.529409   -3.096516    0.920950
    20          1           0       -4.069776   -3.324519    0.332744
    21          1           0       -2.576850    3.114972   -0.901521
    22          1           0       -4.123328    3.297110   -0.313248
    23          1           0       -2.777634   -3.298778   -0.682643
    24          1           0       -4.237805   -1.046942    0.498645
    25          1           0       -4.239572    1.023414   -0.515606
    26          1           0       -2.832870    3.284990    0.704481
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6009841           0.2721949           0.1880009
 Leave Link  202 at Sat Sep 26 00:50:13 2026, MaxMem=    805306368 cpu:                0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
```

Supporting Information file

Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1011.0783133502 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0154179136 Hartrees.
Nuclear repulsion after empirical dispersion term = 1011.0628954366 Hartrees.
Leave Link 301 at Sat Sep 26 00:50:13 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23237 LenP2D= 51999.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.81D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 00:50:14 2026, MaxMem= 805306368 cpu: 7.1 elap: 1.2
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 00:50:15 2026, MaxMem= 805306368 cpu: 0.9 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 0.000000 0.000000
Rot= 0.999998 0.000123 -0.000054 -0.001791 Ang= 0.21 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.

Supporting Information file

Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.982012766550
Leave Link 401 at Sat Sep 26 00:50:23 2026, MaxMem= 805306368 cpu: 52.9 elap: 8.8
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.411351190900
DIIS: error= 1.05D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.411351190900 IErMin= 1 ErrMin= 1.05D-03
ErrMax= 1.05D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-03 BMatP= 1.55D-03
IDIUse=3 WtCom= 9.90D-01 WtEn= 1.05D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.702 Goal= None Shift= 0.000
GapD= 0.702 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=1.06D-02 MaxDP=3.58D-01 OVMax= 9.74D-03

Cycle 2 Pass 0 IDiag 1:
RMSU= 8.17D-03 CP: 1.60D+00

E= -723.412491398603 Delta-E= -0.001140207703 Rises=F Damp=F
DIIS: error= 8.75D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.412491398603 IErMin= 2 ErrMin= 8.75D-04
ErrMax= 8.75D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-04 BMatP= 1.55D-03
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.75D-03
Coeff-Com: 0.490D-01 0.951D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.486D-01 0.951D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.25D-02 MaxDP=4.20D-01 DE=-1.14D-03 OVMax= 4.36D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 4.50D-03 CP: 8.58D-01 9.54D-03
E= -723.412539986292 Delta-E= -0.000048587689 Rises=F Damp=F
DIIS: error= 3.34D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.412539986292 IErMin= 2 ErrMin= 8.75D-04
ErrMax= 3.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.59D-04 BMatP= 1.34D-04
IDIUse=3 WtCom= 1.47D-01 WtEn= 8.53D-01
Coeff-Com: -0.266D-01 0.700D+00 0.327D+00
Coeff-En: 0.000D+00 0.298D+00 0.702D+00
Coeff: -0.392D-02 0.357D+00 0.647D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=7.87D+02 MaxDP=3.28D+04 DE=-4.86D-05 OVMax= 9.80D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.412346230021 Delta-E= 0.000193756270 Rises=F Damp=F
DIIS: error= 8.34D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.412346230021 IErMin= 1 ErrMin= 8.34D-04
ErrMax= 8.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-04 BMatP= 1.83D-04
IDIUse=3 WtCom= 9.92D-01 WtEn= 8.34D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=4.20D-03 MaxDP=1.04D-01 DE= 1.94D-04 OVMax= 3.24D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.15D-03 CP: 9.41D-01
E= -723.412459149414 Delta-E= -0.000112919392 Rises=F Damp=F
DIIS: error= 1.46D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.412459149414 IErMin= 2 ErrMin= 1.46D-04
ErrMax= 1.46D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.00D-05 BMatP= 1.83D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.46D-03
Coeff-Com: 0.514D-01 0.949D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.513D-01 0.949D+00

Gap= 0.177 Goal= None Shift= 0.000
RMSDP=5.44D-04 MaxDP=2.09D-02 DE=-1.13D-04 OVMax= 2.73D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.32D-04 CP: 9.61D-01 1.09D+00
E= -723.412450087691 Delta-E= 0.000009061723 Rises=F Damp=F
DIIS: error= 1.80D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.412459149414 IErMin= 2 ErrMin= 1.46D-04
ErrMax= 1.80D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-05 BMatP= 1.00D-05
IDIUse=3 WtCom= 4.27D-01 WtEn= 5.73D-01
Coeff-Com: -0.203D-01 0.602D+00 0.419D+00
Coeff-En: 0.000D+00 0.622D+00 0.378D+00
Coeff: -0.866D-02 0.614D+00 0.395D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=7.81D-05 MaxDP=3.20D-03 DE= 9.06D-06 OVMax= 1.20D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.54D-05 CP: 9.64D-01 1.10D+00 1.15D+00
E= -723.412472277937 Delta-E= -0.000022190246 Rises=F Damp=F
DIIS: error= 2.52D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.412472277937 IErMin= 4 ErrMin= 2.52D-05
ErrMax= 2.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-07 BMatP= 1.00D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.832D-02 0.192D+00 0.117D+00 0.699D+00
Coeff: -0.832D-02 0.192D+00 0.117D+00 0.699D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=5.31D-05 MaxDP=2.22D-03 DE=-2.22D-05 OVMax= 6.14D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 7.27D-06 CP: 9.66D-01 1.11D+00 1.25D+00 1.51D+00
E= -723.412472838410 Delta-E= -0.000000560474 Rises=F Damp=F
DIIS: error= 2.33D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.412472838410 IErMin= 5 ErrMin= 2.33D-05
ErrMax= 2.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.35D-08 BMatP= 1.81D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.579D-02-0.199D+00-0.151D+00 0.398D+00 0.947D+00
Coeff: 0.579D-02-0.199D+00-0.151D+00 0.398D+00 0.947D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=5.60D-05 MaxDP=2.39D-03 DE=-5.60D-07 OVMax= 6.90D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.41D-06 CP: 9.69D-01 1.12D+00 1.36D+00 2.07D+00 2.44D+00
E= -723.412473357206 Delta-E= -0.000000518796 Rises=F Damp=F
DIIS: error= 1.03D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.412473357206 IErMin= 6 ErrMin= 1.03D-05
ErrMax= 1.03D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-08 BMatP= 9.35D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.418D-02-0.123D+00-0.880D-01 0.126D-01 0.340D+00 0.854D+00

Coeff: 0.418D-02-0.123D+00-0.880D-01 0.126D-01 0.340D+00 0.854D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.28D-05 MaxDP=5.61D-04 DE=-5.19D-07 OVMax= 4.17D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.74D-06 CP: 9.69D-01 1.12D+00 1.38D+00 2.25D+00 2.93D+00
CP: 1.46D+00
E= -723.412473497603 Delta-E= -0.000000140397 Rises=F Damp=F
DIIS: error= 8.79D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.412473497603 IErMin= 7 ErrMin= 8.79D-06
ErrMax= 8.79D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.17D-09 BMatP= 1.81D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.332D-03 0.221D-01 0.178D-01-0.154D+00-0.224D+00 0.428D+00
Coeff-Com: 0.911D+00
Coeff: -0.332D-03 0.221D-01 0.178D-01-0.154D+00-0.224D+00 0.428D+00
Coeff: 0.911D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=3.03D-06 MaxDP=1.50D-04 DE=-1.40D-07 OVMax= 2.77D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 9.70D-07 CP: 9.69D-01 1.12D+00 1.38D+00 2.29D+00 3.00D+00
CP: 1.79D+00 2.12D+00
E= -723.412473549887 Delta-E= -0.000000052284 Rises=F Damp=F
DIIS: error= 3.45D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.412473549887 IErMin= 8 ErrMin= 3.45D-06
ErrMax= 3.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.28D-09 BMatP= 7.17D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.126D-02 0.442D-01 0.324D-01-0.938D-01-0.217D+00 0.390D-01
Coeff-Com: 0.517D+00 0.680D+00
Coeff: -0.126D-02 0.442D-01 0.324D-01-0.938D-01-0.217D+00 0.390D-01
Coeff: 0.517D+00 0.680D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.83D-06 MaxDP=7.90D-05 DE=-5.23D-08 OVMax= 1.24D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 3.74D-07 CP: 9.69D-01 1.12D+00 1.38D+00 2.28D+00 3.00D+00
CP: 1.88D+00 2.62D+00 1.22D+00
E= -723.412473559488 Delta-E= -0.000000009601 Rises=F Damp=F
DIIS: error= 2.15D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.412473559488 IErMin= 9 ErrMin= 2.15D-06
ErrMax= 2.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-10 BMatP= 2.28D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.396D-03 0.115D-01 0.782D-02 0.195D-02-0.284D-01-0.789D-01
Coeff-Com: -0.332D-01 0.254D+00 0.866D+00
Coeff: -0.396D-03 0.115D-01 0.782D-02 0.195D-02-0.284D-01-0.789D-01
Coeff: -0.332D-01 0.254D+00 0.866D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=6.86D-07 MaxDP=2.69D-05 DE=-9.60D-09 OVMax= 4.53D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 2.46D-07 CP: 9.69D-01 1.12D+00 1.37D+00 2.27D+00 3.00D+00
CP: 1.88D+00 2.75D+00 1.23D+00 2.14D+00
E= -723.412473561334 Delta-E= -0.000000001846 Rises=F Damp=F
DIIS: error= 6.70D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.412473561334 IErMin=10 ErrMin= 6.70D-07
ErrMax= 6.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-10 BMatP= 3.50D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.128D-03-0.576D-02-0.458D-02 0.254D-01 0.416D-01-0.485D-01
Coeff-Com: -0.157D+00-0.442D-01 0.450D+00 0.743D+00
Coeff: 0.128D-03-0.576D-02-0.458D-02 0.254D-01 0.416D-01-0.485D-01
Coeff: -0.157D+00-0.442D-01 0.450D+00 0.743D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=3.39D-07 MaxDP=1.52D-05 DE=-1.85D-09 OVMax= 2.24D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 9.63D-08 CP: 9.69D-01 1.12D+00 1.37D+00 2.26D+00 3.00D+00
CP: 1.86D+00 2.75D+00 1.20D+00 2.77D+00 1.42D+00
E= -723.412473561753 Delta-E= -0.000000000419 Rises=F Damp=F
DIIS: error= 5.31D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.412473561753 IErMin=11 ErrMin= 5.31D-07
ErrMax= 5.31D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.22D-11 BMatP= 1.17D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.152D-03-0.554D-02-0.416D-02 0.136D-01 0.285D-01-0.113D-01
Coeff-Com: -0.828D-01-0.742D-01 0.741D-01 0.423D+00 0.638D+00
Coeff: 0.152D-03-0.554D-02-0.416D-02 0.136D-01 0.285D-01-0.113D-01
Coeff: -0.828D-01-0.742D-01 0.741D-01 0.423D+00 0.638D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.70D-07 MaxDP=9.67D-06 DE=-4.19D-10 OVMax= 8.41D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 3.92D-08 CP: 9.69D-01 1.12D+00 1.37D+00 2.26D+00 3.00D+00
CP: 1.85D+00 2.72D+00 1.20D+00 2.97D+00 1.62D+00
CP: 1.66D+00
E= -723.412473561855 Delta-E= -0.000000000101 Rises=F Damp=F
DIIS: error= 9.65D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.412473561855 IErMin=12 ErrMin= 9.65D-08
ErrMax= 9.65D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.98D-12 BMatP= 3.22D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.273D-05 0.384D-03 0.363D-03-0.386D-02-0.523D-02 0.102D-01
Coeff-Com: 0.242D-01 0.646D-04-0.103D+00-0.109D+00 0.107D+00 0.108D+01
Coeff: -0.273D-05 0.384D-03 0.363D-03-0.386D-02-0.523D-02 0.102D-01
Coeff: 0.242D-01 0.646D-04-0.103D+00-0.109D+00 0.107D+00 0.108D+01
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=1.31D-07 MaxDP=7.84D-06 DE=-1.01D-10 OVMax= 4.76D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.00D-08 CP: 9.69D-01 1.12D+00 1.37D+00 2.26D+00 3.00D+00
CP: 1.84D+00 2.69D+00 1.20D+00 3.00D+00 1.76D+00
CP: 2.34D+00 2.18D+00
E= -723.412473561884 Delta-E= -0.000000000030 Rises=F Damp=F
DIIS: error= 5.43D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.412473561884 IErMin=13 ErrMin= 5.43D-08
ErrMax= 5.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.43D-13 BMatP= 2.98D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.252D-04 0.105D-02 0.820D-03-0.373D-02-0.666D-02 0.644D-02
Coeff-Com: 0.241D-01 0.116D-01-0.596D-01-0.122D+00-0.578D-01 0.502D+00
Coeff-Com: 0.704D+00
Coeff: -0.252D-04 0.105D-02 0.820D-03-0.373D-02-0.666D-02 0.644D-02
Coeff: 0.241D-01 0.116D-01-0.596D-01-0.122D+00-0.578D-01 0.502D+00
Coeff: 0.704D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=9.01D-08 MaxDP=5.39D-06 DE=-2.96D-11 OVMax= 1.72D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 8.67D-09 CP: 9.69D-01 1.12D+00 1.37D+00 2.25D+00 3.00D+00
CP: 1.83D+00 2.68D+00 1.19D+00 3.00D+00 1.82D+00
CP: 2.52D+00 2.55D+00 1.57D+00
E= -723.412473561890 Delta-E= -0.000000000006 Rises=F Damp=F
DIIS: error= 2.74D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.412473561890 IErMin=14 ErrMin= 2.74D-08
ErrMax= 2.74D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-13 BMatP= 9.43D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.823D-05 0.300D-03 0.227D-03-0.692D-03-0.153D-02 0.523D-03
Coeff-Com: 0.470D-02 0.432D-02-0.439D-02-0.258D-01-0.391D-01 0.645D-02
Coeff-Com: 0.260D+00 0.795D+00
Coeff: -0.823D-05 0.300D-03 0.227D-03-0.692D-03-0.153D-02 0.523D-03
Coeff: 0.470D-02 0.432D-02-0.439D-02-0.258D-01-0.391D-01 0.645D-02
Coeff: 0.260D+00 0.795D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=4.20D-08 MaxDP=2.47D-06 DE=-5.91D-12 OVMax= 7.49D-07

Cycle 18 Pass 1 IDiag 1:
RMSU= 4.62D-09 CP: 9.69D-01 1.12D+00 1.37D+00 2.25D+00 3.00D+00
CP: 1.83D+00 2.68D+00 1.19D+00 3.00D+00 1.85D+00
CP: 2.55D+00 2.66D+00 1.80D+00 1.62D+00
E= -723.412473561886 Delta-E= 0.000000000004 Rises=F Damp=F
DIIS: error= 1.43D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=14 EnMin= -723.412473561890 IErMin=15 ErrMin= 1.43D-08
ErrMax= 1.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.96D-14 BMatP= 1.53D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.389D-05-0.188D-03-0.153D-03 0.899D-03 0.145D-02-0.202D-02
Coeff-Com: -0.574D-02-0.134D-02 0.189D-01 0.284D-01-0.513D-02-0.179D+00
Coeff-Com: -0.825D-01 0.483D+00 0.744D+00
Coeff: 0.389D-05-0.188D-03-0.153D-03 0.899D-03 0.145D-02-0.202D-02

Supporting Information file

Coeff: -0.574D-02-0.134D-02 0.189D-01 0.284D-01-0.513D-02-0.179D+00
Coeff: -0.825D-01 0.483D+00 0.744D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=2.22D-08 MaxDP=1.35D-06 DE= 3.64D-12 OVMax= 5.78D-07

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.76D-09 CP: 9.69D-01 1.12D+00 1.37D+00 2.25D+00 3.00D+00
CP: 1.83D+00 2.68D+00 1.19D+00 3.00D+00 1.86D+00
CP: 2.56D+00 2.71D+00 1.93D+00 2.08D+00 1.86D+00
E= -723.412473561901 Delta-E= -0.000000000015 Rises=F Damp=F
DIIS: error= 9.72D-09 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.412473561901 IErMin=16 ErrMin= 9.72D-09
ErrMax= 9.72D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.67D-15 BMatP= 6.96D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.262D-05-0.110D-03-0.858D-04 0.393D-03 0.727D-03-0.713D-03
Coeff-Com: -0.259D-02-0.115D-02 0.651D-02 0.131D-01 0.472D-02-0.549D-01
Coeff-Com: -0.709D-01 0.102D-01 0.224D+00 0.870D+00
Coeff: 0.262D-05-0.110D-03-0.858D-04 0.393D-03 0.727D-03-0.713D-03
Coeff: -0.259D-02-0.115D-02 0.651D-02 0.131D-01 0.472D-02-0.549D-01
Coeff: -0.709D-01 0.102D-01 0.224D+00 0.870D+00
Gap= 0.177 Goal= None Shift= 0.000
RMSDP=3.44D-09 MaxDP=2.14D-07 DE=-1.46D-11 OVMax= 3.25D-07

SCF Done: E(RwB97XD) = -723.412473562 A.U. after 19 cycles
NFock= 19 Conv=0.34D-08 -V/T= 2.0046
KE= 7.200877571313D+02 PE=-3.703297657250D+03 EE= 1.248734531120D+03
Leave Link 502 at Sat Sep 26 01:16:24 2026, MaxMem= 805306368 cpu: 9359.4 elap: 1560.4
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23237 LenP2D= 51999.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 01:16:24 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 01:16:24 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.

Supporting Information file

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 01:35:58 2026, MaxMem= 805306368 cpu: 7040.8 elap: 1173.8
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.76798184D+00 2.03311670D-02 2.95971738D-02
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000685293	0.002417193	0.000269899
2	6	0.001416957	-0.001801191	-0.000216271
3	6	-0.000651784	-0.002450887	-0.000263108
4	6	-0.001786655	0.000854052	0.000075994
5	6	0.001425586	0.001870854	0.000209778
6	6	0.001711464	-0.000395518	-0.000246145
7	6	-0.001868203	-0.000914996	-0.000058938
8	6	-0.000173502	0.000236219	0.000079794
9	6	0.001820173	0.000468709	0.000183981
10	6	0.000059929	-0.000338812	0.000824911
11	6	-0.000491076	-0.000286857	-0.000144177
12	6	0.000048286	-0.004785353	-0.001646576
13	6	0.000040572	-0.000265485	-0.000708794
14	6	0.000520061	0.002175645	0.001744014
15	6	0.001871787	0.001448959	0.002352006
16	6	-0.000032413	-0.000004608	-0.002340571
17	7	-0.004439913	-0.000955092	-0.000379789
18	7	-0.001635117	0.002471897	0.000621079
19	1	0.000622049	0.000483634	-0.000989386
20	1	-0.000648258	0.001685833	0.000324681
21	1	0.000583982	-0.000680413	0.001042397
22	1	-0.000597509	-0.001295162	-0.000301283
23	1	0.000938289	0.000800595	0.000421807
24	1	0.000660197	0.000494967	-0.001294778
25	1	0.000387384	-0.000421711	0.000969873
26	1	0.000903009	-0.000812471	-0.000530396

Cartesian Forces: Max 0.004785353 RMS 0.001324422
Leave Link 716 at Sat Sep 26 01:35:58 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Supporting Information file

Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.004865849 RMS 0.001075513
Search for a local minimum.
Step number 13 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .10755D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 10 11 12 13
DE= -3.05D-04 DEPred=-2.82D-04 R= 1.08D+00
TightC=F SS= 1.41D+00 RLast= 1.43D-01 DXNew= 2.4000D+00 4.2819D-01
Trust test= 1.08D+00 RLast= 1.43D-01 DXMaxT set to 1.43D+00
ITU= 1 1 1 1 1 1 1 1 1 0 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00445	0.00487	0.01118	0.01668	0.01745
Eigenvalues ---	0.01972	0.02394	0.02694	0.02803	0.03114
Eigenvalues ---	0.03123	0.03611	0.03758	0.03939	0.04359
Eigenvalues ---	0.04438	0.04466	0.05026	0.06279	0.06883
Eigenvalues ---	0.08660	0.09957	0.10293	0.11350	0.11525
Eigenvalues ---	0.11720	0.12330	0.14881	0.15245	0.15474
Eigenvalues ---	0.16000	0.16000	0.16000	0.16109	0.16118
Eigenvalues ---	0.17946	0.23503	0.24467	0.24997	0.24999
Eigenvalues ---	0.25000	0.25000	0.25000	0.25012	0.25666
Eigenvalues ---	0.28979	0.34637	0.37231	0.37815	0.41852
Eigenvalues ---	0.45106	0.45836	0.46840	0.47679	0.47688
Eigenvalues ---	0.47688	0.47691	0.47891	0.50217	0.54809
Eigenvalues ---	0.54896	0.55104	0.55659	0.55669	0.56341
Eigenvalues ---	0.93718	0.93912	0.95022	0.95461	0.97688
Eigenvalues ---	0.99168	1.36343			

RFO step: Lambda=-6.86595881D-04 EMin= 4.44958897D-03
Quartic linear search produced a step of 0.17348.
Iteration 1 RMS(Cart)= 0.04461817 RMS(Int)= 0.00120199
Iteration 2 RMS(Cart)= 0.00333001 RMS(Int)= 0.00001441
Iteration 3 RMS(Cart)= 0.00000800 RMS(Int)= 0.00001371
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001371
ITry= 1 IFail=0 DXMaxC= 1.53D-01 DCOld= 1.00D+10 DXMaxT= 1.43D+00 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.32965	-0.00147	-0.00035	-0.00331	-0.00366	2.32599
R2	2.52432	0.00111	0.00044	0.00431	0.00475	2.52907
R3	2.52322	0.00089	0.00049	0.00468	0.00517	2.52839
R4	2.32964	-0.00150	-0.00035	-0.00334	-0.00369	2.32595
R5	2.32529	-0.00105	-0.00037	-0.00332	-0.00368	2.32160
R6	2.52326	0.00091	0.00049	0.00471	0.00520	2.52846
R7	2.52710	0.00064	0.00052	0.00472	0.00524	2.53234
R8	2.32526	-0.00113	-0.00037	-0.00340	-0.00377	2.32149
R9	2.32169	0.00053	-0.00027	-0.00226	-0.00253	2.31916

R10	2.52719	0.00066	0.00052	0.00476	0.00529	2.53248
R11	2.62208	0.00044	0.00030	0.00331	0.00361	2.62569
R12	2.32165	0.00028	-0.00026	-0.00249	-0.00275	2.31890
R13	2.70657	-0.00100	-0.00103	-0.00917	-0.01020	2.69637
R14	2.67801	0.00283	0.00148	0.01671	0.01819	2.69620
R15	2.62228	0.00048	0.00031	0.00342	0.00373	2.62601
R16	2.67860	0.00073	0.00171	0.01258	0.01429	2.69289
R17	2.80890	0.00156	-0.00054	-0.00263	-0.00317	2.80573
R18	2.04701	0.00001	0.00057	0.00472	0.00528	2.05229
R19	2.80890	0.00030	-0.00051	-0.00343	-0.00394	2.80496
R20	2.04679	0.00008	0.00055	0.00482	0.00537	2.05216
R21	1.94463	0.00124	0.00032	0.00343	0.00376	1.94838
R22	1.91528	0.00127	0.00013	0.00166	0.00178	1.91707
R23	1.92272	0.00103	-0.00015	-0.00051	-0.00066	1.92205
R24	1.94460	0.00131	0.00032	0.00356	0.00388	1.94848
R25	1.91540	0.00104	0.00015	0.00130	0.00145	1.91685
R26	1.92271	0.00110	-0.00016	-0.00038	-0.00054	1.92217
A1	2.56425	-0.00022	0.00023	0.00172	0.00194	2.56620
A2	2.60569	0.00015	-0.00029	-0.00205	-0.00234	2.60335
A3	2.56467	-0.00027	0.00026	0.00167	0.00193	2.56660
A4	2.72599	-0.00013	0.00046	0.00354	0.00399	2.72997
A5	2.60540	0.00013	-0.00029	-0.00230	-0.00261	2.60280
A6	2.82999	0.00061	-0.00059	-0.00401	-0.00460	2.82539
A7	2.72634	-0.00023	0.00049	0.00322	0.00371	2.73005
A8	2.82992	0.00056	-0.00058	-0.00433	-0.00491	2.82501
A9	2.08888	-0.00068	0.00023	-0.00165	-0.00143	2.08745
A10	2.10792	0.00038	0.00014	0.00304	0.00317	2.11109
A11	2.08637	0.00030	-0.00033	-0.00142	-0.00175	2.08462
A12	2.08802	0.00031	0.00004	0.00137	0.00140	2.08942
A13	2.08658	0.00025	-0.00032	-0.00149	-0.00182	2.08475
A14	2.10858	-0.00057	0.00032	0.00013	0.00044	2.10901
A15	2.08713	-0.00119	-0.00485	-0.05171	-0.05657	2.03056
A16	1.95665	-0.00332	-0.00021	-0.01270	-0.01291	1.94374
A17	2.08346	0.00061	-0.00587	-0.03610	-0.04197	2.04149
A18	1.95262	-0.00150	-0.00122	0.00307	0.00185	1.95447
A19	1.99001	-0.00023	0.00139	0.01068	0.01205	2.00206
A20	1.90821	0.00162	-0.00076	-0.00317	-0.00394	1.90427
A21	1.92018	0.00035	-0.00008	0.00025	0.00014	1.92031
A22	1.90515	-0.00048	-0.00045	-0.00429	-0.00474	1.90041
A23	1.85138	-0.00063	0.00045	0.00221	0.00262	1.85399
A24	1.88573	-0.00074	-0.00061	-0.00641	-0.00704	1.87869
A25	1.98919	0.00009	0.00129	0.01229	0.01356	2.00275
A26	1.90900	0.00111	-0.00060	-0.00573	-0.00634	1.90266
A27	1.92047	0.00037	-0.00009	0.00041	0.00028	1.92075
A28	1.90515	-0.00048	-0.00043	-0.00449	-0.00492	1.90023
A29	1.85123	-0.00060	0.00042	0.00269	0.00306	1.85429
A30	1.88560	-0.00060	-0.00064	-0.00583	-0.00650	1.87910
A31	2.91468	0.00003	-0.00043	-0.00143	-0.00186	2.91282

A32	3.12046	-0.00014	0.00049	0.00216	0.00265	3.12311
A33	2.91586	-0.00015	-0.00020	-0.00484	-0.00505	2.91081
A34	3.11883	0.00002	0.00017	0.00690	0.00707	3.12590
A35	4.04378	-0.00451	-0.00506	-0.06442	-0.06948	3.97430
A36	4.03607	-0.00089	-0.00708	-0.03303	-0.04011	3.99596
A37	3.14656	0.00038	-0.00021	0.00045	0.00026	3.14682
A38	3.12580	0.00075	0.00064	0.00960	0.01023	3.13603
A39	3.14651	0.00042	-0.00022	0.00050	0.00028	3.14679
A40	3.12852	0.00051	0.00121	-0.00018	0.00102	3.12954
A41	3.97437	-0.00487	0.00925	0.01342	0.02267	3.99704
A42	3.95139	0.00022	0.00488	0.09245	0.09733	4.04873
D1	0.01633	0.00028	0.00059	0.00453	0.00511	0.02144
D2	-0.01765	0.00027	-0.00020	-0.00318	-0.00338	-0.02104
D3	-0.01705	0.00015	0.00007	0.00108	0.00114	-0.01591
D4	0.01647	0.00023	0.00062	0.00389	0.00451	0.02099
D5	0.00780	0.00007	0.00002	0.00063	0.00063	0.00843
D6	-0.01673	0.00010	0.00014	-0.00030	-0.00017	-0.01690
D7	0.00297	0.00005	-0.00342	-0.00283	-0.00628	-0.00331
D8	3.13010	-0.00003	0.00018	-0.00182	-0.00164	3.12846
D9	0.00800	0.00001	0.00007	-0.00019	-0.00013	0.00787
D10	0.00473	0.00001	-0.00306	-0.00909	-0.01217	-0.00744
D11	3.13261	-0.00006	0.00068	-0.00872	-0.00805	3.12456
D12	0.00832	-0.00042	0.00307	0.00333	0.00638	0.01471
D13	-3.12733	0.00012	0.00004	0.00215	0.00219	-3.12514
D14	-3.12861	0.00029	-0.00025	0.00871	0.00845	-3.12017
D15	0.01892	0.00082	-0.00328	0.00753	0.00425	0.02317
D16	2.51188	0.00057	-0.00502	-0.04902	-0.05403	2.45785
D17	-0.63442	-0.00015	-0.00165	-0.05447	-0.05613	-0.69055
D18	-0.63804	0.00033	-0.00299	-0.03338	-0.03638	-0.67442
D19	2.50956	0.00087	-0.00605	-0.03458	-0.04063	2.46893
D20	-1.60118	0.00044	0.00671	0.06340	0.07013	-1.53104
D21	0.53658	0.00087	0.00653	0.06291	0.06942	0.60601
D22	2.60483	0.00115	0.00527	0.05331	0.05857	2.66340
D23	-1.60604	0.00053	0.00669	0.06357	0.07030	-1.53574
D24	0.53174	0.00080	0.00658	0.06204	0.06859	0.60033
D25	2.60049	0.00097	0.00537	0.05169	0.05703	2.65752

Item	Value	Threshold	Converged?
Maximum Force	0.004866	0.000450	NO
RMS Force	0.001076	0.000300	NO
Maximum Displacement	0.152624	0.001800	NO
RMS Displacement	0.044329	0.001200	NO

Predicted change in Energy=-3.703869D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 01:35:58 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)

Supporting Information file

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.006027	0.648724	0.054843
2	6	0	3.339045	1.680926	0.123470
3	6	0	4.002467	-0.685827	-0.045557
4	6	0	2.140093	2.273212	0.166594
5	6	0	3.330376	-1.714433	-0.117844
6	6	0	0.912988	2.332541	0.168157
7	6	0	2.128169	-2.299684	-0.167176
8	6	0	-0.379258	1.978832	0.140925
9	6	0	0.900823	-2.351944	-0.174465
10	6	0	-1.458182	1.396123	0.090870
11	6	0	-0.389412	-1.990344	-0.152514
12	6	0	-2.667297	0.713444	0.040047
13	6	0	-1.463651	-1.398981	-0.106702
14	6	0	-2.669414	-0.709193	-0.069575
15	6	0	-3.908746	1.413700	0.104207
16	6	0	-3.911223	-1.404436	-0.141791
17	7	0	-3.744321	2.883708	-0.024061
18	7	0	-3.685785	-2.859211	0.047983
19	1	0	-3.105249	3.181904	-0.776199
20	1	0	-4.653143	3.307296	-0.178200
21	1	0	-3.033440	-3.099198	0.809558
22	1	0	-4.576492	-3.311457	0.224143
23	1	0	-3.367171	3.268581	0.838574
24	1	0	-4.702862	1.046708	-0.539339
25	1	0	-4.720083	-1.033799	0.480842
26	1	0	-3.295748	-3.265109	-0.799217

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.230859	0.000000			
3	C	1.338327	2.463781	0.000000		
4	C	2.476521	1.337964	3.502764	0.000000	
5	C	2.463906	3.403934	1.230837	4.171210	0.000000
6	C	3.523488	2.512440	4.324477	1.228540	4.722664
7	C	3.502678	4.170845	2.476351	4.585076	1.338004
8	C	4.583375	3.730259	5.131734	2.536622	5.241045
9	C	4.324220	4.722047	3.523174	4.800435	2.512440
10	C	5.515205	4.805784	5.845666	3.704403	5.713966
11	C	5.131039	5.239827	4.582773	4.967710	3.730168
12	C	6.673655	6.084335	6.815500	5.055679	6.472372
13	C	5.842651	5.710052	5.512783	5.152346	4.804407
14	C	6.813290	6.469275	6.671965	5.664086	6.083610

15	C	7.951809	7.252742	8.186436	6.109920	7.889196
16	C	8.181502	7.883921	7.946832	7.087921	7.248271
17	N	8.066552	7.186273	8.529640	5.919069	8.438189
18	N	8.453971	8.364615	7.990092	7.765095	7.110875
19	H	7.594596	6.677670	8.124827	5.406311	8.113250
20	H	9.061101	8.161566	9.533216	6.880136	9.431754
21	H	8.010656	7.995553	7.487293	7.486096	6.578434
22	H	9.453641	9.358940	8.975812	8.735237	8.073785
23	H	7.863964	6.928590	8.410148	5.636690	8.402517
24	H	8.738203	8.094061	8.889783	6.987753	8.504968
25	H	8.897042	8.511580	8.745345	7.622145	8.101332
26	H	8.328471	8.326770	7.777187	7.820113	6.839181

		6	7	8	9	10
6	C	0.000000				
7	C	4.800689	0.000000			
8	C	1.340056	4.968683	0.000000		
9	C	4.697013	1.228479	4.526996	0.000000	
10	C	2.550548	5.156306	1.227245	4.436588	0.000000
11	C	4.526192	2.536557	3.980021	1.340128	3.559447
12	C	3.931454	5.667308	2.616583	4.708939	1.389458
13	C	4.432631	3.703525	3.556241	2.550190	2.802083
14	C	4.705556	5.055293	3.537598	3.931441	2.434169
15	C	4.908918	7.092758	3.574634	6.114711	2.450664
16	C	6.110161	6.105438	4.899102	4.904552	3.730238
17	N	4.693746	7.834167	3.488505	7.000859	2.729936
18	N	6.936674	5.844778	5.860752	4.619933	4.803324
19	H	4.214197	7.603117	3.117616	6.858147	2.579468
20	H	5.661442	8.799122	4.486954	7.929285	3.732661
21	H	6.744588	5.313703	5.768720	4.123726	4.817246
22	H	7.873515	6.791855	6.753581	5.574992	5.648268
23	H	4.432312	7.887704	3.328331	7.129679	2.776580
24	H	5.804454	7.615762	4.474949	6.563936	3.323733
25	H	6.569741	6.994351	5.294738	5.810467	4.086147
26	H	7.069863	5.545304	6.073607	4.339977	5.088811

		11	12	13	14	15
11	C	0.000000				
12	C	3.540666	0.000000			
13	C	1.227110	2.435702	0.000000		
14	C	2.616607	1.426856	1.389622	0.000000	
15	C	4.902972	1.426769	3.732847	2.464309	0.000000
16	C	3.570231	2.462891	2.447829	1.425015	2.828853
17	N	5.918471	2.423661	4.852804	3.750524	1.484726
18	N	3.414850	3.715003	2.663471	2.381052	4.279093
19	H	5.875109	2.636542	4.911983	3.978682	2.132433
20	H	6.800372	3.274031	5.685685	4.480978	2.054163
21	H	3.024239	3.906719	2.488876	2.572453	4.650799
22	H	4.406682	4.458559	3.668352	3.239599	4.773613
23	H	6.124181	2.766982	5.128652	4.139358	2.067168

24	H	5.289534	2.142493	4.081796	2.727412	1.086027
25	H	4.480048	2.731499	3.329101	2.147923	2.605834
26	H	3.238833	4.114390	2.705289	2.730821	4.804498

		16	17	18	19	20
16	C	0.000000				
17	N	4.293005	0.000000			
18	N	1.484320	5.743669	0.000000		
19	H	4.699637	1.031041	6.124653	0.000000	
20	H	4.769926	1.014468	6.246019	1.664122	0.000000
21	H	2.132554	6.082387	1.031089	6.478582	6.681487
22	H	2.052613	6.255732	1.014356	6.732680	6.631414
23	H	4.805642	1.017108	6.186791	1.638172	1.639833
24	H	2.606309	2.135153	4.078676	2.677225	2.289793
25	H	1.085955	4.068648	2.142258	4.686149	4.391346
26	H	2.067153	6.213697	1.017168	6.449869	6.739785

		21	22	23	24	25
21	H	0.000000				
22	H	1.663964	0.000000			
23	H	6.376584	6.718399	0.000000		
24	H	4.668515	4.426339	2.935887	0.000000	
25	H	2.686763	2.296572	4.524247	2.317234	0.000000
26	H	1.638441	1.640036	6.736213	4.543047	2.940413

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=2 Diff= 1.74D-02
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.508548	-0.693523	-0.027996
2	6	0	3.832593	-1.721690	-0.059170
3	6	0	4.516615	0.643808	0.022985
4	6	0	2.628527	-2.304669	-0.081733
5	6	0	3.853515	1.680216	0.056421
6	6	0	1.400949	-2.353291	-0.082502
7	6	0	2.656449	2.277373	0.082707
8	6	0	0.111835	-1.987540	-0.069843
9	6	0	1.429603	2.340588	0.086658
10	6	0	-0.961976	-1.393974	-0.042600
11	6	0	0.136263	1.989710	0.076619
12	6	0	-2.165097	-0.699345	-0.018435

13	6	0	-0.943084	1.406466	0.051479
14	6	0	-2.154822	0.726337	0.038506
15	6	0	-3.412589	-1.390621	-0.058075
16	6	0	-3.390542	1.434599	0.083548
17	7	0	-3.261171	-2.856260	0.124648
18	7	0	-3.152195	2.879334	-0.159631
19	1	0	-2.625356	-3.132007	0.888026
20	1	0	-4.173800	-3.265901	0.293306
21	1	0	-2.497147	3.085282	-0.928813
22	1	0	-4.038756	3.332521	-0.353409
23	1	0	-2.886707	-3.276054	-0.722735
24	1	0	-4.203980	-0.993155	0.570554
25	1	0	-4.202113	1.048268	-0.525877
26	1	0	-2.759305	3.312865	0.672426

Rotational constants (GHZ): 0.6009501 0.2718282 0.1878314
Leave Link 202 at Sat Sep 26 01:35:58 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.6354131096 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0154114684 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.6200016412 Hartrees.
Leave Link 301 at Sat Sep 26 01:35:59 2026, MaxMem= 805306368 cpu: 0.5 elap: 0.1
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23238 LenP2D= 51971.

Supporting Information file

LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.79D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 01:36:00 2026, MaxMem= 805306368 cpu: 11.1 elap: 1.9
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 01:36:01 2026, MaxMem= 805306368 cpu: 1.4 elap: 0.3
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 -0.000000 -0.000000
Rot= 0.999987 0.000091 0.000161 0.005071 Ang= 0.58 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.980451859020
Leave Link 401 at Sat Sep 26 01:36:18 2026, MaxMem= 805306368 cpu: 103.1 elap: 17.2
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.

Supporting Information file

```
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
      NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
      wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
      NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
Symmetry not used in FoFCou.
E= -723.409010930287
DIIS: error= 1.55D-03 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -723.409010930287     IErMin= 1 ErrMin= 1.55D-03
ErrMax= 1.55D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.70D-03 BMatP= 3.70D-03
IDIUse=3 WtCom= 9.84D-01 WtEn= 1.55D-02
Coeff-Com:  0.100D+01
Coeff-En:   0.100D+01
Coeff:      0.100D+01
Gap=     0.706 Goal=   None    Shift=    0.000
GapD=    0.706 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=1.36D-02 MaxDP=4.64D-01              OVMax= 1.67D-02

Cycle   2  Pass 0  IDiag  1:
RMSU=  1.03D-02    CP:  1.78D+00
E= -723.412172563489     Delta-E=       -0.003161633202 Rises=F Damp=F
DIIS: error= 8.23D-04 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.412172563489     IErMin= 2 ErrMin= 8.23D-04
ErrMax= 8.23D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-04 BMatP= 3.70D-03
IDIUse=3 WtCom= 9.92D-01 WtEn= 8.23D-03
Coeff-Com: -0.144D-01 0.101D+01
Coeff-En:   0.000D+00 0.100D+01
Coeff:     -0.142D-01 0.101D+01
Gap=     0.179 Goal=   None    Shift=    0.000
RMSDP=1.13D-02 MaxDP=4.00D-01 DE=-3.16D-03 OVMax= 6.92D-03

Cycle   3  Pass 0  IDiag  1:
RMSU=  4.05D-03    CP:  1.10D+00  3.02D-01
E= -723.412361862040     Delta-E=       -0.000189298551 Rises=F Damp=F
DIIS: error= 4.31D-03 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -723.412361862040     IErMin= 2 ErrMin= 8.23D-04
ErrMax= 4.31D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 7.49D-04 BMatP= 2.09D-04
IDIUse=3 WtCom= 1.32D-01 WtEn= 8.68D-01
Coeff-Com: -0.383D-01 0.751D+00 0.287D+00
Coeff-En:   0.000D+00 0.000D+00 0.100D+01
Coeff:     -0.506D-02 0.993D-01 0.906D+00
Gap=     0.179 Goal=   None    Shift=    0.000
RMSDP=7.93D+02 MaxDP=3.32D+04 DE=-1.89D-04 OVMax= 9.61D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle   4  Pass 1  IDiag  1:
E= -723.412110843718     Delta-E=       0.000251018323 Rises=F Damp=F
DIIS: error= 9.20D-04 at cycle   1 NSaved=   1.
```

NSaved= 1 IEnMin= 1 EnMin= -723.412110843718 IErMin= 1 ErrMin= 9.20D-04
ErrMax= 9.20D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.55D-04 BMatP= 2.55D-04
IDIUse=3 WtCom= 9.91D-01 WtEn= 9.20D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.52D-03 MaxDP=1.79D-01 DE= 2.51D-04 OVMax= 7.05D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.02D-03 CP: 7.18D-01
E= -723.412249733740 Delta-E= -0.000138890022 Rises=F Damp=F
DIIS: error= 3.09D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.412249733740 IErMin= 2 ErrMin= 3.09D-04
ErrMax= 3.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.04D-05 BMatP= 2.55D-04
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.09D-03
Coeff-Com: 0.212D+00 0.788D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.211D+00 0.789D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.52D-04 MaxDP=9.87D-03 DE=-1.39D-04 OVMax= 5.77D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.17D-04 CP: 7.21D-01 1.03D+00
E= -723.412259615382 Delta-E= -0.000009881643 Rises=F Damp=F
DIIS: error= 3.07D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.412259615382 IErMin= 3 ErrMin= 3.07D-04
ErrMax= 3.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.67D-05 BMatP= 5.04D-05
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.07D-03
Coeff-Com: -0.182D-01 0.494D+00 0.525D+00
Coeff-En: 0.000D+00 0.461D+00 0.539D+00
Coeff: -0.181D-01 0.494D+00 0.525D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=9.98D-05 MaxDP=4.54D-03 DE=-9.88D-06 OVMax= 2.89D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 3.63D-05 CP: 7.23D-01 1.04D+00 1.36D+00
E= -723.412312928285 Delta-E= -0.000053312902 Rises=F Damp=F
DIIS: error= 7.30D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.412312928285 IErMin= 4 ErrMin= 7.30D-05
ErrMax= 7.30D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.43D-07 BMatP= 4.67D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.123D-01 0.219D+00 0.248D+00 0.545D+00
Coeff: -0.123D-01 0.219D+00 0.248D+00 0.545D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.57D-05 MaxDP=1.27D-03 DE=-5.33D-05 OVMax= 6.85D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.04D-06 CP: 7.24D-01 1.04D+00 1.45D+00 1.18D+00
E= -723.412314553402 Delta-E= -0.000001625117 Rises=F Damp=F
DIIS: error= 3.99D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.412314553402 IErMin= 5 ErrMin= 3.99D-05
ErrMax= 3.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.07D-07 BMatP= 8.43D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.381D-02-0.135D+00-0.138D+00 0.193D+00 0.108D+01
Coeff: 0.381D-02-0.135D+00-0.138D+00 0.193D+00 0.108D+01
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.23D-05 MaxDP=2.17D-03 DE=-1.63D-06 OVMax= 1.24D-03

Cycle 9 Pass 1 IDiag 1:
RMSU= 5.58D-06 CP: 7.26D-01 1.04D+00 1.58D+00 1.42D+00 2.80D+00
E= -723.412315927601 Delta-E= -0.000001374199 Rises=F Damp=F
DIIS: error= 2.43D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.412315927601 IErMin= 6 ErrMin= 2.43D-05
ErrMax= 2.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.44D-08 BMatP= 2.07D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.573D-02-0.137D+00-0.147D+00-0.548D-01 0.532D+00 0.801D+00
Coeff: 0.573D-02-0.137D+00-0.147D+00-0.548D-01 0.532D+00 0.801D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.83D-05 MaxDP=9.24D-04 DE=-1.37D-06 OVMax= 7.10D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 6.17D-06 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.49D+00
E= -723.412316357045 Delta-E= -0.000000429444 Rises=F Damp=F
DIIS: error= 1.02D-05 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.412316357045 IErMin= 7 ErrMin= 1.02D-05
ErrMax= 1.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-08 BMatP= 6.44D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.291D-03 0.470D-02 0.256D-02-0.644D-01-0.168D+00 0.194D+00
Coeff-Com: 0.103D+01
Coeff: 0.291D-03 0.470D-02 0.256D-02-0.644D-01-0.168D+00 0.194D+00
Coeff: 0.103D+01
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.02D-06 MaxDP=2.55D-04 DE=-4.29D-07 OVMax= 4.39D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.94D-06 CP: 7.27D-01 1.04D+00 1.63D+00 1.53D+00 3.00D+00
CP: 1.74D+00 1.49D+00
E= -723.412316466040 Delta-E= -0.000000108995 Rises=F Damp=F
DIIS: error= 6.75D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.412316466040 IErMin= 8 ErrMin= 6.75D-06
ErrMax= 6.75D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.80D-09 BMatP= 1.21D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.148D-02 0.427D-01 0.439D-01-0.248D-01-0.255D+00-0.105D+00
Coeff-Com: 0.613D+00 0.688D+00

Coeff: -0.148D-02 0.427D-01 0.439D-01-0.248D-01-0.255D+00-0.105D+00
Coeff: 0.613D+00 0.688D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.95D-06 MaxDP=8.89D-05 DE=-1.09D-07 OVMax= 1.63D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.26D-07 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.80D+00 1.64D+00 1.59D+00
E= -723.412316489756 Delta-E= -0.000000023716 Rises=F Damp=F
DIIS: error= 1.91D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.412316489756 IErMin= 9 ErrMin= 1.91D-06
ErrMax= 1.91D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.96D-10 BMatP= 5.80D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.642D-03 0.156D-01 0.165D-01 0.454D-02-0.597D-01-0.773D-01
Coeff-Com: -0.257D-02 0.266D+00 0.838D+00
Coeff: -0.642D-03 0.156D-01 0.165D-01 0.454D-02-0.597D-01-0.773D-01
Coeff: -0.257D-02 0.266D+00 0.838D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=6.54D-07 MaxDP=2.65D-05 DE=-2.37D-08 OVMax= 6.63D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 3.12D-07 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.79D+00 1.62D+00 1.81D+00 1.70D+00
E= -723.412316493764 Delta-E= -0.000000004008 Rises=F Damp=F
DIIS: error= 1.39D-06 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.412316493764 IErMin=10 ErrMin= 1.39D-06
ErrMax= 1.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-10 BMatP= 7.96D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.105D-03-0.422D-02-0.414D-02 0.797D-02 0.391D-01-0.304D-02
Coeff-Com: -0.157D+00-0.664D-01 0.343D+00 0.844D+00
Coeff: 0.105D-03-0.422D-02-0.414D-02 0.797D-02 0.391D-01-0.304D-02
Coeff: -0.157D+00-0.664D-01 0.343D+00 0.844D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.60D-07 MaxDP=1.90D-05 DE=-4.01D-09 OVMax= 2.96D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 1.13D-07 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.76D+00 1.59D+00 1.85D+00 2.20D+00 1.80D+00
E= -723.412316494643 Delta-E= -0.000000000879 Rises=F Damp=F
DIIS: error= 5.36D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.412316494643 IErMin=11 ErrMin= 5.36D-07
ErrMax= 5.36D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.84D-11 BMatP= 1.98D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.185D-03-0.546D-02-0.557D-02 0.349D-02 0.332D-01 0.119D-01
Coeff-Com: -0.900D-01-0.884D-01 0.484D-01 0.482D+00 0.610D+00
Coeff: 0.185D-03-0.546D-02-0.557D-02 0.349D-02 0.332D-01 0.119D-01
Coeff: -0.900D-01-0.884D-01 0.484D-01 0.482D+00 0.610D+00
Gap= 0.179 Goal= None Shift= 0.000

RMSDP=1.87D-07 MaxDP=8.54D-06 DE=-8.79D-10 OVMax= 1.25D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 5.27D-08 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.76D+00 1.58D+00 1.84D+00 2.37D+00 2.17D+00
CP: 1.44D+00
E= -723.412316494841 Delta-E= -0.000000000197 Rises=F Damp=F
DIIS: error= 2.96D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.412316494841 IErMin=12 ErrMin= 2.96D-07
ErrMax= 2.96D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.70D-12 BMatP= 6.84D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.472D-04-0.114D-02-0.118D-02-0.557D-03 0.365D-02 0.500D-02
Coeff-Com: 0.256D-02-0.197D-01-0.611D-01-0.144D-01 0.245D+00 0.842D+00
Coeff: 0.472D-04-0.114D-02-0.118D-02-0.557D-03 0.365D-02 0.500D-02
Coeff: 0.256D-02-0.197D-01-0.611D-01-0.144D-01 0.245D+00 0.842D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.31D-07 MaxDP=7.46D-06 DE=-1.97D-10 OVMax= 5.61D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 3.49D-08 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.75D+00 1.57D+00 1.83D+00 2.48D+00 2.39D+00
CP: 1.93D+00 1.92D+00
E= -723.412316494871 Delta-E= -0.000000000030 Rises=F Damp=F
DIIS: error= 9.68D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.412316494871 IErMin=13 ErrMin= 9.68D-08
ErrMax= 9.68D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.43D-12 BMatP= 9.70D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.250D-04 0.850D-03 0.869D-03-0.962D-03-0.631D-02-0.695D-03
Coeff-Com: 0.235D-01 0.137D-01-0.397D-01-0.132D+00-0.495D-01 0.391D+00
Coeff-Com: 0.799D+00
Coeff: -0.250D-04 0.850D-03 0.869D-03-0.962D-03-0.631D-02-0.695D-03
Coeff: 0.235D-01 0.137D-01-0.397D-01-0.132D+00-0.495D-01 0.391D+00
Coeff: 0.799D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.04D-07 MaxDP=7.53D-06 DE=-3.00D-11 OVMax= 2.98D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 1.20D-08 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.75D+00 1.57D+00 1.83D+00 2.53D+00 2.49D+00
CP: 2.20D+00 2.56D+00 1.64D+00
E= -723.412316494884 Delta-E= -0.000000000013 Rises=F Damp=F
DIIS: error= 3.66D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.412316494884 IErMin=14 ErrMin= 3.66D-08
ErrMax= 3.66D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.38D-13 BMatP= 2.43D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.168D-04 0.514D-03 0.529D-03-0.361D-03-0.329D-02-0.966D-03
Coeff-Com: 0.102D-01 0.847D-02-0.105D-01-0.575D-01-0.513D-01 0.722D-01
Coeff-Com: 0.354D+00 0.678D+00

Coeff: -0.168D-04 0.514D-03 0.529D-03-0.361D-03-0.329D-02-0.966D-03
Coeff: 0.102D-01 0.847D-02-0.105D-01-0.575D-01-0.513D-01 0.722D-01
Coeff: 0.354D+00 0.678D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.72D-08 MaxDP=2.07D-06 DE=-1.34D-11 OVMax= 9.64D-07

Cycle 18 Pass 1 IDiag 1:
RMSU= 5.89D-09 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.75D+00 1.57D+00 1.83D+00 2.55D+00 2.51D+00
CP: 2.27D+00 2.76D+00 1.91D+00 1.47D+00
E= -723.412316494886 Delta-E= -0.000000000002 Rises=F Damp=F
DIIS: error= 2.04D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.412316494886 IErMin=15 ErrMin= 2.04D-08
ErrMax= 2.04D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-13 BMatP= 4.38D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.359D-06-0.451D-04-0.444D-04 0.178D-03 0.651D-03-0.298D-03
Coeff-Com: -0.346D-02-0.594D-03 0.102D-01 0.204D-01-0.110D-01-0.117D+00
Coeff-Com: -0.108D+00 0.382D+00 0.827D+00
Coeff: 0.359D-06-0.451D-04-0.444D-04 0.178D-03 0.651D-03-0.298D-03
Coeff: -0.346D-02-0.594D-03 0.102D-01 0.204D-01-0.110D-01-0.117D+00
Coeff: -0.108D+00 0.382D+00 0.827D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.95D-08 MaxDP=1.46D-06 DE=-1.59D-12 OVMax= 8.96D-07

Cycle 19 Pass 1 IDiag 1:
RMSU= 2.37D-09 CP: 7.27D-01 1.04D+00 1.63D+00 1.52D+00 3.00D+00
CP: 1.75D+00 1.57D+00 1.83D+00 2.55D+00 2.52D+00
CP: 2.31D+00 2.91D+00 2.11D+00 2.00D+00 2.02D+00
E= -723.412316494879 Delta-E= 0.000000000006 Rises=F Damp=F
DIIS: error= 1.49D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=15 EnMin= -723.412316494886 IErMin=16 ErrMin= 1.49D-08
ErrMax= 1.49D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.97D-14 BMatP= 1.56D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.346D-05-0.121D-03-0.123D-03 0.145D-03 0.949D-03 0.511D-04
Coeff-Com: -0.353D-02-0.196D-02 0.655D-02 0.200D-01 0.559D-02-0.650D-01
Coeff-Com: -0.118D+00 0.339D-01 0.363D+00 0.759D+00
Coeff: 0.346D-05-0.121D-03-0.123D-03 0.145D-03 0.949D-03 0.511D-04
Coeff: -0.353D-02-0.196D-02 0.655D-02 0.200D-01 0.559D-02-0.650D-01
Coeff: -0.118D+00 0.339D-01 0.363D+00 0.759D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.64D-09 MaxDP=3.69D-07 DE= 6.37D-12 OVMax= 4.80D-07

SCF Done: E(RwB97XD) = -723.412316495 A.U. after 19 cycles
NFock= 19 Conv=0.56D-08 -V/T= 2.0046
KE= 7.200737314585D+02 PE=-3.702367417802D+03 EE= 1.248261368207D+03
Leave Link 502 at Sat Sep 26 02:14:36 2026, MaxMem= 805306368 cpu: 13781.3 elap: 2297.9
(Enter /home/user/gauss16/g16/l701.exe)

Supporting Information file

... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23238 LenP2D= 51971.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 02:14:37 2026, MaxMem= 805306368 cpu: 6.2 elap: 1.1
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 02:14:37 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 02:34:52 2026, MaxMem= 805306368 cpu: 7285.6 elap: 1214.5
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.54414646D+00-4.65954117D-02-7.12957174D-02
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000077083	0.001035628	0.000015666
2	6	-0.000125126	-0.001046034	-0.000042379
3	6	-0.000054500	-0.000936816	-0.000032141
4	6	-0.000050448	0.001135796	0.000042728
5	6	-0.000112972	0.000841615	0.000052549
6	6	0.000052233	-0.001310945	-0.000066383
7	6	0.000151343	-0.000950707	-0.000076270
8	6	0.000639997	0.001020894	0.000205601
9	6	-0.000250541	0.001117473	0.000224279
10	6	-0.001322760	0.000504174	0.000547097
11	6	0.001467565	-0.000950432	-0.000061118
12	6	0.000093149	0.002486477	-0.000721854
13	6	-0.001335060	0.001120744	-0.000896042
14	6	-0.000967591	0.004137113	0.000597059
15	6	0.001167664	-0.006022656	0.000244175

```
    16        6        0.005779546   0.002431332  -0.000510218
    17        7       -0.000027281  -0.000488366  -0.001855576
    18        7       -0.006883045  -0.003464929   0.001469751
    19        1        0.000134749   0.000036124  -0.000049644
    20        1       -0.000112951   0.000639435   0.000296057
    21        1        0.000133337   0.000393795  -0.000133379
    22        1       -0.000237059  -0.001612954  -0.000387455
    23        1        0.001322952   0.000482226   0.000511432
    24        1       -0.000794620   0.001637595   0.000418289
    25        1       -0.000101768  -0.001775527   0.000454834
    26        1        0.001356103  -0.000461053  -0.000247056
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.006883045 RMS     0.001609945
 Leave Link  716 at Sat Sep 26 02:34:52 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.1
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.009375658 RMS     0.001727675
 Search for a local minimum.
 Step number  14 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .17277D-02 SwitMx=.10000D-02 MixMth= 1
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points   10   11   12   14   13
 DE=  1.57D-04 DEPred=-3.70D-04 R=-4.24D-01
 Trust test=-4.24D-01 RLast= 2.43D-01 DXMaxT set to 7.14D-01
 ITU= -1  1  1  1  1  1  1  1  1  1  0  0  1  0
 Use linear search instead of GDIIS.
    Eigenvalues ---    0.00448   0.00650   0.01120   0.01679   0.01748
    Eigenvalues ---    0.02177   0.02391   0.02674   0.02800   0.02980
    Eigenvalues ---    0.03128   0.03310   0.03615   0.03785   0.04347
    Eigenvalues ---    0.04438   0.04466   0.05026   0.06815   0.07053
    Eigenvalues ---    0.09953   0.10078   0.11051   0.11282   0.11597
    Eigenvalues ---    0.11738   0.13607   0.15116   0.15358   0.15868
    Eigenvalues ---    0.16000   0.16000   0.16000   0.16107   0.16641
    Eigenvalues ---    0.21611   0.22381   0.24421   0.24999   0.24999
    Eigenvalues ---    0.25000   0.25000   0.25001   0.25083   0.28781
    Eigenvalues ---    0.29047   0.34095   0.37231   0.37916   0.43538
    Eigenvalues ---    0.45059   0.45808   0.45926   0.47640   0.47688
    Eigenvalues ---    0.47688   0.47776   0.47856   0.48513   0.50728
    Eigenvalues ---    0.54812   0.55094   0.55383   0.55659   0.55670
    Eigenvalues ---    0.93065   0.93733   0.95026   0.95421   0.97712
    Eigenvalues ---    0.98514   1.36980
 RFO step:  Lambda=-4.46730733D-04 EMin= 4.47522917D-03
```

Supporting Information file

Quartic linear search produced a step of -0.58453.
Iteration 1 RMS(Cart)= 0.03967055 RMS(Int)= 0.00082804
Iteration 2 RMS(Cart)= 0.00134677 RMS(Int)= 0.00002831
Iteration 3 RMS(Cart)= 0.00000141 RMS(Int)= 0.00002831
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002831
ITry= 1 IFail=0 DXMaxC= 1.53D-01 DCOld= 1.00D+10 DXMaxT= 7.14D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.32599	-0.00051	0.00214	-0.00214	-0.00000	2.32599
R2	2.52907	0.00042	-0.00278	0.00298	0.00020	2.52927
R3	2.52839	0.00009	-0.00302	0.00276	-0.00026	2.52812
R4	2.32595	-0.00043	0.00216	-0.00214	0.00002	2.32596
R5	2.32160	-0.00020	0.00215	-0.00185	0.00031	2.32191
R6	2.52846	0.00005	-0.00304	0.00276	-0.00028	2.52818
R7	2.53234	-0.00027	-0.00306	0.00232	-0.00074	2.53160
R8	2.32149	0.00002	0.00220	-0.00184	0.00036	2.32185
R9	2.31916	0.00067	0.00148	-0.00065	0.00083	2.31999
R10	2.53248	-0.00033	-0.00309	0.00231	-0.00078	2.53170
R11	2.62569	-0.00021	-0.00211	0.00194	-0.00017	2.62553
R12	2.31890	0.00132	0.00161	-0.00063	0.00098	2.31988
R13	2.69637	-0.00034	0.00596	-0.00500	0.00097	2.69734
R14	2.69620	-0.00331	-0.01063	0.00574	-0.00489	2.69131
R15	2.62601	-0.00037	-0.00218	0.00188	-0.00030	2.62571
R16	2.69289	0.00212	-0.00835	0.00617	-0.00219	2.69070
R17	2.80573	0.00090	0.00185	0.00097	0.00283	2.80855
R18	2.05229	-0.00022	-0.00309	0.00148	-0.00161	2.05068
R19	2.80496	0.00428	0.00230	0.00107	0.00337	2.80833
R20	2.05216	-0.00027	-0.00314	0.00157	-0.00157	2.05059
R21	1.94838	0.00013	-0.00220	0.00253	0.00033	1.94871
R22	1.91707	0.00032	-0.00104	0.00161	0.00056	1.91763
R23	1.92205	0.00111	0.00039	0.00171	0.00209	1.92415
R24	1.94848	-0.00011	-0.00227	0.00248	0.00021	1.94869
R25	1.91685	0.00086	-0.00085	0.00162	0.00077	1.91763
R26	1.92217	0.00091	0.00032	0.00169	0.00200	1.92417
A1	2.56620	-0.00039	-0.00114	-0.00037	-0.00151	2.56468
A2	2.60335	0.00041	0.00137	0.00015	0.00151	2.60486
A3	2.56660	-0.00024	-0.00113	-0.00026	-0.00139	2.56521
A4	2.72997	-0.00070	-0.00233	-0.00001	-0.00235	2.72763
A5	2.60280	0.00044	0.00152	0.00004	0.00156	2.60436
A6	2.82539	0.00092	0.00269	0.00100	0.00370	2.82909
A7	2.73005	-0.00042	-0.00217	0.00006	-0.00211	2.72794
A8	2.82501	0.00104	0.00287	0.00093	0.00381	2.82883
A9	2.08745	0.00140	0.00083	-0.00012	0.00066	2.08811
A10	2.11109	-0.00164	-0.00185	-0.00139	-0.00332	2.10777
A11	2.08462	0.00024	0.00103	0.00137	0.00232	2.08694
A12	2.08942	-0.00111	-0.00082	-0.00040	-0.00130	2.08811
A13	2.08475	0.00039	0.00106	0.00149	0.00244	2.08720

A14	2.10901	0.00072	-0.00025	-0.00113	-0.00150	2.10751
A15	2.03056	0.00474	0.03307	-0.00837	0.02470	2.05526
A16	1.94374	-0.00158	0.00755	-0.00830	-0.00075	1.94298
A17	2.04149	0.00033	0.02453	-0.00914	0.01539	2.05688
A18	1.95447	-0.00580	-0.00108	-0.00847	-0.00955	1.94491
A19	2.00206	-0.00036	-0.00704	0.00429	-0.00274	1.99931
A20	1.90427	0.00096	0.00230	0.00359	0.00590	1.91016
A21	1.92031	0.00006	-0.00008	0.00067	0.00060	1.92092
A22	1.90041	-0.00006	0.00277	-0.00290	-0.00013	1.90028
A23	1.85399	-0.00062	-0.00153	-0.00282	-0.00433	1.84966
A24	1.87869	-0.00000	0.00412	-0.00353	0.00059	1.87928
A25	2.00275	-0.00114	-0.00792	0.00424	-0.00368	1.99907
A26	1.90266	0.00221	0.00371	0.00381	0.00751	1.91018
A27	1.92075	0.00005	-0.00016	0.00074	0.00059	1.92134
A28	1.90023	-0.00008	0.00287	-0.00298	-0.00011	1.90012
A29	1.85429	-0.00069	-0.00179	-0.00280	-0.00457	1.84972
A30	1.87910	-0.00041	0.00380	-0.00370	0.00009	1.87920
A31	2.91282	-0.00050	0.00109	-0.00243	-0.00133	2.91149
A32	3.12311	-0.00022	-0.00155	0.00185	0.00032	3.12343
A33	2.91081	-0.00005	0.00295	-0.00243	0.00053	2.91134
A34	3.12590	-0.00056	-0.00413	0.00208	-0.00204	3.12386
A35	3.97430	0.00316	0.04061	-0.01667	0.02395	3.99825
A36	3.99596	-0.00547	0.02345	-0.01761	0.00584	4.00180
A37	3.14682	0.00025	-0.00015	0.00328	0.00309	3.14991
A38	3.13603	-0.00002	-0.00598	0.00941	0.00345	3.13948
A39	3.14679	0.00017	-0.00016	0.00339	0.00318	3.14997
A40	3.12954	0.00060	-0.00060	0.00944	0.00887	3.13840
A41	3.99704	0.00436	-0.01325	0.00790	-0.00536	3.99169
A42	4.04873	-0.00938	-0.05689	-0.00543	-0.06232	3.98640
D1	0.02144	0.00005	-0.00299	0.00308	0.00008	0.02152
D2	-0.02104	0.00015	0.00198	0.00127	0.00323	-0.01780
D3	-0.01591	-0.00002	-0.00067	0.00145	0.00079	-0.01512
D4	0.02099	0.00016	-0.00264	0.00312	0.00047	0.02146
D5	0.00843	-0.00007	-0.00037	0.00030	-0.00003	0.00840
D6	-0.01690	0.00014	0.00010	0.00150	0.00161	-0.01529
D7	-0.00331	0.00017	0.00367	0.00630	0.00999	0.00668
D8	3.12846	-0.00027	0.00096	-0.01008	-0.00905	3.11941
D9	0.00787	0.00009	0.00008	0.00036	0.00047	0.00834
D10	-0.00744	0.00029	0.00711	0.00637	0.01351	0.00608
D11	3.12456	-0.00023	0.00470	-0.01148	-0.00673	3.11783
D12	0.01471	-0.00045	-0.00373	-0.01465	-0.01835	-0.00364
D13	-3.12514	0.00052	-0.00128	0.01000	0.00874	-3.11640
D14	-3.12017	0.00004	-0.00494	0.00850	0.00361	-3.11656
D15	0.02317	0.00101	-0.00248	0.03315	0.03070	0.05387
D16	2.45785	0.00149	0.03158	0.01156	0.04312	2.50097
D17	-0.69055	0.00101	0.03281	-0.01191	0.02092	-0.66963
D18	-0.67442	-0.00014	0.02127	-0.01146	0.00981	-0.66461
D19	2.46893	0.00084	0.02375	0.01347	0.03721	2.50614

D20	-1.53104	0.00031	-0.04100	0.03685	-0.00416	-1.53520
D21	0.60601	0.00071	-0.04058	0.03883	-0.00175	0.60426
D22	2.66340	0.00131	-0.03423	0.03708	0.00286	2.66625
D23	-1.53574	0.00011	-0.04109	0.03709	-0.00402	-1.53976
D24	0.60033	0.00090	-0.04009	0.03908	-0.00101	0.59932
D25	2.65752	0.00175	-0.03334	0.03728	0.00396	2.66148

Item	Value	Threshold	Converged?
Maximum Force	0.009376	0.000450	NO
RMS Force	0.001728	0.000300	NO
Maximum Displacement	0.152528	0.001800	NO
RMS Displacement	0.039722	0.001200	NO

Predicted change in Energy=-3.765332D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 02:34:52 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.012860	0.667764	0.044870
2	6	0	3.341652	1.697545	0.108474
3	6	0	4.012704	-0.667634	-0.045246
4	6	0	2.141324	2.286657	0.152454
5	6	0	3.341803	-1.697612	-0.108664
6	6	0	0.913782	2.339596	0.159335
7	6	0	2.141323	-2.286515	-0.152236
8	6	0	-0.377649	1.983797	0.141515
9	6	0	0.913817	-2.339620	-0.158622
10	6	0	-1.455496	1.397708	0.097286
11	6	0	-0.377611	-1.983650	-0.140158
12	6	0	-2.663018	0.712245	0.048558
13	6	0	-1.455229	-1.397307	-0.095296
14	6	0	-2.662924	-0.711900	-0.047322
15	6	0	-3.901279	1.411242	0.128571
16	6	0	-3.900605	-1.411156	-0.128304
17	7	0	-3.724070	2.878027	-0.032662
18	7	0	-3.724554	-2.878063	0.031979
19	1	0	-3.112576	3.152166	-0.816453
20	1	0	-4.631037	3.316443	-0.154932
21	1	0	-3.114154	-3.152961	0.816335
22	1	0	-4.631917	-3.315957	0.153173
23	1	0	-3.300271	3.272767	0.804797
24	1	0	-4.727940	1.045277	-0.471680
25	1	0	-4.730223	-1.043926	0.466991
26	1	0	-3.300197	-3.272854	-0.805190

Supporting Information file

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.230859	0.000000			
3	C	1.338435	2.463333	0.000000		
4	C	2.476900	1.337825	3.502710	0.000000	
5	C	2.463512	3.402093	1.230847	4.169380	0.000000
6	C	3.523124	2.511846	4.323031	1.228702	4.718703
7	C	3.502751	4.169111	2.476749	4.583311	1.337855
8	C	4.584523	3.730447	5.132267	2.537138	5.239245
9	C	4.323173	4.718519	3.522994	4.796455	2.511928
10	C	5.517108	4.806523	5.846978	3.705454	5.712923
11	C	5.132296	5.238887	4.584296	4.966506	3.730529
12	C	6.676027	6.085267	6.817487	5.056805	6.472248
13	C	5.846722	5.712241	5.516631	5.154432	4.806441
14	C	6.817482	6.471834	6.675775	5.666750	6.085403
15	C	7.949425	7.248616	8.184318	6.105733	7.885651
16	C	8.183814	7.884819	7.948596	7.089256	7.248097
17	N	8.046823	7.165046	8.510554	5.898037	8.418361
18	N	8.511206	8.418629	8.047181	7.816482	7.165657
19	H	7.595127	6.680455	8.121283	5.412149	8.104339
20	H	9.042808	8.139656	9.518359	6.857101	9.418549
21	H	8.123264	8.105918	7.596794	7.592775	6.682293
22	H	9.519134	9.418864	9.043365	8.790112	8.140503
23	H	7.800347	6.861584	8.350385	5.568566	8.346031
24	H	8.764184	8.116672	8.917105	7.008378	8.530883
25	H	8.919056	8.532255	8.766000	7.642636	8.118885
26	H	8.350561	8.345886	7.800206	7.838074	6.861683

		6	7	8	9	10
6	C	0.000000				
7	C	4.796336	0.000000			
8	C	1.339666	4.966596	0.000000		
9	C	4.690006	1.228671	4.522157	0.000000	
10	C	2.550389	5.154888	1.227686	4.432466	0.000000
11	C	4.521930	2.537106	3.977434	1.339718	3.556936
12	C	3.931163	5.666972	2.616945	4.706437	1.389368
13	C	4.431873	3.705283	3.556561	2.550361	2.801642
14	C	4.706077	5.056798	3.539057	3.931277	2.435003
15	C	4.903835	7.089803	3.569868	6.110368	2.446020
16	C	6.109763	6.105057	4.899972	4.903226	3.730839
17	N	4.672948	7.815986	3.468216	6.982099	2.711948
18	N	6.982432	5.898507	5.903513	4.673408	4.840982
19	H	4.221847	7.591040	3.124518	6.841366	2.580495
20	H	5.638973	8.789653	4.467117	7.920636	3.718766
21	H	6.842814	5.413770	5.859192	4.223342	4.896608
22	H	7.920864	6.857828	6.796052	5.639647	5.684312
23	H	4.364135	7.837888	3.262378	7.084180	2.723897

```
  24  H    5.822583   7.641313   4.492423   6.586726   3.340183
  25  H    6.587691   7.010394   5.312057   5.824552   4.101475
  26  H    7.084316   5.568605   6.088508   4.364275   5.102111
                11         12         13         14         15
  11  C    0.000000
  12  C    3.539286   0.000000
  13  C    1.227628   2.435089   0.000000
  14  C    2.616987   1.427369   1.389465   0.000000
  15  C    4.900382   1.424180   3.731116   2.464182   0.000000
  16  C    3.569226   2.464088   2.445638   1.423858   2.834063
  17  N    5.903071   2.413098   4.840460   3.743504   1.486222
  18  N    3.468665   3.743988   2.712688   2.413630   4.294031
  19  H    5.857816   2.627463   4.895362   3.965445   2.132120
  20  H    6.795795   3.270528   5.684079   4.484707   2.059784
  21  H    3.125834   3.966462   2.581749   2.628363   4.682365
  22  H    4.467684   4.484853   3.719449   3.270817   4.783393
  23  H    6.088087   2.744862   5.101367   4.124305   2.069727
  24  H    5.311277   2.155333   4.101039   2.744457   1.085173
  25  H    4.494101   2.744551   3.341651   2.156035   2.613337
  26  H    3.262794   4.125033   2.724983   2.745718   4.813935
                16         17         18         19         20
  16  C    0.000000
  17  N    4.293880   0.000000
  18  N    1.486103   5.756454   0.000000
  19  H    4.681713   1.031215   6.120295   0.000000
  20  H    4.783767   1.014765   6.263270   1.664428   0.000000
  21  H    2.131839   6.120916   1.031200   6.513112   6.715466
  22  H    2.059688   6.262919   1.014763   6.714550   6.639552
  23  H    4.813545   1.018215   6.213693   1.636528   1.641319
  24  H    2.614661   2.135291   4.080815   2.677172   2.295194
  25  H    1.085127   4.079671   2.136508   4.676665   4.405615
  26  H    2.069924   6.213679   1.018229   6.427769   6.753725
                21         22         23         24         25
  21  H    0.000000
  22  H    1.664318   0.000000
  23  H    6.428434   6.753457   0.000000
  24  H    4.678514   4.406815   2.937575   0.000000
  25  H    2.679879   2.295707   4.559904   2.290388   0.000000
  26  H    1.636561   1.641278   6.740714   4.560256   2.937948
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 1.28D-02
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
```

Supporting Information file

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.517403	-0.668845	-0.021370
2	6	0	3.846197	-1.700219	-0.049016
3	6	0	4.517245	0.668883	0.022109
4	6	0	2.645870	-2.290509	-0.072424
5	6	0	3.846342	1.700446	0.049558
6	6	0	1.418328	-2.343657	-0.077459
7	6	0	2.645862	2.290508	0.072558
8	6	0	0.126896	-1.987456	-0.072066
9	6	0	1.418356	2.343802	0.077082
10	6	0	-0.950952	-1.400181	-0.048312
11	6	0	0.126927	1.987402	0.071043
12	6	0	-2.158475	-0.713437	-0.023528
13	6	0	-0.950689	1.399850	0.046656
14	6	0	-2.158383	0.713185	0.022616
15	6	0	-3.396735	-1.414803	-0.079114
16	6	0	-3.396065	1.414838	0.079153
17	7	0	-3.219524	-2.875071	0.133186
18	7	0	-3.220016	2.875262	-0.132201
19	1	0	-2.608033	-3.121701	0.926065
20	1	0	-4.126491	-3.308955	0.270672
21	1	0	-2.609613	3.122634	-0.925667
22	1	0	-4.127378	3.308660	-0.268600
23	1	0	-2.795722	-3.298782	-0.689992
24	1	0	-4.223399	-1.028123	0.508002
25	1	0	-4.225681	1.027066	-0.502973
26	1	0	-2.795663	3.299016	0.690688

Rotational constants (GHZ): 0.6003689 0.2712430 0.1874571
Leave Link 202 at Sat Sep 26 02:34:52 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1009.8980973706 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0154101663 Hartrees.
Nuclear repulsion after empirical dispersion term = 1009.8826872042 Hartrees.
Leave Link 301 at Sat Sep 26 02:34:52 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23220 LenP2D= 51932.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.81D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 02:34:53 2026, MaxMem= 805306368 cpu: 8.6 elap: 1.4
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 02:34:54 2026, MaxMem= 805306368 cpu: 1.0 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Lowest energy guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 0.000000 -0.000000
Rot= 0.999999 -0.000024 0.000039 0.001442 Ang= -0.17 deg.
Guess basis will be translated and rotated to current coordinates.
B after Tr= -0.000000 0.000000 -0.000000
Rot= 0.999993 -0.000110 -0.000121 -0.003626 Ang= -0.42 deg.
Guess basis will be translated and rotated to current coordinates.
CkInt1: FT= 4.15D-01
Max alpha theta= 1.776 degrees.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Sat Sep 26 02:34:56 2026, MaxMem= 805306368 cpu: 12.1 elap: 2.1
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666

Supporting Information file

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.411291503359
DIIS: error= 1.51D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.411291503359 IErMin= 1 ErrMin= 1.51D-03
ErrMax= 1.51D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-03 BMatP= 2.09D-03
IDIUse=3 WtCom= 9.85D-01 WtEn= 1.51D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 10.559 Goal= None Shift= 0.000
GapD= 10.559 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=1.08D-02 MaxDP=3.88D-01 OVMax= 8.40D-03

Cycle 2 Pass 0 IDiag 1:
RMSU= 8.52D-03 CP: 1.60D+00
E= -723.412884570865 Delta-E= -0.001593067506 Rises=F Damp=F
DIIS: error= 7.93D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.412884570865 IErMin= 2 ErrMin= 7.93D-04
ErrMax= 7.93D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-04 BMatP= 2.09D-03
IDIUse=3 WtCom= 9.92D-01 WtEn= 7.93D-03
Coeff-Com: 0.241D-01 0.976D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.239D-01 0.976D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=9.47D-03 MaxDP=3.25D-01 DE=-1.59D-03 OVMax= 3.60D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 3.83D-03 CP: 1.04D+00 2.85D-01
E= -723.412976814609 Delta-E= -0.000092243744 Rises=F Damp=F
DIIS: error= 5.02D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.412976814609 IErMin= 2 ErrMin= 7.93D-04
ErrMax= 5.02D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.52D-04 BMatP= 1.56D-04
IDIUse=3 WtCom= 1.24D-01 WtEn= 8.76D-01
Coeff-Com: -0.128D-01 0.791D+00 0.221D+00

Coeff-En: 0.000D+00 0.107D-01 0.989D+00
Coeff: -0.158D-02 0.107D+00 0.894D+00
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=8.21D+02 MaxDP=3.38D+04 DE=-9.22D-05 OVMax= 9.73D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.412747486314 Delta-E= 0.000229328295 Rises=F Damp=F
DIIS: error= 8.91D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.412747486314 IErMin= 1 ErrMin= 8.91D-04
ErrMax= 8.91D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-04 BMatP= 2.01D-04
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.91D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=4.79D-03 MaxDP=1.29D-01 DE= 2.29D-04 OVMax= 2.49D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.73D-03 CP: 7.56D-01
E= -723.412873602104 Delta-E= -0.000126115790 Rises=F Damp=F
DIIS: error= 1.14D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.412873602104 IErMin= 2 ErrMin= 1.14D-04
ErrMax= 1.14D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.51D-06 BMatP= 2.01D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.14D-03
Coeff-Com: 0.248D-01 0.975D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.248D-01 0.975D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.68D-04 MaxDP=1.13D-02 DE=-1.26D-04 OVMax= 1.73D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.23D-04 CP: 7.59D-01 1.04D+00
E= -723.412872953600 Delta-E= 0.000000648504 Rises=F Damp=F
DIIS: error= 1.40D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.412873602104 IErMin= 2 ErrMin= 1.14D-04
ErrMax= 1.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.66D-06 BMatP= 6.51D-06
IDIUse=3 WtCom= 4.58D-01 WtEn= 5.42D-01
Coeff-Com: -0.172D-01 0.544D+00 0.473D+00
Coeff-En: 0.000D+00 0.522D+00 0.478D+00
Coeff: -0.790D-02 0.532D+00 0.476D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.89D-05 MaxDP=1.88D-03 DE= 6.49D-07 OVMax= 7.48D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.28D-05 CP: 7.60D-01 1.04D+00 1.14D+00
E= -723.412881390552 Delta-E= -0.000008436952 Rises=F Damp=F

DIIS: error= 4.58D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.412881390552 IErMin= 4 ErrMin= 4.58D-05
ErrMax= 4.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-07 BMatP= 6.51D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.950D-02 0.238D+00 0.251D+00 0.521D+00
Coeff: -0.950D-02 0.238D+00 0.251D+00 0.521D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.19D-05 MaxDP=1.06D-03 DE=-8.44D-06 OVMax= 3.55D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 4.09D-06 CP: 7.61D-01 1.04D+00 1.22D+00 1.37D+00
E= -723.412881943482 Delta-E= -0.000000552930 Rises=F Damp=F
DIIS: error= 2.13D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.412881943482 IErMin= 5 ErrMin= 2.13D-05
ErrMax= 2.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.79D-08 BMatP= 3.39D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.508D-02-0.174D+00-0.134D+00 0.171D+00 0.113D+01
Coeff: 0.508D-02-0.174D+00-0.134D+00 0.171D+00 0.113D+01
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=3.26D-05 MaxDP=1.59D-03 DE=-5.53D-07 OVMax= 6.27D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 2.53D-06 CP: 7.63D-01 1.04D+00 1.33D+00 2.04D+00 2.57D+00
E= -723.412882330406 Delta-E= -0.000000386924 Rises=F Damp=F
DIIS: error= 9.04D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.412882330406 IErMin= 6 ErrMin= 9.04D-06
ErrMax= 9.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-08 BMatP= 5.79D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.333D-02-0.999D-01-0.846D-01-0.470D-02 0.363D+00 0.823D+00
Coeff: 0.333D-02-0.999D-01-0.846D-01-0.470D-02 0.363D+00 0.823D+00
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=5.92D-06 MaxDP=2.71D-04 DE=-3.87D-07 OVMax= 3.08D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.12D-06 CP: 7.63D-01 1.04D+00 1.35D+00 2.19D+00 2.94D+00
CP: 1.21D+00
E= -723.412882420402 Delta-E= -0.000000089995 Rises=F Damp=F
DIIS: error= 8.13D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.412882420402 IErMin= 7 ErrMin= 8.13D-06
ErrMax= 8.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.12D-09 BMatP= 1.24D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.870D-03 0.380D-01 0.275D-01-0.880D-01-0.446D+00 0.479D+00
Coeff-Com: 0.990D+00
Coeff: -0.870D-03 0.380D-01 0.275D-01-0.880D-01-0.446D+00 0.479D+00
Coeff: 0.990D+00
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=2.72D-06 MaxDP=1.00D-04 DE=-9.00D-08 OVMax= 2.81D-04

```
Cycle  11  Pass 1  IDiag  1:
RMSU=  9.89D-07    CP:  7.63D-01  1.04D+00  1.35D+00  2.25D+00  3.00D+00
               CP:  1.33D+00  2.27D+00
E= -723.412882468091     Delta-E=       -0.000000047690 Rises=F Damp=F
DIIS: error= 1.82D-06 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -723.412882468091     IErMin= 8 ErrMin= 1.82D-06
ErrMax= 1.82D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-09 BMatP= 6.12D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.104D-02 0.369D-01 0.300D-01-0.384D-01-0.286D+00 0.787D-01
Coeff-Com:  0.492D+00 0.688D+00
Coeff:     -0.104D-02 0.369D-01 0.300D-01-0.384D-01-0.286D+00 0.787D-01
Coeff:      0.492D+00 0.688D+00
Gap=     0.178 Goal=   None    Shift=    0.000
RMSDP=1.06D-06 MaxDP=5.13D-05 DE=-4.77D-08 OVMax= 9.12D-05

Cycle  12  Pass 1  IDiag  1:
RMSU=  3.57D-07    CP:  7.63D-01  1.04D+00  1.35D+00  2.23D+00  3.00D+00
               CP:  1.29D+00  2.70D+00  1.13D+00
E= -723.412882473056     Delta-E=       -0.000000004964 Rises=F Damp=F
DIIS: error= 1.56D-06 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.412882473056     IErMin= 9 ErrMin= 1.56D-06
ErrMax= 1.56D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-10 BMatP= 1.25D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.278D-03 0.806D-02 0.797D-02 0.525D-02-0.302D-01-0.814D-01
Coeff-Com: -0.683D-02 0.322D+00 0.775D+00
Coeff:     -0.278D-03 0.806D-02 0.797D-02 0.525D-02-0.302D-01-0.814D-01
Coeff:     -0.683D-02 0.322D+00 0.775D+00
Gap=     0.178 Goal=   None    Shift=    0.000
RMSDP=7.78D-07 MaxDP=3.42D-05 DE=-4.96D-09 OVMax= 3.11D-05

Cycle  13  Pass 1  IDiag  1:
RMSU=  1.49D-07    CP:  7.63D-01  1.04D+00  1.34D+00  2.21D+00  3.00D+00
               CP:  1.25D+00  2.86D+00  1.13D+00  1.96D+00
E= -723.412882474074     Delta-E=       -0.000000001018 Rises=F Damp=F
DIIS: error= 5.55D-07 at cycle  10 NSaved=  10.
NSaved=10 IEnMin=10 EnMin= -723.412882474074     IErMin=10 ErrMin= 5.55D-07
ErrMax= 5.55D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 6.95D-11 BMatP= 2.73D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.129D-03-0.552D-02-0.363D-02 0.133D-01 0.583D-01-0.618D-01
Coeff-Com: -0.134D+00-0.164D-01 0.406D+00 0.744D+00
Coeff:      0.129D-03-0.552D-02-0.363D-02 0.133D-01 0.583D-01-0.618D-01
Coeff:     -0.134D+00-0.164D-01 0.406D+00 0.744D+00
Gap=     0.178 Goal=   None    Shift=    0.000
RMSDP=3.88D-07 MaxDP=1.56D-05 DE=-1.02D-09 OVMax= 1.55D-05

Cycle  14  Pass 1  IDiag  1:
RMSU=  5.95D-08    CP:  7.63D-01  1.04D+00  1.34D+00  2.20D+00  3.00D+00
               CP:  1.23D+00  2.89D+00  1.12D+00  2.50D+00  1.35D+00
```

E= -723.412882474299 Delta-E= -0.000000000225 Rises=F Damp=F
DIIS: error= 3.88D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.412882474299 IErMin=11 ErrMin= 3.88D-07
ErrMax= 3.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-11 BMatP= 6.95D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.905D-04-0.338D-02-0.251D-02 0.494D-02 0.282D-01-0.151D-01
Coeff-Com: -0.558D-01-0.490D-01 0.623D-01 0.336D+00 0.694D+00
Coeff: 0.905D-04-0.338D-02-0.251D-02 0.494D-02 0.282D-01-0.151D-01
Coeff: -0.558D-01-0.490D-01 0.623D-01 0.336D+00 0.694D+00
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=8.34D-08 MaxDP=3.91D-06 DE=-2.25D-10 OVMax= 4.17D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 2.44D-08 CP: 7.63D-01 1.04D+00 1.34D+00 2.20D+00 3.00D+00
CP: 1.22D+00 2.89D+00 1.12D+00 2.62D+00 1.50D+00
CP: 1.35D+00
E= -723.412882474329 Delta-E= -0.000000000030 Rises=F Damp=F
DIIS: error= 1.08D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.412882474329 IErMin=12 ErrMin= 1.08D-07
ErrMax= 1.08D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-12 BMatP= 1.06D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.723D-05-0.910D-04-0.186D-03-0.129D-02-0.265D-02 0.945D-02
Coeff-Com: 0.910D-02-0.195D-01-0.808D-01-0.337D-01 0.310D+00 0.809D+00
Coeff: 0.723D-05-0.910D-04-0.186D-03-0.129D-02-0.265D-02 0.945D-02
Coeff: 0.910D-02-0.195D-01-0.808D-01-0.337D-01 0.310D+00 0.809D+00
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=3.66D-08 MaxDP=1.60D-06 DE=-2.96D-11 OVMax= 2.29D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.12D-08 CP: 7.63D-01 1.04D+00 1.34D+00 2.20D+00 3.00D+00
CP: 1.22D+00 2.89D+00 1.12D+00 2.66D+00 1.56D+00
CP: 1.62D+00 1.81D+00
E= -723.412882474328 Delta-E= 0.000000000001 Rises=F Damp=F
DIIS: error= 5.10D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=12 EnMin= -723.412882474329 IErMin=13 ErrMin= 5.10D-08
ErrMax= 5.10D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.37D-13 BMatP= 2.27D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.161D-04 0.696D-03 0.456D-03-0.176D-02-0.759D-02 0.867D-02
Coeff-Com: 0.175D-01 0.471D-03-0.582D-01-0.943D-01 0.172D-01 0.434D+00
Coeff-Com: 0.683D+00
Coeff: -0.161D-04 0.696D-03 0.456D-03-0.176D-02-0.759D-02 0.867D-02
Coeff: 0.175D-01 0.471D-03-0.582D-01-0.943D-01 0.172D-01 0.434D+00
Coeff: 0.683D+00
Gap= 0.178 Goal= None Shift= 0.000
RMSDP=1.70D-08 MaxDP=9.26D-07 DE= 6.82D-13 OVMax= 8.86D-07

Cycle 17 Pass 1 IDiag 1:
RMSU= 5.35D-09 CP: 7.63D-01 1.04D+00 1.34D+00 2.20D+00 3.00D+00

```
               CP:  1.21D+00  2.89D+00  1.12D+00  2.66D+00  1.57D+00
               CP:  1.71D+00  2.22D+00  1.52D+00
 E= -723.412882474336     Delta-E=       -0.000000000008 Rises=F Damp=F
 DIIS: error= 2.13D-08 at cycle  14 NSaved=  14.
 NSaved=14 IEnMin=14 EnMin= -723.412882474336     IErMin=14 ErrMin= 2.13D-08
 ErrMax= 2.13D-08  0.00D+00 EMaxC= 1.00D-01 BMatC= 5.13D-14 BMatP= 6.37D-13
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: -0.282D-05 0.881D-04 0.723D-04 0.222D-06-0.291D-03-0.491D-03
 Coeff-Com:  0.566D-03 0.338D-02 0.597D-02-0.658D-02-0.468D-01-0.747D-01
 Coeff-Com:  0.735D-01 0.105D+01
 Coeff:     -0.282D-05 0.881D-04 0.723D-04 0.222D-06-0.291D-03-0.491D-03
 Coeff:      0.566D-03 0.338D-02 0.597D-02-0.658D-02-0.468D-01-0.747D-01
 Coeff:      0.735D-01 0.105D+01
 Gap=     0.178 Goal=   None    Shift=    0.000
 RMSDP=9.28D-09 MaxDP=5.00D-07 DE=-7.96D-12 OVMax= 5.19D-07

 SCF Done:  E(RwB97XD) =  -723.412882474     A.U. after   17 cycles
          NFock= 17  Conv=0.93D-08     -V/T= 2.0047
 KE= 7.200517590388D+02 PE=-3.700917821495D+03 EE= 1.247570492777D+03
 Leave Link  502 at Sat Sep 26 02:51:20 2026, MaxMem=    805306368 cpu:             5900.5 elap:
983.7
 (Enter /home/user/gauss16/g16/l701.exe)
 ... and contract with generalized density number  0.
 Compute integral first derivatives.
 R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23220 LenP2D=   51932.
 LDataN:  DoStor=T MaxTD1= 7 Len=  274
 Leave Link  701 at Sat Sep 26 02:51:20 2026, MaxMem=    805306368 cpu:                2.9 elap:
0.5
 (Enter /home/user/gauss16/g16/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link  702 at Sat Sep 26 02:51:20 2026, MaxMem=    805306368 cpu:                0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l703.exe)
 Integral derivatives from FoFJK, PRISM(SPDF).
 Compute integral first derivatives, UseDBF=F ICtDFT=          0.
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 FoFJK:  IHMeth= 1 ICntrl=    2127 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=         800
       NFxFlg=          0 DoJE=F BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=      2527 IOpCl=  0 I1Cent=          0 NGrid=          0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 Leave Link  703 at Sat Sep 26 03:01:24 2026, MaxMem=    805306368 cpu:             3621.6 elap:
603.7
```

Supporting Information file

(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.67348988D+00 4.93643576D-03 3.26659661D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000051443	0.000770606	0.000012023
2	6	-0.000069351	-0.000757081	0.000002220
3	6	0.000032706	-0.000766916	-0.000012467
4	6	-0.000087898	0.000887452	0.000058168
5	6	-0.000047801	0.000752127	-0.000005373
6	6	0.000102179	-0.000922771	0.000036415
7	6	-0.000112006	-0.000883279	-0.000056318
8	6	0.000235354	0.000501147	-0.000057686
9	6	0.000139869	0.000905885	-0.000025511
10	6	-0.000776092	0.000219698	-0.000061032
11	6	0.000203898	-0.000462936	0.000084191
12	6	-0.000573862	0.000464899	0.001410127
13	6	-0.000732610	-0.000297845	0.000002804
14	6	-0.000697443	-0.000507795	-0.001369297
15	6	0.000869835	-0.002601226	0.000320501
16	6	0.000922059	0.002679752	-0.000408558
17	7	-0.000696205	0.000220117	-0.001206046
18	7	-0.000724093	-0.000111019	0.001260156
19	1	-0.000251337	-0.000044364	0.000113514
20	1	0.000032825	0.000340041	0.000326591
21	1	-0.000245770	0.000047429	-0.000119733
22	1	0.000019310	-0.000340544	-0.000317593
23	1	0.000913364	0.000033421	0.000066935
24	1	0.000250767	0.001024177	-0.000426767
25	1	0.000313393	-0.001134037	0.000448458
26	1	0.000927466	-0.000016937	-0.000075724

Cartesian Forces: Max 0.002679752 RMS 0.000695716
Leave Link 716 at Sat Sep 26 03:01:24 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002031966 RMS 0.000583946
Search for a local minimum.
Step number 15 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .58395D-03 SwitMx=.10000D-02 MixMth= 2

Supporting Information file

Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 11 12 14 13 15
DE= -4.09D-04 DEPred=-3.77D-04 R= 1.09D+00
TightC=F SS= 1.41D+00 RLast= 1.94D-01 DXNew= 1.2000D+00 5.8195D-01
Trust test= 1.09D+00 RLast= 1.94D-01 DXMaxT set to 7.14D-01
ITU= 1 -1 1 1 1 1 1 1 1 1 1 0 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00412	0.00447	0.01119	0.01679	0.01752
Eigenvalues ---	0.02050	0.02393	0.02643	0.02800	0.02943
Eigenvalues ---	0.03124	0.03465	0.03634	0.03789	0.04359
Eigenvalues ---	0.04438	0.04466	0.05026	0.07005	0.07148
Eigenvalues ---	0.09871	0.09955	0.11290	0.11333	0.11712
Eigenvalues ---	0.11766	0.14536	0.15246	0.15291	0.15678
Eigenvalues ---	0.15914	0.16000	0.16000	0.16002	0.16222
Eigenvalues ---	0.21495	0.22117	0.24525	0.24997	0.24998
Eigenvalues ---	0.24998	0.25000	0.25000	0.25150	0.28399
Eigenvalues ---	0.29667	0.33541	0.37232	0.38580	0.44330
Eigenvalues ---	0.44637	0.45839	0.46816	0.47609	0.47688
Eigenvalues ---	0.47688	0.47759	0.47859	0.50262	0.53777
Eigenvalues ---	0.54810	0.55363	0.55643	0.55659	0.59884
Eigenvalues ---	0.92780	0.93731	0.95027	0.95408	0.97715
Eigenvalues ---	0.98522	1.37097			

RFO step: Lambda=-3.85175544D-04 EMin= 4.12306900D-03
Quartic linear search produced a step of 0.16690.
Iteration 1 RMS(Cart)= 0.02865232 RMS(Int)= 0.00067733
Iteration 2 RMS(Cart)= 0.00168370 RMS(Int)= 0.00000630
Iteration 3 RMS(Cart)= 0.00000192 RMS(Int)= 0.00000615
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000615
ITry= 1 IFail=0 DXMaxC= 1.06D-01 DCOld= 1.00D+10 DXMaxT= 7.14D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.32599	-0.00030	-0.00061	-0.00162	-0.00223	2.32376
R2	2.52927	0.00038	0.00083	0.00196	0.00278	2.53206
R3	2.52812	0.00014	0.00082	0.00169	0.00250	2.53063
R4	2.32596	-0.00030	-0.00061	-0.00161	-0.00223	2.32374
R5	2.32191	-0.00013	-0.00056	-0.00129	-0.00186	2.32005
R6	2.52818	0.00015	0.00082	0.00172	0.00254	2.53072
R7	2.53160	-0.00011	0.00075	0.00126	0.00201	2.53361
R8	2.32185	-0.00014	-0.00057	-0.00130	-0.00187	2.31999
R9	2.31999	0.00025	-0.00028	-0.00004	-0.00033	2.31966
R10	2.53170	-0.00009	0.00075	0.00133	0.00208	2.53378
R11	2.62553	-0.00032	0.00057	0.00007	0.00064	2.62617
R12	2.31988	0.00023	-0.00030	-0.00003	-0.00033	2.31955
R13	2.69734	-0.00021	-0.00154	-0.00343	-0.00497	2.69237
R14	2.69131	-0.00152	0.00222	0.00407	0.00629	2.69760
R15	2.62571	-0.00026	0.00057	0.00021	0.00078	2.62649
R16	2.69070	-0.00165	0.00202	0.00446	0.00648	2.69718

R17	2.80855	0.00062	-0.00006	0.00843	0.00838	2.81693
R18	2.05068	-0.00030	0.00061	0.00181	0.00243	2.05311
R19	2.80833	0.00049	-0.00009	0.00844	0.00835	2.81668
R20	2.05059	-0.00038	0.00063	0.00159	0.00223	2.05282
R21	1.94871	-0.00025	0.00068	0.00069	0.00138	1.95009
R22	1.91763	0.00008	0.00039	0.00125	0.00164	1.91927
R23	1.92415	0.00045	0.00024	0.00117	0.00141	1.92556
R24	1.94869	-0.00025	0.00068	0.00065	0.00133	1.95001
R25	1.91763	0.00009	0.00037	0.00134	0.00171	1.91934
R26	1.92417	0.00046	0.00024	0.00116	0.00140	1.92558
A1	2.56468	-0.00021	0.00007	-0.00044	-0.00038	2.56431
A2	2.60486	0.00037	-0.00014	0.00040	0.00025	2.60511
A3	2.56521	-0.00020	0.00009	-0.00021	-0.00013	2.56508
A4	2.72763	-0.00050	0.00027	-0.00034	-0.00007	2.72755
A5	2.60436	0.00036	-0.00017	0.00030	0.00012	2.60448
A6	2.82909	0.00070	-0.00015	0.00177	0.00162	2.83071
A7	2.72794	-0.00049	0.00027	-0.00010	0.00017	2.72811
A8	2.82883	0.00069	-0.00018	0.00181	0.00162	2.83045
A9	2.08811	0.00024	-0.00013	0.00230	0.00217	2.09028
A10	2.10777	-0.00087	-0.00002	-0.00245	-0.00249	2.10528
A11	2.08694	0.00064	0.00009	0.00028	0.00036	2.08730
A12	2.08811	0.00025	0.00002	0.00178	0.00179	2.08990
A13	2.08720	0.00064	0.00010	0.00039	0.00048	2.08767
A14	2.10751	-0.00089	-0.00018	-0.00207	-0.00226	2.10524
A15	2.05526	0.00198	-0.00532	-0.00670	-0.01202	2.04324
A16	1.94298	-0.00124	-0.00228	-0.02299	-0.02527	1.91771
A17	2.05688	0.00203	-0.00444	-0.00889	-0.01333	2.04355
A18	1.94491	-0.00131	-0.00129	-0.02571	-0.02700	1.91792
A19	1.99931	-0.00015	0.00155	0.00092	0.00246	2.00177
A20	1.91016	0.00059	0.00033	0.00583	0.00615	1.91631
A21	1.92092	-0.00018	0.00012	-0.00310	-0.00298	1.91794
A22	1.90028	-0.00003	-0.00081	0.00017	-0.00066	1.89963
A23	1.84966	-0.00033	-0.00029	-0.00322	-0.00351	1.84615
A24	1.87928	0.00009	-0.00108	-0.00102	-0.00210	1.87718
A25	1.99907	-0.00015	0.00165	0.00067	0.00230	2.00137
A26	1.91018	0.00059	0.00020	0.00639	0.00657	1.91675
A27	1.92134	-0.00021	0.00014	-0.00331	-0.00317	1.91817
A28	1.90012	-0.00003	-0.00084	0.00018	-0.00067	1.89945
A29	1.84972	-0.00033	-0.00025	-0.00329	-0.00355	1.84617
A30	1.87920	0.00011	-0.00107	-0.00105	-0.00211	1.87708
A31	2.91149	-0.00027	-0.00053	-0.00228	-0.00281	2.90868
A32	3.12343	-0.00032	0.00050	-0.00098	-0.00047	3.12296
A33	2.91134	-0.00026	-0.00075	-0.00110	-0.00185	2.90949
A34	3.12386	-0.00036	0.00084	-0.00291	-0.00207	3.12179
A35	3.99825	0.00073	-0.00760	-0.02970	-0.03730	3.96095
A36	4.00180	0.00072	-0.00572	-0.03460	-0.04033	3.96147
A37	3.14991	-0.00023	0.00056	-0.00223	-0.00167	3.14823
A38	3.13948	-0.00027	0.00228	0.00146	0.00375	3.14322

A39	3.14997	-0.00025	0.00058	-0.00261	-0.00204	3.14793
A40	3.13840	-0.00022	0.00165	0.00652	0.00817	3.14658
A41	3.99169	0.00082	0.00289	0.05787	0.06076	4.05244
A42	3.98640	0.00093	0.00584	0.04144	0.04728	4.03369
D1	0.02152	-0.00013	0.00087	0.00223	0.00310	0.02462
D2	-0.01780	-0.00014	-0.00003	-0.00233	-0.00236	-0.02016
D3	-0.01512	-0.00006	0.00032	-0.00095	-0.00063	-0.01576
D4	0.02146	-0.00012	0.00083	0.00264	0.00347	0.02493
D5	0.00840	-0.00002	0.00010	-0.00029	-0.00019	0.00821
D6	-0.01529	-0.00004	0.00024	-0.00003	0.00022	-0.01507
D7	0.00668	-0.00001	0.00062	-0.00956	-0.00894	-0.00226
D8	3.11941	0.00001	-0.00179	-0.00474	-0.00652	3.11289
D9	0.00834	-0.00001	0.00006	0.00029	0.00035	0.00869
D10	0.00608	-0.00002	0.00022	-0.00718	-0.00695	-0.00088
D11	3.11783	0.00004	-0.00247	-0.00010	-0.00256	3.11527
D12	-0.00364	0.00014	-0.00200	0.00594	0.00395	0.00030
D13	-3.11640	-0.00011	0.00182	0.00229	0.00412	-3.11228
D14	-3.11656	-0.00012	0.00201	0.00086	0.00288	-3.11368
D15	0.05387	-0.00037	0.00583	-0.00278	0.00305	0.05692
D16	2.50097	0.00014	-0.00182	-0.01758	-0.01940	2.48157
D17	-0.66963	0.00042	-0.00588	-0.01237	-0.01824	-0.68788
D18	-0.66461	0.00040	-0.00443	-0.01585	-0.02028	-0.68489
D19	2.50614	0.00012	-0.00057	-0.01960	-0.02018	2.48597
D20	-1.53520	0.00046	0.01101	0.06094	0.07194	-1.46326
D21	0.60426	0.00075	0.01129	0.06630	0.07761	0.68187
D22	2.66625	0.00111	0.01025	0.06673	0.07698	2.74323
D23	-1.53976	0.00044	0.01106	0.06092	0.07197	-1.46779
D24	0.59932	0.00075	0.01128	0.06653	0.07783	0.67715
D25	2.66148	0.00112	0.01018	0.06714	0.07731	2.73879

Item	Value	Threshold	Converged?
Maximum Force	0.002032	0.000450	NO
RMS Force	0.000584	0.000300	NO
Maximum Displacement	0.105805	0.001800	NO
RMS Displacement	0.029117	0.001200	NO

Predicted change in Energy=-2.034609D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 03:01:24 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.008765	0.672413	0.050021
2	6	0	3.337298	1.700087	0.121637

3	6	0	4.009280	-0.663660	-0.051274
4	6	0	2.135430	2.288570	0.171875
5	6	0	3.339420	-1.692430	-0.122009
6	6	0	0.908841	2.340425	0.181157
7	6	0	2.138042	-2.282145	-0.170829
8	6	0	-0.383936	1.985531	0.162976
9	6	0	0.911563	-2.335880	-0.179135
10	6	0	-1.460542	1.397589	0.117899
11	6	0	-0.381735	-1.982576	-0.160415
12	6	0	-2.666753	0.709604	0.062918
13	6	0	-1.459481	-1.396845	-0.115354
14	6	0	-2.666421	-0.710181	-0.055779
15	6	0	-3.907665	1.408754	0.158365
16	6	0	-3.906634	-1.410522	-0.148214
17	7	0	-3.713885	2.872405	-0.047133
18	7	0	-3.727851	-2.878124	0.041080
19	1	0	-3.131674	3.119916	-0.862410
20	1	0	-4.616316	3.329496	-0.137664
21	1	0	-3.148917	-3.140167	0.854095
22	1	0	-4.634765	-3.327440	0.125973
23	1	0	-3.244282	3.276850	0.761680
24	1	0	-4.724491	1.053361	-0.463632
25	1	0	-4.723263	-1.054500	0.473419
26	1	0	-3.261512	-3.278452	-0.771675

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229679	0.000000			
3	C	1.339907	2.463485	0.000000		
4	C	2.477135	1.339150	3.503822	0.000000	
5	C	2.463757	3.401256	1.229668	4.169451	0.000000
6	C	3.522639	2.512166	4.323340	1.227720	4.718426
7	C	3.503968	4.169163	2.476958	4.583545	1.339200
8	C	4.586159	3.732394	5.134633	2.537541	5.241373
9	C	4.323772	4.718442	3.522573	4.796520	2.512326
10	C	5.517590	4.807368	5.847762	3.705101	5.713616
11	C	5.135148	5.241448	4.586117	4.968826	3.732647
12	C	6.675634	6.085486	6.816767	5.056280	6.471328
13	C	5.849008	5.714564	5.518062	5.156372	4.808000
14	C	6.817688	6.471902	6.675865	5.665872	6.085994
15	C	7.951340	7.250912	8.186383	6.106821	7.887724
16	C	8.187274	7.888172	7.951660	7.091705	7.251583
17	N	8.030488	7.149965	8.494178	5.882459	8.401931
18	N	8.512439	8.419195	8.048328	7.816003	7.167899
19	H	7.603202	6.695660	8.121984	5.431691	8.098267
20	H	9.027034	8.122942	9.505454	6.838524	9.408173
21	H	8.149522	8.126226	7.628405	7.606638	6.719169

22	H	9.524453	9.424958	9.046914	8.796432	8.143855
23	H	7.739266	6.798017	8.294738	5.501442	8.295769
24	H	8.756639	8.108837	8.910497	6.999152	8.525417
25	H	8.911218	8.525500	8.757019	7.636015	8.109769
26	H	8.315134	8.314334	7.760189	7.810826	6.819812

		6	7	8	9	10
6	C	0.000000				
7	C	4.796142	0.000000			
8	C	1.340728	4.968385	0.000000		
9	C	4.690165	1.227683	4.524373	0.000000	
10	C	2.550866	5.154959	1.227513	4.433272	0.000000
11	C	4.524444	2.537543	3.981264	1.340819	3.559045
12	C	3.931721	5.664914	2.617108	4.705095	1.389709
13	C	4.434417	3.705267	3.560160	2.551020	2.804152
14	C	4.705830	5.056399	3.538991	3.931931	2.434544
15	C	4.905840	7.090958	3.570625	6.112378	2.447484
16	C	6.112846	6.107237	4.903001	4.906350	3.733587
17	N	4.658832	7.799342	3.452428	6.966953	2.698124
18	N	6.982248	5.899898	5.903539	4.676183	4.840281
19	H	4.245280	7.578288	3.144569	6.824980	2.592316
20	H	5.622034	8.781398	4.450805	7.915532	3.708974
21	H	6.852382	5.453312	5.864772	4.266373	4.897328
22	H	7.928386	6.859420	6.804306	5.642521	5.692245
23	H	4.296781	7.793677	3.194923	7.046909	2.669795
24	H	5.814355	7.635816	4.483526	6.582781	3.333172
25	H	6.582669	6.999977	5.307347	5.815413	4.096887
26	H	7.061976	5.523480	6.071535	4.319039	5.089223

		11	12	13	14	15
11	C	0.000000				
12	C	3.538223	0.000000			
13	C	1.227455	2.434424	0.000000		
14	C	2.617198	1.424739	1.389878	0.000000	
15	C	4.902543	1.427510	3.733620	2.465042	0.000000
16	C	3.571037	2.465120	2.447412	1.427287	2.835897
17	N	5.889559	2.405474	4.828405	3.732584	1.490655
18	N	3.469740	3.741417	2.713699	2.415780	4.292251
19	H	5.838697	2.623354	4.873957	3.941670	2.138275
20	H	6.793401	3.271828	5.683696	4.486400	2.068590
21	H	3.166472	3.959695	2.614038	2.639224	4.663949
22	H	4.469781	4.491634	3.723958	3.279856	4.791791
23	H	6.058547	2.722601	5.079186	4.110788	2.072160
24	H	5.307390	2.151676	4.096963	2.740817	1.086457
25	H	4.484633	2.740403	3.334086	2.151559	2.613825
26	H	3.216527	4.117630	2.686730	2.731786	4.822073

		16	17	18	19	20
16	C	0.000000				
17	N	4.288453	0.000000			
18	N	1.490521	5.751223	0.000000		

```
 19  H    4.651398   1.031944   6.094933   0.000000
 20  H    4.792862   1.015632   6.273425   1.665335   0.000000
 21  H    2.137856   6.105933   1.031903   6.491173   6.707710
 22  H    2.068798   6.270252   1.015670   6.693622   6.662179
 23  H    4.820588   1.018961   6.215852   1.635536   1.641362
 24  H    2.615167   2.122196   4.087127   2.639458   2.301901
 25  H    1.086307   4.087836   2.122114   4.662976   4.427672
 26  H    2.072209   6.209883   1.018972   6.400328   6.775134
            21         22         23         24         25
 21  H    0.000000
 22  H    1.665226   0.000000
 23  H    6.418391   6.778953   0.000000
 24  H    4.669531   4.421210   2.938761   0.000000
 25  H    2.640736   2.301044   4.585965   2.306761   0.000000
 26  H    1.635520   1.641339   6.732270   4.582554   2.938186
            26
 26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=3 Diff= 6.97D-03
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.517285   -0.663652   -0.023754
    2          6           0        3.847919   -1.694720   -0.054736
    3          6           0        4.515070    0.675371    0.024876
    4          6           0        2.647255   -2.287181   -0.081539
    5          6           0        3.843109    1.704756    0.055195
    6          6           0        1.420774   -2.341870   -0.088533
    7          6           0        2.640529    2.293476    0.081002
    8          6           0        0.127274   -1.989181   -0.084082
    9          6           0        1.413944    2.344988    0.087426
   10          6           0       -0.950531   -1.402123   -0.061970
   11          6           0        0.121371    1.988577    0.082879
   12          6           0       -2.158145   -0.714976   -0.033875
   13          6           0       -0.955176    1.399323    0.061116
   14          6           0       -2.160712    0.708379    0.028849
   15          6           0       -3.397631   -1.419878   -0.101487
   16          6           0       -3.402348    1.409277    0.093891
   17          7           0       -3.200825   -2.873907    0.161421
   18          7           0       -3.226598    2.868654   -0.153054
   19          1           0       -2.618014   -3.087946    0.985694
```

```
    20        1        0     -4.102306   -3.328925    0.270049
    21        1        0     -2.648296    3.099678   -0.975866
    22        1        0     -4.134442    3.312424   -0.255389
    23        1        0     -2.730485   -3.308911   -0.630939
    24        1        0     -4.215113   -1.041950    0.506199
    25        1        0     -4.218317    1.027394   -0.513088
    26        1        0     -2.760988    3.301614    0.643223
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6004686           0.2713964           0.1876134
 Leave Link  202 at Sat Sep 26 03:01:24 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1009.9468232607 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0154359885 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1009.9313872722 Hartrees.
 Leave Link  301 at Sat Sep 26 03:01:24 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23233 LenP2D=   51946.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.81D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=         32
 NSgBfM=   683   683   683   683   683 MxSgAt=    26 MxSgA2=    26.
```

Supporting Information file

```
 Leave Link  302 at Sat Sep 26 03:01:25 2026, MaxMem=    805306368 cpu:                5.7 elap:
1.0
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Sat Sep 26 03:01:25 2026, MaxMem=    805306368 cpu:                0.7 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=     0.000000   -0.000000    0.000000
       Rot=    1.000000    0.000126   -0.000027   -0.000853 Ang=   0.10 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Generating alternative initial guess.
 ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn=          5 AccDes=
0.00D+00
 Harris functional with IExCor= 4639 and IRadAn=       5 diagonalized for initial guess.
 HarFok:  IExCor= 4639 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Petite list used in FoFCou.
 Harris En= -691.982385785267
 Leave Link  401 at Sat Sep 26 03:01:35 2026, MaxMem=    805306368 cpu:               56.4 elap:
9.4
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.410992246524
 DIIS: error= 1.37D-03 at cycle   1 NSaved=   1.
```

NSaved= 1 IEnMin= 1 EnMin= -723.410992246524 IErMin= 1 ErrMin= 1.37D-03
ErrMax= 1.37D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-03 BMatP= 1.86D-03
IDIUse=3 WtCom= 9.86D-01 WtEn= 1.37D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.706 Goal= None Shift= 0.000
GapD= 0.706 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=8.51D-03 MaxDP=3.36D-01 OVMax= 1.10D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 7.12D-03 CP: 1.46D+00
E= -723.413033033551 Delta-E= -0.002040787027 Rises=F Damp=F
DIIS: error= 9.45D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413033033551 IErMin= 2 ErrMin= 9.45D-04
ErrMax= 9.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-04 BMatP= 1.86D-03
IDIUse=3 WtCom= 9.91D-01 WtEn= 9.45D-03
Coeff-Com: 0.205D-01 0.980D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.203D-01 0.980D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.06D-02 MaxDP=3.64D-01 DE=-2.04D-03 OVMax= 4.41D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 4.24D-03 CP: 8.28D-01 -1.99D-02
E= -723.413083703967 Delta-E= -0.000050670415 Rises=F Damp=F
DIIS: error= 3.24D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.413083703967 IErMin= 2 ErrMin= 9.45D-04
ErrMax= 3.24D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.56D-04 BMatP= 1.80D-04
IDIUse=3 WtCom= 1.49D-01 WtEn= 8.51D-01
Coeff-Com: -0.620D-01 0.709D+00 0.353D+00
Coeff-En: 0.000D+00 0.330D+00 0.670D+00
Coeff: -0.926D-02 0.387D+00 0.623D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=7.98D+02 MaxDP=3.31D+04 DE=-5.07D-05 OVMax= 9.56D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.412937321315 Delta-E= 0.000146382652 Rises=F Damp=F
DIIS: error= 9.44D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.412937321315 IErMin= 1 ErrMin= 9.44D-04
ErrMax= 9.44D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-04 BMatP= 1.89D-04
IDIUse=3 WtCom= 9.91D-01 WtEn= 9.44D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.181 Goal= None Shift= 0.000

RMSDP=4.00D-03 MaxDP=9.65D-02 DE= 1.46D-04 OVMax= 5.23D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.96D-03 CP: 9.41D-01
E= -723.413009682611 Delta-E= -0.000072361296 Rises=F Damp=F
DIIS: error= 4.53D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413009682611 IErMin= 2 ErrMin= 4.53D-04
ErrMax= 4.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.71D-05 BMatP= 1.89D-04
IDIUse=3 WtCom= 9.95D-01 WtEn= 4.53D-03
Coeff-Com: 0.279D+00 0.721D+00
Coeff-En: 0.100D+00 0.900D+00
Coeff: 0.279D+00 0.721D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.71D-04 MaxDP=1.24D-02 DE=-7.24D-05 OVMax= 4.04D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.30D-04 CP: 9.52D-01 1.07D+00
E= -723.413008335684 Delta-E= 0.000001346927 Rises=F Damp=F
DIIS: error= 4.29D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413009682611 IErMin= 3 ErrMin= 4.29D-04
ErrMax= 4.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.87D-05 BMatP= 5.71D-05
IDIUse=3 WtCom= 9.96D-01 WtEn= 4.29D-03
Coeff-Com: -0.172D-01 0.508D+00 0.510D+00
Coeff-En: 0.000D+00 0.504D+00 0.496D+00
Coeff: -0.172D-01 0.508D+00 0.510D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.99D-04 MaxDP=7.23D-03 DE= 1.35D-06 OVMax= 3.08D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 4.01D-05 CP: 9.58D-01 1.10D+00 1.53D+00
E= -723.413076592411 Delta-E= -0.000068256727 Rises=F Damp=F
DIIS: error= 4.83D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413076592411 IErMin= 4 ErrMin= 4.83D-05
ErrMax= 4.83D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.02D-07 BMatP= 5.71D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.128D-01 0.234D+00 0.246D+00 0.533D+00
Coeff: -0.128D-01 0.234D+00 0.246D+00 0.533D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.02D-05 MaxDP=1.65D-03 DE=-6.83D-05 OVMax= 3.85D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 9.18D-06 CP: 9.60D-01 1.11D+00 1.65D+00 1.14D+00
E= -723.413077519305 Delta-E= -0.000000926894 Rises=F Damp=F
DIIS: error= 1.48D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413077519305 IErMin= 5 ErrMin= 1.48D-05
ErrMax= 1.48D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.86D-08 BMatP= 6.02D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.540D-02-0.149D+00-0.153D+00-0.471D-01 0.134D+01

Coeff: 0.540D-02-0.149D+00-0.153D+00-0.471D-01 0.134D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=6.41D-05 MaxDP=2.64D-03 DE=-9.27D-07 OVMax= 8.83D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 4.51D-06 CP: 9.63D-01 1.12D+00 1.84D+00 1.42D+00 2.61D+00
E= -723.413078081364 Delta-E= -0.000000562059 Rises=F Damp=F
DIIS: error= 1.17D-05 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413078081364 IErMin= 6 ErrMin= 1.17D-05
ErrMax= 1.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.81D-08 BMatP= 5.86D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.463D-02-0.111D+00-0.115D+00-0.985D-01 0.720D+00 0.601D+00
Coeff: 0.463D-02-0.111D+00-0.115D+00-0.985D-01 0.720D+00 0.601D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.86D-06 MaxDP=4.00D-04 DE=-5.62D-07 OVMax= 2.67D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.31D-06 CP: 9.63D-01 1.12D+00 1.87D+00 1.46D+00 2.98D+00
CP: 1.11D+00
E= -723.413078184852 Delta-E= -0.000000103488 Rises=F Damp=F
DIIS: error= 7.95D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413078184852 IErMin= 7 ErrMin= 7.95D-06
ErrMax= 7.95D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.40D-09 BMatP= 2.81D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.117D-02 0.378D-01 0.389D-01-0.102D-01-0.444D+00 0.154D+00
Coeff-Com: 0.122D+01
Coeff: -0.117D-02 0.378D-01 0.389D-01-0.102D-01-0.444D+00 0.154D+00
Coeff: 0.122D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.78D-06 MaxDP=1.21D-04 DE=-1.03D-07 OVMax= 3.27D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 2.49D-06 CP: 9.63D-01 1.12D+00 1.87D+00 1.47D+00 3.00D+00
CP: 1.20D+00 2.75D+00
E= -723.413078243161 Delta-E= -0.000000058309 Rises=F Damp=F
DIIS: error= 2.93D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413078243161 IErMin= 8 ErrMin= 2.93D-06
ErrMax= 2.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.82D-09 BMatP= 5.40D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.134D-02 0.372D-01 0.386D-01 0.134D-01-0.339D+00-0.290D-01
Coeff-Com: 0.636D+00 0.644D+00
Coeff: -0.134D-02 0.372D-01 0.386D-01 0.134D-01-0.339D+00-0.290D-01
Coeff: 0.636D+00 0.644D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.45D-07 MaxDP=3.46D-05 DE=-5.83D-08 OVMax= 8.63D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 3.72D-07 CP: 9.63D-01 1.12D+00 1.86D+00 1.47D+00 3.00D+00

```
              CP:  1.20D+00  3.00D+00  1.08D+00
E= -723.413078250046     Delta-E=       -0.000000006885 Rises=F Damp=F
DIIS: error= 2.01D-06 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.413078250046     IErMin= 9 ErrMin= 2.01D-06
ErrMax= 2.01D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-10 BMatP= 1.82D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.945D-04 0.677D-03 0.992D-03 0.109D-01 0.297D-01-0.760D-01
Coeff-Com: -0.184D+00 0.226D+00 0.992D+00
Coeff:     -0.945D-04 0.677D-03 0.992D-03 0.109D-01 0.297D-01-0.760D-01
Coeff:     -0.184D+00 0.226D+00 0.992D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=5.69D-07 MaxDP=2.21D-05 DE=-6.89D-09 OVMax= 5.26D-05

Cycle  13  Pass 1  IDiag  1:
RMSU=  1.99D-07    CP:  9.63D-01  1.12D+00  1.86D+00  1.47D+00  3.00D+00
              CP:  1.18D+00  3.00D+00  1.01D+00  2.15D+00
E= -723.413078252306     Delta-E=       -0.000000002260 Rises=F Damp=F
DIIS: error= 7.22D-07 at cycle  10 NSaved=  10.
NSaved=10 IEnMin=10 EnMin= -723.413078252306     IErMin=10 ErrMin= 7.22D-07
ErrMax= 7.22D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 9.21D-11 BMatP= 3.43D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.229D-03-0.725D-02-0.730D-02 0.214D-02 0.797D-01-0.320D-01
Coeff-Com: -0.208D+00-0.212D-01 0.471D+00 0.723D+00
Coeff:      0.229D-03-0.725D-02-0.730D-02 0.214D-02 0.797D-01-0.320D-01
Coeff:     -0.208D+00-0.212D-01 0.471D+00 0.723D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=2.80D-07 MaxDP=1.33D-05 DE=-2.26D-09 OVMax= 1.86D-05

Cycle  14  Pass 1  IDiag  1:
RMSU=  1.13D-07    CP:  9.63D-01  1.12D+00  1.86D+00  1.47D+00  3.00D+00
              CP:  1.17D+00  3.00D+00  9.79D-01  2.44D+00  1.46D+00
E= -723.413078252712     Delta-E=       -0.000000000406 Rises=F Damp=F
DIIS: error= 4.94D-07 at cycle  11 NSaved=  11.
NSaved=11 IEnMin=11 EnMin= -723.413078252712     IErMin=11 ErrMin= 4.94D-07
ErrMax= 4.94D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.25D-11 BMatP= 9.21D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com:  0.130D-03-0.361D-02-0.367D-02-0.132D-02 0.316D-01 0.388D-03
Coeff-Com: -0.582D-01-0.542D-01 0.964D-02 0.346D+00 0.733D+00
Coeff:      0.130D-03-0.361D-02-0.367D-02-0.132D-02 0.316D-01 0.388D-03
Coeff:     -0.582D-01-0.542D-01 0.964D-02 0.346D+00 0.733D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=1.37D-07 MaxDP=5.89D-06 DE=-4.06D-10 OVMax= 7.37D-06

Cycle  15  Pass 1  IDiag  1:
RMSU=  4.35D-08    CP:  9.63D-01  1.12D+00  1.86D+00  1.47D+00  3.00D+00
              CP:  1.17D+00  3.00D+00  9.55D-01  2.44D+00  1.77D+00
              CP:  1.81D+00
E= -723.413078252789     Delta-E=       -0.000000000077 Rises=F Damp=F
```

DIIS: error= 1.55D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413078252789 IErMin=12 ErrMin= 1.55D-07
ErrMax= 1.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.23D-12 BMatP= 2.25D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.105D-04 0.557D-03 0.564D-03-0.121D-02-0.962D-02 0.949D-02
Coeff-Com: 0.364D-01-0.178D-01-0.145D+00-0.737D-01 0.314D+00 0.886D+00
Coeff: -0.105D-04 0.557D-03 0.564D-03-0.121D-02-0.962D-02 0.949D-02
Coeff: 0.364D-01-0.178D-01-0.145D+00-0.737D-01 0.314D+00 0.886D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.59D-07 MaxDP=7.92D-06 DE=-7.66D-11 OVMax= 5.08D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.73D-08 CP: 9.63D-01 1.12D+00 1.86D+00 1.47D+00 3.00D+00
CP: 1.18D+00 3.00D+00 9.34D-01 2.41D+00 1.96D+00
CP: 2.38D+00 1.87D+00
E= -723.413078252818 Delta-E= -0.000000000030 Rises=F Damp=F
DIIS: error= 6.81D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.413078252818 IErMin=13 ErrMin= 6.81D-08
ErrMax= 6.81D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-12 BMatP= 5.23D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.282D-04 0.907D-03 0.919D-03-0.311D-03-0.100D-01 0.433D-02
Coeff-Com: 0.273D-01 0.152D-02-0.678D-01-0.100D+00 0.681D-02 0.410D+00
Coeff-Com: 0.726D+00
Coeff: -0.282D-04 0.907D-03 0.919D-03-0.311D-03-0.100D-01 0.433D-02
Coeff: 0.273D-01 0.152D-02-0.678D-01-0.100D+00 0.681D-02 0.410D+00
Coeff: 0.726D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.25D-08 MaxDP=3.84D-06 DE=-2.96D-11 OVMax= 1.78D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 8.13D-09 CP: 9.63D-01 1.12D+00 1.86D+00 1.47D+00 3.00D+00
CP: 1.18D+00 3.00D+00 9.25D-01 2.40D+00 1.99D+00
CP: 2.54D+00 2.18D+00 1.45D+00
E= -723.413078252814 Delta-E= 0.000000000004 Rises=F Damp=F
DIIS: error= 3.20D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.413078252818 IErMin=14 ErrMin= 3.20D-08
ErrMax= 3.20D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-13 BMatP= 1.15D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.427D-05 0.923D-04 0.926D-04 0.189D-03-0.172D-03-0.103D-02
Coeff-Com: -0.128D-02 0.503D-02 0.164D-01-0.122D-01-0.706D-01-0.783D-01
Coeff-Com: 0.212D+00 0.930D+00
Coeff: -0.427D-05 0.923D-04 0.926D-04 0.189D-03-0.172D-03-0.103D-02
Coeff: -0.128D-02 0.503D-02 0.164D-01-0.122D-01-0.706D-01-0.783D-01
Coeff: 0.212D+00 0.930D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.93D-08 MaxDP=1.71D-06 DE= 4.32D-12 OVMax= 8.61D-07

Cycle 18 Pass 1 IDiag 1:

RMSU= 3.91D-09 CP: 9.63D-01 1.12D+00 1.86D+00 1.47D+00 3.00D+00
CP: 1.18D+00 3.00D+00 9.21D-01 2.40D+00 1.99D+00
CP: 2.56D+00 2.31D+00 1.76D+00 1.68D+00
E= -723.413078252819 Delta-E= -0.000000000005 Rises=F Damp=F
DIIS: error= 1.56D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.413078252819 IErMin=15 ErrMin= 1.56D-08
ErrMax= 1.56D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.49D-14 BMatP= 1.69D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.406D-05-0.151D-03-0.152D-03 0.132D-03 0.196D-02-0.144D-02
Coeff-Com: -0.640D-02 0.198D-02 0.212D-01 0.157D-01-0.347D-01-0.122D+00
Coeff-Com: -0.621D-01 0.402D+00 0.784D+00
Coeff: 0.406D-05-0.151D-03-0.152D-03 0.132D-03 0.196D-02-0.144D-02
Coeff: -0.640D-02 0.198D-02 0.212D-01 0.157D-01-0.347D-01-0.122D+00
Coeff: -0.621D-01 0.402D+00 0.784D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.67D-09 MaxDP=2.50D-07 DE=-5.23D-12 OVMax= 4.23D-07

SCF Done: E(RwB97XD) = -723.413078253 A.U. after 18 cycles
NFock= 18 Conv=0.47D-08 -V/T= 2.0047
KE= 7.200424048256D+02 PE=-3.700953772473D+03 EE= 1.247566902123D+03
Leave Link 502 at Sat Sep 26 03:23:29 2026, MaxMem= 805306368 cpu: 7885.5 elap: 1314.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23233 LenP2D= 51946.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 03:23:30 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 03:23:30 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.

Supporting Information file

Leave Link 703 at Sat Sep 26 03:35:45 2026, MaxMem= 805306368 cpu: 4410.3 elap: 735.1
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.49002090D+00 1.86359609D-02 1.97534472D-02
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000505243	-0.000313222	-0.000205439
2	6	-0.000891792	-0.000020454	0.000181232
3	6	0.000490198	0.000296849	0.000212305
4	6	0.000792593	0.000826100	-0.000037046
5	6	-0.000859675	0.000046984	-0.000178434
6	6	-0.000701886	-0.000957683	0.000149313
7	6	0.000714982	-0.000841992	0.000041107
8	6	0.000001633	0.000165395	-0.000066141
9	6	-0.000605776	0.000980155	-0.000209091
10	6	0.000244006	0.000061462	-0.000432365
11	6	-0.000240904	-0.000143388	0.000004880
12	6	-0.001053544	-0.000218129	0.001202297
13	6	0.000370891	-0.000472822	0.000615646
14	6	-0.000965239	-0.001315927	-0.001193675
15	6	0.000809116	-0.000255808	-0.001851623
16	6	-0.000222667	0.001128416	0.001693381
17	7	-0.000426398	0.002162712	-0.000106863
18	7	0.001064728	-0.001186764	0.000288985
19	1	-0.000855869	-0.000330183	0.000652037
20	1	0.000507046	-0.000530817	0.000388019
21	1	-0.000855232	0.000249600	-0.000606065
22	1	0.000533786	0.000746416	-0.000357116
23	1	0.000517959	-0.000390382	-0.000306515
24	1	0.000334038	-0.000428929	0.000223554
25	1	0.000257690	0.000357592	-0.000356467
26	1	0.000535075	0.000384816	0.000254085

Cartesian Forces: Max 0.002162712 RMS 0.000689690
Leave Link 716 at Sat Sep 26 03:35:45 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003027034 RMS 0.000619919
Search for a local minimum.
Step number 16 out of a maximum of 103

Supporting Information file

All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .61992D-03 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 12 14 13 15 16
DE= -1.96D-04 DEPred=-2.03D-04 R= 9.62D-01
TightC=F SS= 1.41D+00 RLast= 2.18D-01 DXNew= 1.2000D+00 6.5279D-01
Trust test= 9.62D-01 RLast= 2.18D-01 DXMaxT set to 7.14D-01
ITU= 1 1 -1 1 1 1 1 1 1 1 1 1 0 0 1 0
Eigenvalues --- 0.00424 0.00448 0.01126 0.01591 0.01681
Eigenvalues --- 0.01753 0.02397 0.02643 0.02800 0.02919
Eigenvalues --- 0.03123 0.03463 0.03642 0.03793 0.04363
Eigenvalues --- 0.04438 0.04466 0.05026 0.07102 0.07733
Eigenvalues --- 0.09963 0.10676 0.11169 0.11269 0.11652
Eigenvalues --- 0.11705 0.14036 0.15040 0.15340 0.15886
Eigenvalues --- 0.16000 0.16000 0.16002 0.16117 0.16645
Eigenvalues --- 0.21440 0.22759 0.24622 0.24996 0.24997
Eigenvalues --- 0.24998 0.25000 0.25000 0.25156 0.29268
Eigenvalues --- 0.30455 0.33335 0.37232 0.38476 0.44339
Eigenvalues --- 0.45436 0.45843 0.47281 0.47660 0.47688
Eigenvalues --- 0.47688 0.47856 0.48208 0.50243 0.54520
Eigenvalues --- 0.54810 0.55362 0.55652 0.55659 0.65941
Eigenvalues --- 0.93183 0.93744 0.95031 0.95417 0.97724
Eigenvalues --- 0.99446 1.37601
En-DIIS/RFO-DIIS/Sim-DIIS IScMMF= -3 using points: 16 15
RFO step: Lambda=-2.42172247D-04.
NNeg= 0 NGDIIS= 2 SimSw= 2.50D-03 Rises=F DC= -1.96D-04 SmlDif= 1.00D-05
NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj= 3.0
RMS Error= 0.1145809052D-01 NUsed= 2 OKEnD=T EnDIS=F
InvSVX: RCond= 1.03D-02 Info= 0 Equed=N FErr= 2.06D-15 BErr= 6.98D-18
DidBck=F Rises=F RFO-DIIS coefs: 1.36774 -0.36774
Iteration 1 RMS(Cart)= 0.02800497 RMS(Int)= 0.00073356
Iteration 2 RMS(Cart)= 0.00077456 RMS(Int)= 0.00000337
Iteration 3 RMS(Cart)= 0.00000054 RMS(Int)= 0.00000335
ITry= 1 IFail=0 DXMaxC= 1.12D-01 DCOld= 1.00D+10 DXMaxT= 7.14D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.32376	0.00049	-0.00082	-0.00045	-0.00127	2.32249
R2	2.53206	-0.00008	0.00102	0.00135	0.00237	2.53443
R3	2.53063	-0.00023	0.00092	0.00090	0.00182	2.53245
R4	2.32374	0.00046	-0.00082	-0.00046	-0.00128	2.32246
R5	2.32005	0.00039	-0.00068	-0.00036	-0.00104	2.31901
R6	2.53072	-0.00022	0.00093	0.00091	0.00185	2.53257
R7	2.53361	-0.00038	0.00074	0.00041	0.00115	2.53475
R8	2.31999	0.00032	-0.00069	-0.00039	-0.00107	2.31891
R9	2.31966	-0.00036	-0.00012	-0.00055	-0.00067	2.31899
R10	2.53378	-0.00036	0.00077	0.00043	0.00120	2.53498

R11	2.62617	-0.00014	0.00024	0.00106	0.00130	2.62747
R12	2.31955	-0.00056	-0.00012	-0.00063	-0.00075	2.31881
R13	2.69237	-0.00017	-0.00183	-0.00174	-0.00357	2.68880
R14	2.69760	-0.00073	0.00231	-0.00162	0.00070	2.69830
R15	2.62649	-0.00003	0.00029	0.00122	0.00151	2.62800
R16	2.69718	-0.00202	0.00238	-0.00213	0.00025	2.69744
R17	2.81693	0.00077	0.00308	-0.00241	0.00067	2.81760
R18	2.05311	-0.00024	0.00089	-0.00095	-0.00005	2.05305
R19	2.81668	-0.00009	0.00307	-0.00254	0.00053	2.81721
R20	2.05282	-0.00028	0.00082	-0.00109	-0.00027	2.05255
R21	1.95009	-0.00108	0.00051	-0.00020	0.00031	1.95040
R22	1.91927	-0.00072	0.00060	-0.00053	0.00008	1.91934
R23	1.92556	-0.00016	0.00052	0.00089	0.00141	1.92697
R24	1.95001	-0.00102	0.00049	-0.00019	0.00030	1.95032
R25	1.91934	-0.00084	0.00063	-0.00053	0.00009	1.91943
R26	1.92558	-0.00011	0.00052	0.00092	0.00143	1.92701
A1	2.56431	-0.00029	-0.00014	-0.00177	-0.00191	2.56240
A2	2.60511	0.00039	0.00009	0.00209	0.00219	2.60730
A3	2.56508	-0.00029	-0.00005	-0.00169	-0.00174	2.56334
A4	2.72755	-0.00062	-0.00003	-0.00309	-0.00312	2.72443
A5	2.60448	0.00036	0.00004	0.00199	0.00203	2.60651
A6	2.83071	0.00073	0.00060	0.00432	0.00491	2.83562
A7	2.72811	-0.00066	0.00006	-0.00307	-0.00301	2.72510
A8	2.83045	0.00070	0.00060	0.00425	0.00484	2.83529
A9	2.09028	-0.00032	0.00080	-0.00075	0.00005	2.09032
A10	2.10528	0.00017	-0.00092	-0.00119	-0.00211	2.10317
A11	2.08730	0.00015	0.00013	0.00199	0.00213	2.08942
A12	2.08990	0.00021	0.00066	-0.00062	0.00003	2.08993
A13	2.08767	0.00012	0.00017	0.00201	0.00218	2.08986
A14	2.10524	-0.00033	-0.00083	-0.00129	-0.00213	2.10312
A15	2.04324	0.00017	-0.00442	0.00588	0.00146	2.04470
A16	1.91771	0.00022	-0.00929	0.00610	-0.00319	1.91452
A17	2.04355	0.00116	-0.00490	0.00657	0.00167	2.04523
A18	1.91792	0.00105	-0.00993	0.00610	-0.00382	1.91409
A19	2.00177	-0.00005	0.00090	0.00298	0.00388	2.00565
A20	1.91631	-0.00024	0.00226	0.00011	0.00237	1.91868
A21	1.91794	-0.00025	-0.00109	-0.00039	-0.00148	1.91646
A22	1.89963	0.00019	-0.00024	-0.00157	-0.00183	1.89780
A23	1.84615	0.00001	-0.00129	-0.00211	-0.00340	1.84275
A24	1.87718	0.00039	-0.00077	0.00082	0.00005	1.87723
A25	2.00137	0.00013	0.00085	0.00307	0.00391	2.00528
A26	1.91675	-0.00053	0.00242	-0.00011	0.00230	1.91905
A27	1.91817	-0.00025	-0.00117	-0.00040	-0.00156	1.91661
A28	1.89945	0.00020	-0.00025	-0.00152	-0.00178	1.89767
A29	1.84617	0.00003	-0.00131	-0.00211	-0.00341	1.84275
A30	1.87708	0.00048	-0.00078	0.00091	0.00013	1.87721
A31	2.90868	0.00001	-0.00103	-0.00066	-0.00169	2.90699
A32	3.12296	-0.00011	-0.00017	-0.00022	-0.00039	3.12257

A33	2.90949	-0.00008	-0.00068	-0.00076	-0.00145	2.90804
A34	3.12179	-0.00003	-0.00076	-0.00000	-0.00077	3.12103
A35	3.96095	0.00039	-0.01372	0.01198	-0.00173	3.95922
A36	3.96147	0.00221	-0.01483	0.01268	-0.00215	3.95932
A37	3.14823	-0.00035	-0.00062	-0.00004	-0.00065	3.14758
A38	3.14322	-0.00050	0.00138	-0.00030	0.00108	3.14431
A39	3.14793	-0.00031	-0.00075	0.00021	-0.00053	3.14740
A40	3.14658	-0.00074	0.00301	-0.00522	-0.00221	3.14437
A41	4.05244	-0.00303	0.02234	-0.04072	-0.01838	4.03407
A42	4.03369	0.00020	0.01739	-0.03143	-0.01404	4.01964
D1	0.02462	-0.00024	0.00114	-0.00077	0.00037	0.02499
D2	-0.02016	-0.00023	-0.00087	0.00076	-0.00011	-0.02027
D3	-0.01576	-0.00007	-0.00023	0.00069	0.00046	-0.01530
D4	0.02493	-0.00028	0.00128	-0.00121	0.00006	0.02499
D5	0.00821	-0.00001	-0.00007	-0.00020	-0.00027	0.00794
D6	-0.01507	-0.00013	0.00008	-0.00030	-0.00022	-0.01530
D7	-0.00226	0.00022	-0.00329	-0.00115	-0.00444	-0.00669
D8	3.11289	-0.00016	-0.00240	0.00079	-0.00162	3.11127
D9	0.00869	-0.00007	0.00013	-0.00068	-0.00055	0.00814
D10	-0.00088	0.00020	-0.00256	-0.00363	-0.00619	-0.00707
D11	3.11527	-0.00019	-0.00094	-0.00364	-0.00459	3.11069
D12	0.00030	0.00015	0.00145	0.00557	0.00703	0.00733
D13	-3.11228	-0.00005	0.00151	0.00176	0.00328	-3.10900
D14	-3.11368	0.00009	0.00106	0.00347	0.00452	-3.10915
D15	0.05692	-0.00011	0.00112	-0.00034	0.00077	0.05770
D16	2.48157	-0.00027	-0.00713	0.01879	0.01165	2.49322
D17	-0.68788	-0.00021	-0.00671	0.02092	0.01421	-0.67366
D18	-0.68489	0.00007	-0.00746	0.02271	0.01525	-0.66964
D19	2.48597	-0.00014	-0.00742	0.01885	0.01143	2.49740
D20	-1.46326	0.00069	0.02646	0.01498	0.04143	-1.42183
D21	0.68187	0.00071	0.02854	0.01516	0.04371	0.72558
D22	2.74323	0.00089	0.02831	0.01599	0.04430	2.78754
D23	-1.46779	0.00074	0.02647	0.01514	0.04160	-1.42619
D24	0.67715	0.00068	0.02862	0.01528	0.04391	0.72106
D25	2.73879	0.00080	0.02843	0.01608	0.04451	2.78331

Item	Value	Threshold	Converged?
Maximum Force	0.003027	0.000450	NO
RMS Force	0.000620	0.000300	NO
Maximum Displacement	0.111967	0.001800	NO
RMS Displacement	0.028082	0.001200	NO

Predicted change in Energy=-1.226078D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 03:35:45 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Supporting Information file

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.017251	0.672506	0.048655
2	6	0	3.344270	1.698538	0.118088
3	6	0	4.017655	-0.665003	-0.050254
4	6	0	2.141749	2.287973	0.167260
5	6	0	3.346283	-1.692115	-0.118991
6	6	0	0.915573	2.336424	0.176509
7	6	0	2.144153	-2.282595	-0.166864
8	6	0	-0.378547	1.984080	0.159631
9	6	0	0.918095	-2.332894	-0.174840
10	6	0	-1.455109	1.396629	0.116874
11	6	0	-0.376537	-1.982044	-0.156664
12	6	0	-2.661963	0.708294	0.063029
13	6	0	-1.454284	-1.397028	-0.113141
14	6	0	-2.661807	-0.709384	-0.058203
15	6	0	-3.901624	1.410274	0.159457
16	6	0	-3.900638	-1.412032	-0.153670
17	7	0	-3.725987	2.876551	-0.046191
18	7	0	-3.737449	-2.880857	0.042315
19	1	0	-3.190925	3.136298	-0.889686
20	1	0	-4.632977	3.332265	-0.082006
21	1	0	-3.206314	-3.150323	0.885190
22	1	0	-4.648087	-3.329704	0.073323
23	1	0	-3.211649	3.276295	0.738322
24	1	0	-4.723979	1.050632	-0.452686
25	1	0	-4.724040	-1.051123	0.455838
26	1	0	-3.224601	-3.279580	-0.743723

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229010	0.000000			
3	C	1.341161	2.463354	0.000000		
4	C	2.478166	1.340115	3.505196	0.000000	
5	C	2.463683	3.398932	1.228993	4.168207	0.000000
6	C	3.522127	2.511749	4.322372	1.227168	4.714319
7	C	3.505363	4.167841	2.477945	4.582766	1.340178
8	C	4.588636	3.733983	5.136952	2.538563	5.240840
9	C	4.322863	4.714295	3.522024	4.792366	2.511935
10	C	5.520483	4.808866	5.850590	3.705998	5.713961
11	C	5.137525	5.240857	4.588555	4.967871	3.734283
12	C	6.679325	6.087565	6.820269	5.057855	6.472566
13	C	5.852080	5.715078	5.521044	5.156483	4.809632
14	C	6.821352	6.473185	6.679614	5.666492	6.088235
15	C	7.953940	7.251744	8.189367	6.106782	7.888886

16	C	8.190189	7.889119	7.954125	7.092495	7.252415
17	N	8.051369	7.169605	8.515081	5.901043	8.419918
18	N	8.530052	8.433703	8.065991	7.829265	7.184594
19	H	7.675191	6.766945	8.192567	5.502200	8.163494
20	H	9.050847	8.145280	9.529564	6.859271	9.429441
21	H	8.215455	8.185967	7.696596	7.661088	6.787583
22	H	9.544966	9.442616	9.067027	8.813002	8.162637
23	H	7.714425	6.771565	8.271549	5.473735	8.272036
24	H	8.763756	8.114321	8.917484	7.003826	8.530132
25	H	8.918904	8.530670	8.764841	7.640150	8.116120
26	H	8.288019	8.287005	7.730923	7.786222	6.788730

		6	7	8	9	10
6	C	0.000000				
7	C	4.791937	0.000000			
8	C	1.341334	4.967407	0.000000		
9	C	4.682519	1.227115	4.519891	0.000000	
10	C	2.550864	5.154793	1.227157	4.430185	0.000000
11	C	4.519925	2.538565	3.978717	1.341453	3.557187
12	C	3.932232	5.665423	2.617432	4.703426	1.390396
13	C	4.431567	3.706192	3.558582	2.551045	2.803110
14	C	4.704220	5.058068	3.537722	3.932567	2.433529
15	C	4.905449	7.091910	3.569500	6.111689	2.446924
16	C	6.111942	6.107172	4.902741	4.905978	3.733951
17	N	4.678184	7.816002	3.470479	6.980140	2.715445
18	N	6.992042	5.915650	5.913003	4.692708	4.848869
19	H	4.317394	7.638712	3.215298	6.878016	2.655686
20	H	5.643132	8.801326	4.469471	7.932026	3.726269
21	H	6.899027	5.521527	5.906335	4.336197	4.932728
22	H	7.941660	6.876674	6.817090	5.660176	5.703966
23	H	4.270006	7.772081	3.167203	7.025073	2.646654
24	H	5.818393	7.639590	4.486540	6.584712	3.336109
25	H	6.584734	7.005451	5.308814	5.820169	4.097840
26	H	7.037569	5.490925	6.051627	4.287396	5.073329

		11	12	13	14	15
11	C	0.000000				
12	C	3.536857	0.000000			
13	C	1.227060	2.433496	0.000000		
14	C	2.617598	1.422852	1.390678	0.000000	
15	C	4.902448	1.427878	3.734264	2.465253	0.000000
16	C	3.569904	2.465169	2.446736	1.427422	2.839624
17	N	5.902285	2.417729	4.840309	3.740528	1.491009
18	N	3.484708	3.746880	2.727409	2.425367	4.295868
19	H	5.886895	2.661329	4.916298	3.969962	2.141251
20	H	6.809166	3.284990	5.698357	4.496777	2.070563
21	H	3.233879	3.982611	2.672137	2.672950	4.670031
22	H	4.485000	4.500025	3.737698	3.290697	4.799168
23	H	6.040612	2.711606	5.064906	4.101514	2.072000
24	H	5.308955	2.152921	4.098443	2.739676	1.086430

```
  25  H    4.488046   2.738979   3.336868   2.152633   2.612026
  26  H    3.184291   4.107378   2.660011   2.718931   4.823778
                16         17         18         19         20
  16  C    0.000000
  17  N    4.293483   0.000000
  18  N    1.490801   5.758100   0.000000
  19  H    4.661837   1.032106   6.113385   0.000000
  20  H    4.801022   1.015672   6.278560   1.664411   0.000000
  21  H    2.140787   6.120518   1.032062   6.532383   6.707815
  22  H    2.070669   6.275520   1.015720   6.697753   6.663796
  23  H    4.821906   1.019706   6.218635   1.634148   1.642024
  24  H    2.613812   2.120190   4.083488   2.625115   2.313338
  25  H    1.086161   4.083474   2.119503   4.657829   4.417200
  26  H    2.071938   6.215778   1.019730   6.417627   6.792488
                21         22         23         24         25
  21  H    0.000000
  22  H    1.664336   0.000000
  23  H    6.428298   6.792996   0.000000
  24  H    4.662750   4.412458   2.942655   0.000000
  25  H    2.625733   2.311713   4.592784   2.289714   0.000000
  26  H    1.634136   1.642069   6.721319   4.591686   2.941647
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=3 Diff= 1.29D-03
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.522436   -0.665542   -0.022980
    2          6           0        3.851181   -1.694617   -0.052726
    3          6           0        4.520594    0.674784    0.024329
    4          6           0        2.649651   -2.287531   -0.078958
    5          6           0        3.847497    1.702651    0.053557
    6          6           0        1.423558   -2.338365   -0.086133
    7          6           0        2.644377    2.292514    0.078844
    8          6           0        0.128847   -1.987809   -0.082629
    9          6           0        1.418236    2.341020    0.085076
   10          6           0       -0.948701   -1.400959   -0.062359
   11          6           0        0.124197    1.987553    0.080641
   12          6           0       -2.156709   -0.713092   -0.034874
   13          6           0       -0.952566    1.399483    0.059863
```

```
    14        6        0       -2.158932    0.708202    0.031653
    15        6        0       -3.395193   -1.420349   -0.103986
    16        6        0       -3.398938    1.411922    0.100184
    17        7        0       -3.217062   -2.877318    0.157968
    18        7        0       -3.238246    2.872380   -0.152267
    19        1        0       -2.681480   -3.103478    1.010755
    20        1        0       -4.123279   -3.332839    0.211460
    21        1        0       -2.707650    3.110067   -1.004984
    22        1        0       -4.149643    3.318166   -0.200395
    23        1        0       -2.702128   -3.306122   -0.610648
    24        1        0       -4.218093   -1.038776    0.493983
    25        1        0       -4.221789    1.026416   -0.494834
    26        1        0       -2.725994    3.301950    0.617744
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6003882           0.2706893           0.1872589
 Leave Link  202 at Sat Sep 26 03:35:45 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1009.2901458406 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0154321563 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1009.2747136843 Hartrees.
 Leave Link  301 at Sat Sep 26 03:35:45 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23228 LenP2D=   51915.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
```

Supporting Information file

NBasis= 606 RedAO= T EigKep= 1.82D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 03:35:46 2026, MaxMem= 805306368 cpu: 5.7 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 03:35:46 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 0.000000 -0.000000
Rot= 1.000000 -0.000088 0.000004 0.000162 Ang= -0.02 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.983934851255
Leave Link 401 at Sat Sep 26 03:35:54 2026, MaxMem= 805306368 cpu: 48.4 elap: 8.1
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

```
      NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
      wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
      NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
Symmetry not used in FoFCou.
E= -723.411555540842
DIIS: error= 1.49D-03 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -723.411555540842     IErMin= 1 ErrMin= 1.49D-03
ErrMax= 1.49D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-03 BMatP= 1.47D-03
IDIUse=3 WtCom= 9.85D-01 WtEn= 1.49D-02
Coeff-Com:  0.100D+01
Coeff-En:   0.100D+01
Coeff:      0.100D+01
Gap=     0.708 Goal=   None    Shift=    0.000
GapD=    0.708 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=9.43D-03 MaxDP=3.56D-01              OVMax= 9.91D-03

Cycle   2  Pass 0  IDiag  1:
RMSU=  7.90D-03    CP:  1.51D+00
E= -723.413222393183     Delta-E=       -0.001666852341 Rises=F Damp=F
DIIS: error= 1.05D-03 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.413222393183     IErMin= 2 ErrMin= 1.05D-03
ErrMax= 1.05D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-04 BMatP= 1.47D-03
IDIUse=3 WtCom= 9.90D-01 WtEn= 1.05D-02
Coeff-Com:  0.343D-01 0.966D+00
Coeff-En:   0.000D+00 0.100D+01
Coeff:      0.340D-01 0.966D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=9.92D-03 MaxDP=3.44D-01 DE=-1.67D-03 OVMax= 3.07D-03

Cycle   3  Pass 0  IDiag  1:
RMSU=  3.74D-03    CP:  9.25D-01  1.08D-01
E= -723.413282594942     Delta-E=       -0.000060201759 Rises=F Damp=F
DIIS: error= 3.54D-03 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -723.413282594942     IErMin= 2 ErrMin= 1.05D-03
ErrMax= 3.54D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 5.45D-04 BMatP= 1.68D-04
IDIUse=3 WtCom= 1.44D-01 WtEn= 8.56D-01
Coeff-Com: -0.601D-01 0.718D+00 0.342D+00
Coeff-En:   0.000D+00 0.217D+00 0.783D+00
Coeff:     -0.864D-02 0.289D+00 0.719D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=7.87D+02 MaxDP=3.24D+04 DE=-6.02D-05 OVMax= 9.39D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle   4  Pass 1  IDiag  1:
E= -723.413118150692     Delta-E=        0.000164444250 Rises=F Damp=F
DIIS: error= 8.15D-04 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -723.413118150692     IErMin= 1 ErrMin= 8.15D-04
```

ErrMax= 8.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-04 BMatP= 1.75D-04
IDIUse=3 WtCom= 9.92D-01 WtEn= 8.15D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=3.69D-03 MaxDP=9.64D-02 DE= 1.64D-04 OVMax= 2.04D-03

Cycle   5 Pass 1 IDiag 1:
RMSU= 3.60D-03   CP: 9.19D-01
E= -723.413225653452   Delta-E=   -0.000107502761 Rises=F Damp=F
DIIS: error= 1.56D-04 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.413225653452   IErMin= 2 ErrMin= 1.56D-04
ErrMax= 1.56D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.23D-06 BMatP= 1.75D-04
IDIUse=3 WtCom= 9.98D-01 WtEn= 1.56D-03
Coeff-Com: 0.223D-01 0.978D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.223D-01 0.978D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=3.88D-04 MaxDP=1.45D-02 DE=-1.08D-04 OVMax= 2.70D-03

Cycle   6 Pass 1 IDiag 1:
RMSU= 2.59D-04   CP: 9.32D-01 1.07D+00
E= -723.413214411971   Delta-E=   0.000011241481 Rises=F Damp=F
DIIS: error= 3.04D-04 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 2 EnMin= -723.413225653452   IErMin= 2 ErrMin= 1.56D-04
ErrMax= 3.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-05 BMatP= 6.23D-06
IDIUse=3 WtCom= 3.65D-01 WtEn= 6.35D-01
Coeff-Com: -0.201D-01 0.631D+00 0.389D+00
Coeff-En: 0.000D+00 0.681D+00 0.319D+00
Coeff: -0.732D-02 0.663D+00 0.345D+00
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=4.06D-05 MaxDP=1.55D-03 DE= 1.12D-05 OVMax= 1.25D-03

Cycle   7 Pass 1 IDiag 1:
RMSU= 1.28D-05   CP: 9.33D-01 1.08D+00 1.11D+00
E= -723.413234008486   Delta-E=   -0.000019596515 Rises=F Damp=F
DIIS: error= 3.36D-05 at cycle   4 NSaved=   4.
NSaved= 4 IEnMin= 4 EnMin= -723.413234008486   IErMin= 4 ErrMin= 3.36D-05
ErrMax= 3.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.87D-07 BMatP= 6.23D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.879D-02 0.214D+00 0.800D-01 0.715D+00
Coeff: -0.879D-02 0.214D+00 0.800D-01 0.715D+00
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=3.99D-05 MaxDP=1.67D-03 DE=-1.96D-05 OVMax= 2.75D-04

Cycle   8 Pass 1 IDiag 1:
RMSU= 6.08D-06   CP: 9.35D-01 1.08D+00 1.22D+00 1.42D+00

E= -723.413234323892 Delta-E= -0.000000315406 Rises=F Damp=F
DIIS: error= 1.21D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413234323892 IErMin= 5 ErrMin= 1.21D-05
ErrMax= 1.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.17D-08 BMatP= 1.87D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.372D-02-0.134D+00-0.966D-01 0.231D+00 0.996D+00
Coeff: 0.372D-02-0.134D+00-0.966D-01 0.231D+00 0.996D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.32D-05 MaxDP=1.45D-03 DE=-3.15D-07 OVMax= 3.11D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 1.83D-06 CP: 9.36D-01 1.09D+00 1.32D+00 1.76D+00 2.12D+00
E= -723.413234460140 Delta-E= -0.000000136249 Rises=F Damp=F
DIIS: error= 7.45D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413234460140 IErMin= 6 ErrMin= 7.45D-06
ErrMax= 7.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.81D-09 BMatP= 3.17D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.221D-02-0.702D-01-0.447D-01 0.415D-01 0.350D+00 0.722D+00
Coeff: 0.221D-02-0.702D-01-0.447D-01 0.415D-01 0.350D+00 0.722D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.84D-06 MaxDP=1.80D-04 DE=-1.36D-07 OVMax= 1.35D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 7.17D-07 CP: 9.37D-01 1.09D+00 1.33D+00 1.81D+00 2.35D+00
CP: 1.25D+00
E= -723.413234488330 Delta-E= -0.000000028190 Rises=F Damp=F
DIIS: error= 5.66D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413234488330 IErMin= 7 ErrMin= 5.66D-06
ErrMax= 5.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.36D-09 BMatP= 5.81D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.955D-03 0.397D-01 0.320D-01-0.104D+00-0.439D+00 0.468D+00
Coeff-Com: 0.100D+01
Coeff: -0.955D-03 0.397D-01 0.320D-01-0.104D+00-0.439D+00 0.468D+00
Coeff: 0.100D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.48D-06 MaxDP=1.14D-04 DE=-2.82D-08 OVMax= 1.79D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 4.41D-07 CP: 9.37D-01 1.09D+00 1.33D+00 1.84D+00 2.55D+00
CP: 1.60D+00 2.49D+00
E= -723.413234511307 Delta-E= -0.000000022977 Rises=F Damp=F
DIIS: error= 2.78D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413234511307 IErMin= 8 ErrMin= 2.78D-06
ErrMax= 2.78D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.32D-10 BMatP= 3.36D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.835D-03 0.300D-01 0.214D-01-0.423D-01-0.253D+00 0.368D-01
Coeff-Com: 0.390D+00 0.818D+00
Coeff: -0.835D-03 0.300D-01 0.214D-01-0.423D-01-0.253D+00 0.368D-01

Coeff: 0.390D+00 0.818D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.76D-07 MaxDP=1.48D-05 DE=-2.30D-08 OVMax= 6.92D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.13D-07 CP: 9.37D-01 1.09D+00 1.33D+00 1.84D+00 2.56D+00
CP: 1.64D+00 2.97D+00 1.41D+00
E= -723.413234514910 Delta-E= -0.000000003603 Rises=F Damp=F
DIIS: error= 1.08D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413234514910 IErMin= 9 ErrMin= 1.08D-06
ErrMax= 1.08D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-10 BMatP= 5.32D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.524D-04 0.227D-03-0.972D-03 0.169D-01 0.252D-01-0.125D+00
Coeff-Com: -0.156D+00 0.351D+00 0.889D+00
Coeff: -0.524D-04 0.227D-03-0.972D-03 0.169D-01 0.252D-01-0.125D+00
Coeff: -0.156D+00 0.351D+00 0.889D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.60D-07 MaxDP=1.37D-05 DE=-3.60D-09 OVMax= 3.85D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.16D-07 CP: 9.37D-01 1.09D+00 1.33D+00 1.84D+00 2.53D+00
CP: 1.61D+00 3.00D+00 1.68D+00 1.90D+00
E= -723.413234515774 Delta-E= -0.000000000865 Rises=F Damp=F
DIIS: error= 4.22D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413234515774 IErMin=10 ErrMin= 4.22D-07
ErrMax= 4.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.52D-11 BMatP= 1.51D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.150D-03-0.629D-02-0.514D-02 0.191D-01 0.674D-01-0.749D-01
Coeff-Com: -0.169D+00 0.170D-01 0.489D+00 0.663D+00
Coeff: 0.150D-03-0.629D-02-0.514D-02 0.191D-01 0.674D-01-0.749D-01
Coeff: -0.169D+00 0.170D-01 0.489D+00 0.663D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.78D-07 MaxDP=7.26D-06 DE=-8.65D-10 OVMax= 1.11D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 6.05D-08 CP: 9.37D-01 1.09D+00 1.33D+00 1.83D+00 2.51D+00
CP: 1.58D+00 3.00D+00 1.77D+00 2.32D+00 1.17D+00
E= -723.413234515928 Delta-E= -0.000000000154 Rises=F Damp=F
DIIS: error= 1.45D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413234515928 IErMin=11 ErrMin= 1.45D-07
ErrMax= 1.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.09D-12 BMatP= 4.52D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.618D-04-0.225D-02-0.166D-02 0.374D-02 0.187D-01-0.357D-02
Coeff-Com: -0.308D-01-0.632D-01 0.148D-01 0.241D+00 0.824D+00
Coeff: 0.618D-04-0.225D-02-0.166D-02 0.374D-02 0.187D-01-0.357D-02
Coeff: -0.308D-01-0.632D-01 0.148D-01 0.241D+00 0.824D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=9.48D-08 MaxDP=4.39D-06 DE=-1.54D-10 OVMax= 4.05D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.82D-08 CP: 9.37D-01 1.09D+00 1.33D+00 1.83D+00 2.51D+00
CP: 1.56D+00 3.00D+00 1.77D+00 2.50D+00 1.24D+00
CP: 1.87D+00
E= -723.413234515940 Delta-E= -0.000000000012 Rises=F Damp=F
DIIS: error= 5.95D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413234515940 IErMin=12 ErrMin= 5.95D-08
ErrMax= 5.95D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-12 BMatP= 5.09D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.709D-05 0.449D-03 0.435D-03-0.264D-02-0.719D-02 0.155D-01
Coeff-Com: 0.252D-01-0.328D-01-0.106D+00-0.453D-01 0.370D+00 0.783D+00
Coeff: -0.709D-05 0.449D-03 0.435D-03-0.264D-02-0.719D-02 0.155D-01
Coeff: 0.252D-01-0.328D-01-0.106D+00-0.453D-01 0.370D+00 0.783D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.99D-08 MaxDP=2.72D-06 DE=-1.23D-11 OVMax= 1.69D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.31D-08 CP: 9.37D-01 1.09D+00 1.33D+00 1.83D+00 2.50D+00
CP: 1.55D+00 2.97D+00 1.76D+00 2.57D+00 1.34D+00
CP: 2.15D+00 1.54D+00
E= -723.413234515952 Delta-E= -0.000000000011 Rises=F Damp=F
DIIS: error= 2.22D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.413234515952 IErMin=13 ErrMin= 2.22D-08
ErrMax= 2.22D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-13 BMatP= 1.23D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.115D-04 0.516D-03 0.434D-03-0.183D-02-0.603D-02 0.850D-02
Coeff-Com: 0.169D-01-0.844D-02-0.565D-01-0.545D-01 0.851D-01 0.401D+00
Coeff-Com: 0.615D+00
Coeff: -0.115D-04 0.516D-03 0.434D-03-0.183D-02-0.603D-02 0.850D-02
Coeff: 0.169D-01-0.844D-02-0.565D-01-0.545D-01 0.851D-01 0.401D+00
Coeff: 0.615D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.56D-08 MaxDP=9.55D-07 DE=-1.11D-11 OVMax= 4.32D-07

Cycle 17 Pass 1 IDiag 1:
RMSU= 2.94D-09 CP: 9.37D-01 1.09D+00 1.33D+00 1.83D+00 2.50D+00
CP: 1.55D+00 2.97D+00 1.76D+00 2.57D+00 1.34D+00
CP: 2.22D+00 1.71D+00 1.37D+00
E= -723.413234515950 Delta-E= 0.000000000002 Rises=F Damp=F
DIIS: error= 1.22D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.413234515952 IErMin=14 ErrMin= 1.22D-08
ErrMax= 1.22D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.06D-14 BMatP= 2.42D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.178D-06-0.159D-04-0.249D-04 0.237D-03 0.574D-03-0.179D-02
Coeff-Com: -0.232D-02 0.501D-02 0.120D-01 0.121D-03-0.546D-01-0.942D-01
Coeff-Com: 0.674D-01 0.107D+01
Coeff: -0.178D-06-0.159D-04-0.249D-04 0.237D-03 0.574D-03-0.179D-02

Coeff: -0.232D-02 0.501D-02 0.120D-01 0.121D-03-0.546D-01-0.942D-01
Coeff: 0.674D-01 0.107D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.41D-09 MaxDP=5.73D-07 DE= 1.82D-12 OVMax= 3.51D-07

SCF Done: E(RwB97XD) = -723.413234516 A.U. after 17 cycles
NFock= 17 Conv=0.84D-08 -V/T= 2.0047
KE= 7.200294715110D+02 PE=-3.699651945262D+03 EE= 1.246934525551D+03
Leave Link 502 at Sat Sep 26 03:53:51 2026, MaxMem= 805306368 cpu: 6456.6 elap: 1076.5
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23228 LenP2D= 51915.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 03:53:51 2026, MaxMem= 805306368 cpu: 3.1 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 03:53:51 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 04:09:03 2026, MaxMem= 805306368 cpu: 5469.5 elap: 911.7
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.53583976D+00 1.34589885D-02 1.35331454D-02
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000681892	-0.001091388	-0.000305371
2	6	-0.001320126	0.000519503	0.000258844
3	6	0.000667586	0.001084790	0.000305833
4	6	0.001377374	0.000524035	-0.000099855

5	6	-0.001301752	-0.000509684	-0.000260332
6	6	-0.001200152	-0.000739308	0.000208676
7	6	0.001345391	-0.000526759	0.000106203
8	6	0.000199554	0.000169888	-0.000041442
9	6	-0.001178629	0.000760125	-0.000215662
10	6	0.000059815	-0.000032024	-0.000483900
11	6	0.000072206	-0.000197758	0.000027340
12	6	-0.001014606	0.002564846	0.000602444
13	6	0.000091285	-0.000186152	0.000469106
14	6	-0.000783930	-0.003701516	-0.000498377
15	6	-0.000940622	-0.000699544	-0.001425063
16	6	-0.001814844	0.001304717	0.001308171
17	7	0.001820806	0.001413771	-0.000092371
18	7	0.002964962	-0.000788306	0.000161669
19	1	-0.000922208	-0.000465138	0.000655599
20	1	0.000498092	-0.000971762	0.000356010
21	1	-0.000913445	0.000409898	-0.000609417
22	1	0.000536855	0.001136873	-0.000345592
23	1	0.000152193	-0.000747506	-0.000379810
24	1	0.000440776	-0.000394979	0.000245388
25	1	0.000320490	0.000439629	-0.000304217
26	1	0.000161036	0.000723750	0.000356125

Cartesian Forces: Max 0.003701516 RMS 0.000960827
Leave Link 716 at Sat Sep 26 04:09:03 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003939698 RMS 0.000886505
Search for a local minimum.
Step number 17 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .88651D-03 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 14 13 15 16 17
DE= -1.56D-04 DEPred=-1.23D-04 R= 1.27D+00
TightC=F SS= 1.41D+00 RLast= 1.14D-01 DXNew= 1.2000D+00 3.4072D-01
Trust test= 1.27D+00 RLast= 1.14D-01 DXMaxT set to 7.14D-01
ITU= 1 1 1 -1 1 1 1 1 1 1 1 1 1 0 0 1 0
Eigenvalues --- 0.00254 0.00446 0.01121 0.01677 0.01741
Eigenvalues --- 0.01774 0.02405 0.02609 0.02797 0.02830
Eigenvalues --- 0.03119 0.03310 0.03630 0.03791 0.04356
Eigenvalues --- 0.04438 0.04467 0.05026 0.06912 0.07254

```
    Eigenvalues ---    0.09965   0.10586   0.10983   0.11245   0.11541
    Eigenvalues ---    0.11700   0.13850   0.15203   0.15365   0.15884
    Eigenvalues ---    0.16000   0.16000   0.16006   0.16128   0.16973
    Eigenvalues ---    0.22172   0.22872   0.24732   0.24995   0.24997
    Eigenvalues ---    0.24998   0.25000   0.25000   0.25077   0.29281
    Eigenvalues ---    0.30020   0.35099   0.37236   0.38299   0.44900
    Eigenvalues ---    0.45795   0.46200   0.47445   0.47651   0.47688
    Eigenvalues ---    0.47688   0.47979   0.48126   0.50605   0.54809
    Eigenvalues ---    0.54946   0.55349   0.55659   0.55663   0.86145
    Eigenvalues ---    0.93725   0.95021   0.95201   0.96170   0.97721
    Eigenvalues ---    1.05868   1.37678
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    17   16   15
 RFO step:  Lambda=-2.61340070D-04.
 NNeg= 0 NGDIIS= 3 SimSw=  2.50D-01 Rises=F DC= -1.56D-04 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.2293182393D-01 NUsed= 3 OKEnD=T EnDIS=F
 InvSVX:  RCond= 5.10D-04 Info=          0 Equed=N FErr=  5.33D-14 BErr=  6.54D-17
 DidBck=F Rises=F RFO-DIIS coefs:    1.76294   -0.20632   -0.55663
 Iteration  1 RMS(Cart)=  0.03446949 RMS(Int)=  0.00125009
 Iteration  2 RMS(Cart)=  0.00130523 RMS(Int)=  0.00000977
 Iteration  3 RMS(Cart)=  0.00000149 RMS(Int)=  0.00000970
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000970
  ITry=  1  IFail=0  DXMaxC=  1.32D-01  DCOld=  1.00D+10  DXMaxT=  7.14D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)   (Quad)   (Total)
   R1       2.32249   0.00091  -0.00221   0.00095  -0.00125   2.32124
   R2       2.53443  -0.00047   0.00336  -0.00109   0.00227   2.53669
   R3       2.53245  -0.00053   0.00279  -0.00110   0.00169   2.53414
   R4       2.32246   0.00089  -0.00221   0.00095  -0.00126   2.32120
   R5       2.31901   0.00072  -0.00183   0.00081  -0.00102   2.31799
   R6       2.53257  -0.00052   0.00282  -0.00112   0.00170   2.53427
   R7       2.53475  -0.00053   0.00199  -0.00096   0.00103   2.53578
   R8       2.31891   0.00069  -0.00186   0.00082  -0.00104   2.31787
   R9       2.31899  -0.00030  -0.00070   0.00011  -0.00059   2.31840
  R10       2.53498  -0.00054   0.00207  -0.00104   0.00104   2.53601
  R11       2.62747  -0.00028   0.00135  -0.00025   0.00110   2.62856
  R12       2.31881  -0.00041  -0.00075   0.00010  -0.00065   2.31816
  R13       2.68880   0.00048  -0.00549   0.00167  -0.00382   2.68498
  R14       2.69830  -0.00187   0.00403  -0.00234   0.00170   2.70000
  R15       2.62800  -0.00026   0.00159  -0.00033   0.00126   2.62926
  R16       2.69744  -0.00272   0.00380  -0.00217   0.00163   2.69907
  R17       2.81760  -0.00065   0.00517  -0.00079   0.00438   2.82198
  R18       2.05305  -0.00034   0.00131  -0.00083   0.00048   2.05353
  R19       2.81721  -0.00122   0.00505  -0.00078   0.00427   2.82148
  R20       2.05255  -0.00027   0.00103  -0.00057   0.00047   2.05301
  R21       1.95040  -0.00113   0.00100  -0.00131  -0.00031   1.95009
  R22       1.91934  -0.00089   0.00097  -0.00101  -0.00004   1.91930
```

R23	1.92697	-0.00051	0.00186	-0.00080	0.00106	1.92803
R24	1.95032	-0.00107	0.00097	-0.00126	-0.00029	1.95002
R25	1.91943	-0.00099	0.00103	-0.00106	-0.00003	1.91940
R26	1.92701	-0.00048	0.00187	-0.00080	0.00107	1.92808
A1	2.56240	-0.00015	-0.00167	-0.00044	-0.00212	2.56028
A2	2.60730	0.00037	0.00181	0.00094	0.00275	2.61005
A3	2.56334	-0.00015	-0.00140	-0.00043	-0.00183	2.56151
A4	2.72443	-0.00058	-0.00242	-0.00164	-0.00407	2.72037
A5	2.60651	0.00035	0.00162	0.00085	0.00246	2.60898
A6	2.83562	0.00044	0.00465	0.00093	0.00558	2.84120
A7	2.72510	-0.00061	-0.00221	-0.00170	-0.00391	2.72119
A8	2.83529	0.00041	0.00460	0.00081	0.00541	2.84070
A9	2.09032	-0.00023	0.00124	-0.00151	-0.00029	2.09003
A10	2.10317	-0.00000	-0.00300	0.00204	-0.00098	2.10219
A11	2.08942	0.00024	0.00182	-0.00081	0.00099	2.09041
A12	2.08993	0.00016	0.00102	-0.00155	-0.00055	2.08938
A13	2.08986	0.00019	0.00193	-0.00093	0.00098	2.09083
A14	2.10312	-0.00035	-0.00288	0.00216	-0.00075	2.10237
A15	2.04470	0.00091	-0.00558	0.00243	-0.00315	2.04155
A16	1.91452	0.00158	-0.01651	0.00754	-0.00896	1.90555
A17	2.04523	0.00161	-0.00614	0.00251	-0.00363	2.04159
A18	1.91409	0.00233	-0.01794	0.00845	-0.00950	1.90460
A19	2.00565	0.00002	0.00433	-0.00080	0.00351	2.00917
A20	1.91868	-0.00079	0.00523	-0.00298	0.00223	1.92092
A21	1.91646	-0.00050	-0.00279	-0.00178	-0.00456	1.91189
A22	1.89780	0.00038	-0.00176	0.00156	-0.00023	1.89757
A23	1.84275	0.00038	-0.00455	0.00220	-0.00235	1.84040
A24	1.87723	0.00060	-0.00113	0.00225	0.00112	1.87835
A25	2.00528	0.00014	0.00427	-0.00085	0.00340	2.00868
A26	1.91905	-0.00101	0.00542	-0.00316	0.00224	1.92129
A27	1.91661	-0.00046	-0.00296	-0.00146	-0.00441	1.91219
A28	1.89767	0.00040	-0.00173	0.00163	-0.00013	1.89753
A29	1.84275	0.00038	-0.00458	0.00218	-0.00240	1.84035
A30	1.87721	0.00065	-0.00108	0.00210	0.00103	1.87824
A31	2.90699	-0.00000	-0.00285	0.00095	-0.00190	2.90509
A32	3.12257	0.00000	-0.00056	0.00057	0.00001	3.12258
A33	2.90804	-0.00008	-0.00213	0.00022	-0.00191	2.90613
A34	3.12103	0.00009	-0.00174	0.00210	0.00037	3.12140
A35	3.95922	0.00250	-0.02208	0.00997	-0.01211	3.94710
A36	3.95932	0.00394	-0.02409	0.01096	-0.01313	3.94619
A37	3.14758	-0.00033	-0.00143	0.00093	-0.00050	3.14707
A38	3.14431	-0.00054	0.00291	-0.00308	-0.00016	3.14414
A39	3.14740	-0.00032	-0.00154	0.00122	-0.00033	3.14707
A40	3.14437	-0.00058	0.00286	-0.00105	0.00182	3.14619
A41	4.03407	0.00056	0.01980	-0.00623	0.01357	4.04763
A42	4.01964	0.00282	0.01561	-0.00408	0.01152	4.03117
D1	0.02499	-0.00026	0.00201	-0.00148	0.00053	0.02551
D2	-0.02027	-0.00022	-0.00139	0.00072	-0.00068	-0.02094

D3	-0.01530	-0.00008	-0.00000	-0.00029	-0.00029	-0.01559
D4	0.02499	-0.00027	0.00198	-0.00135	0.00063	0.02562
D5	0.00794	-0.00002	-0.00031	-0.00055	-0.00086	0.00708
D6	-0.01530	-0.00008	-0.00005	-0.00002	-0.00007	-0.01537
D7	-0.00669	0.00026	-0.00836	0.00950	0.00115	-0.00555
D8	3.11127	-0.00018	-0.00486	-0.00526	-0.01012	3.10115
D9	0.00814	-0.00003	-0.00023	-0.00041	-0.00063	0.00751
D10	-0.00707	0.00025	-0.00859	0.01134	0.00276	-0.00431
D11	3.11069	-0.00017	-0.00493	-0.00336	-0.00829	3.10240
D12	0.00733	0.00002	0.00756	-0.01030	-0.00273	0.00460
D13	-3.10900	-0.00004	0.00479	0.00416	0.00895	-3.10005
D14	-3.10915	-0.00000	0.00505	0.00256	0.00762	-3.10153
D15	0.05770	-0.00006	0.00229	0.01702	0.01931	0.07701
D16	2.49322	-0.00039	-0.00191	0.00099	-0.00092	2.49231
D17	-0.67366	-0.00036	0.00069	-0.01203	-0.01134	-0.68500
D18	-0.66964	-0.00023	0.00034	-0.01454	-0.01419	-0.68384
D19	2.49740	-0.00030	-0.00251	0.00009	-0.00242	2.49498
D20	-1.42183	0.00074	0.07165	0.00246	0.07409	-1.34774
D21	0.72558	0.00063	0.07655	0.00158	0.07815	0.80373
D22	2.78754	0.00060	0.07665	0.00145	0.07810	2.86564
D23	-1.42619	0.00079	0.07180	0.00280	0.07457	-1.35162
D24	0.72106	0.00062	0.07682	0.00183	0.07868	0.79975
D25	2.78331	0.00053	0.07700	0.00162	0.07861	2.86192

Item	Value	Threshold	Converged?
Maximum Force	0.003940	0.000450	NO
RMS Force	0.000887	0.000300	NO
Maximum Displacement	0.131691	0.001800	NO
RMS Displacement	0.034537	0.001200	NO

Predicted change in Energy=-1.294602D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 04:09:03 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.019798	0.673694	0.048556
2	6	0	3.345008	1.697799	0.117132
3	6	0	4.020204	-0.665059	-0.049806
4	6	0	2.142064	2.288421	0.166024
5	6	0	3.347321	-1.690438	-0.117663
6	6	0	0.916265	2.332668	0.174891
7	6	0	2.144760	-2.282109	-0.165263
8	6	0	-0.379136	1.982977	0.157964

9	6	0	0.919094	-2.328385	-0.173016
10	6	0	-1.455570	1.395895	0.115808
11	6	0	-0.376814	-1.980151	-0.155131
12	6	0	-2.663105	0.707514	0.062845
13	6	0	-1.454393	-1.395493	-0.112283
14	6	0	-2.662903	-0.708367	-0.055677
15	6	0	-3.902441	1.410252	0.170580
16	6	0	-3.901388	-1.411904	-0.161444
17	7	0	-3.727186	2.877007	-0.048375
18	7	0	-3.740678	-2.882243	0.042307
19	1	0	-3.252522	3.135002	-0.927602
20	1	0	-4.628321	3.344337	-0.015099
21	1	0	-3.269282	-3.153512	0.919251
22	1	0	-4.646190	-3.340720	0.003635
23	1	0	-3.149458	3.266704	0.696818
24	1	0	-4.726078	1.053719	-0.442106
25	1	0	-4.724514	-1.055485	0.451509
26	1	0	-3.166021	-3.270046	-0.706281

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.228347	0.000000			
3	C	1.342361	2.463098	0.000000		
4	C	2.479320	1.341007	3.506713	0.000000	
5	C	2.463529	3.396363	1.228324	4.167067	0.000000
6	C	3.521374	2.511013	4.321029	1.226629	4.709671
7	C	3.506886	4.166534	2.479006	4.582521	1.341078
8	C	4.590949	3.735270	5.139013	2.539648	5.239888
9	C	4.321566	4.709501	3.521181	4.788059	2.511239
10	C	5.523201	4.810062	5.853124	3.707033	5.713818
11	C	5.139511	5.239599	4.590678	4.966749	3.735574
12	C	6.683003	6.089420	6.823728	5.059601	6.473637
13	C	5.854414	5.714485	5.523463	5.155888	4.810766
14	C	6.824913	6.474140	6.683249	5.667238	6.090245
15	C	7.957341	7.253348	8.192910	6.107965	7.890273
16	C	8.193839	7.890381	7.957503	7.093867	7.254190
17	N	8.054796	7.171740	8.518702	5.902584	8.421105
18	N	8.536375	8.437377	8.071906	7.833117	7.189277
19	H	7.739351	6.832600	8.252486	5.569046	8.215765
20	H	9.051317	8.142637	9.532756	6.854624	9.432408
21	H	8.278665	8.241811	7.763252	7.711333	6.855305
22	H	9.550753	9.447688	9.070193	8.820091	8.162987
23	H	7.651286	6.706385	8.210984	5.407309	8.212477
24	H	8.767868	8.116035	8.922194	7.004690	8.533196
25	H	8.922747	8.532852	8.767773	7.642847	8.116750
26	H	8.231576	8.231099	7.671945	7.735195	6.727945

	6	7	8	9	10

Supporting Information file

6	C	0.000000				
7	C	4.787595	0.000000			
8	C	1.341877	4.966435	0.000000		
9	C	4.674020	1.226564	4.514731	0.000000	
10	C	2.550811	5.154521	1.226847	4.426366	0.000000
11	C	4.514573	2.539610	3.975476	1.342001	3.554547
12	C	3.932629	5.666166	2.617702	4.701539	1.390976
13	C	4.427378	3.707128	3.555737	2.550964	2.800692
14	C	4.702286	5.059871	3.536179	3.933056	2.432072
15	C	4.906200	7.093303	3.569573	6.110865	2.447526
16	C	6.111032	6.108451	4.902396	4.906844	3.733983
17	N	4.680576	7.817281	3.471499	6.978507	2.716779
18	N	6.992853	5.919597	5.914702	4.697510	4.850730
19	H	4.386117	7.684849	3.280543	6.915228	2.709656
20	H	5.639326	8.806478	4.465291	7.935901	3.725575
21	H	6.940537	5.589935	5.942729	4.406402	4.963082
22	H	7.947174	6.875041	6.824465	5.659366	5.712107
23	H	4.204157	7.717594	3.100485	6.972428	2.589740
24	H	5.818284	7.642827	4.485478	6.586275	3.335352
25	H	6.585931	7.005137	5.310436	5.818988	4.099750
26	H	6.987985	5.428915	6.008985	4.226022	5.037110

		11	12	13	14	15
11	C	0.000000				
12	C	3.535277	0.000000			
13	C	1.226718	2.431932	0.000000		
14	C	2.617924	1.420833	1.391346	0.000000	
15	C	4.902138	1.428776	3.734321	2.464993	0.000000
16	C	3.570093	2.464869	2.447544	1.428285	2.841620
17	N	5.901557	2.418954	4.839828	3.740008	1.493327
18	N	3.488313	3.748058	2.731560	2.428361	4.297456
19	H	5.918716	2.687210	4.942003	3.984895	2.145498
20	H	6.815063	3.289526	5.705195	4.504322	2.074141
21	H	3.301128	4.001051	2.729197	2.701281	4.667905
22	H	4.483741	4.508252	3.739642	3.296397	4.811733
23	H	5.995236	2.681029	5.026328	4.074821	2.071309
24	H	5.310633	2.151904	4.100165	2.740615	1.086682
25	H	4.486147	2.740188	3.335740	2.151272	2.614304
26	H	3.122062	4.082336	2.607001	2.690468	4.818339

		16	17	18	19	20
16	C	0.000000				
17	N	4.293936	0.000000			
18	N	1.493063	5.759979	0.000000		
19	H	4.656434	1.031944	6.114430	0.000000	
20	H	4.813696	1.015651	6.289793	1.664123	0.000000
21	H	2.144914	6.124797	1.031906	6.554125	6.703882
22	H	2.074203	6.285492	1.015702	6.689132	6.685107
23	H	4.815743	1.020268	6.211881	1.633007	1.643133
24	H	2.614992	2.115936	4.086253	2.595922	2.332128

```
  25  H    1.086408   4.087669   2.114811   4.650687   4.425540
  26  H    2.071305   6.207577   1.020298   6.409454   6.809267
                21         22         23         24         25
  21  H    0.000000
  22  H    1.664114   0.000000
  23  H    6.425185   6.810196   0.000000
  24  H    4.655786   4.417711   2.946214   0.000000
  25  H    2.595804   2.330027   4.606766   2.290697   0.000000
  26  H    1.632972   1.643131   6.685661   4.604185   2.945108
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=3 Diff= 4.97D-04
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.525210   -0.665294   -0.022924
    2          6           0        3.852418   -1.692590   -0.052102
    3          6           0        4.523006    0.676241    0.024093
    4          6           0        2.650627   -2.286998   -0.078115
    5          6           0        3.848124    1.702152    0.052752
    6          6           0        1.424916   -2.333944   -0.085054
    7          6           0        2.644413    2.292863    0.077879
    8          6           0        0.128835   -1.986390   -0.081292
    9          6           0        1.418660    2.337011    0.084081
   10          6           0       -0.948742   -1.400227   -0.061453
   11          6           0        0.123434    1.985818    0.079787
   12          6           0       -2.157616   -0.712681   -0.034669
   13          6           0       -0.953003    1.397846    0.059562
   14          6           0       -2.160172    0.706698    0.029538
   15          6           0       -3.395585   -1.421447   -0.115181
   16          6           0       -3.400020    1.411351    0.108511
   17          7           0       -3.217436   -2.878395    0.159756
   18          7           0       -3.242211    2.873119   -0.151433
   19          1           0       -2.742171   -3.101599    1.048132
   20          1           0       -4.117657   -3.348414    0.144570
   21          1           0       -2.771444    3.111522   -1.038210
   22          1           0       -4.148615    3.330973   -0.130181
   23          1           0       -2.639028   -3.295218   -0.570072
   24          1           0       -4.219852   -1.043318    0.483552
   25          1           0       -4.222515    1.030112   -0.490188
```

```
    26        1        0      -2.668231    3.290429    0.581647
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6008015           0.2704693           0.1871977
 Leave Link  202 at Sat Sep 26 04:09:03 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1009.1792229651 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.222036 cShort=  0.000000 cLong=
0.777964
  DFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.000000 cShort=  0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0154405701 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1009.1637823950 Hartrees.
 Leave Link  301 at Sat Sep 26 04:09:03 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23232 LenP2D=   51916.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.84D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=          32
 NSgBfM=   683   683   683   683   683 MxSgAt=    26 MxSgA2=    26.
 Leave Link  302 at Sat Sep 26 04:09:04 2026, MaxMem=    805306368 cpu:                  5.7 elap:
1.0
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Sat Sep 26 04:09:04 2026, MaxMem=    805306368 cpu:                  0.7 elap:
0.1
```

Supporting Information file

(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 -0.000000 0.000000
Rot= 1.000000 -0.000069 -0.000002 -0.000117 Ang= -0.02 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.983768668344
Leave Link 401 at Sat Sep 26 04:09:12 2026, MaxMem= 805306368 cpu: 45.1 elap: 7.5
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.410669456987
DIIS: error= 2.10D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.410669456987 IErMin= 1 ErrMin= 2.10D-03
ErrMax= 2.10D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D-03 BMatP= 2.17D-03
IDIUse=3 WtCom= 9.79D-01 WtEn= 2.10D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01

Gap= 0.708 Goal= None Shift= 0.000
GapD= 0.708 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=7.73D-03 MaxDP=3.00D-01 OVMax= 1.26D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 6.58D-03 CP: 1.40D+00
E= -723.413324138091 Delta-E= -0.002654681103 Rises=F Damp=F
DIIS: error= 8.55D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413324138091 IErMin= 2 ErrMin= 8.55D-04
ErrMax= 8.55D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.72D-04 BMatP= 2.17D-03
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.55D-03
Coeff-Com: -0.335D-01 0.103D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.332D-01 0.103D+01
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=8.95D-03 MaxDP=3.14D-01 DE=-2.65D-03 OVMax= 3.21D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 3.84D-03 CP: 8.66D-01 9.00D-02
E= -723.413422094506 Delta-E= -0.000097956415 Rises=F Damp=F
DIIS: error= 3.70D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.413422094506 IErMin= 2 ErrMin= 8.55D-04
ErrMax= 3.70D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.81D-04 BMatP= 1.72D-04
IDIUse=3 WtCom= 1.41D-01 WtEn= 8.59D-01
Coeff-Com: -0.862D-01 0.752D+00 0.334D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.122D-01 0.106D+00 0.906D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=8.03D+02 MaxDP=3.27D+04 DE=-9.80D-05 OVMax= 9.36D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.413266086296 Delta-E= 0.000156008210 Rises=F Damp=F
DIIS: error= 8.61D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413266086296 IErMin= 1 ErrMin= 8.61D-04
ErrMax= 8.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.78D-04 BMatP= 1.78D-04
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.61D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=3.68D-03 MaxDP=9.34D-02 DE= 1.56D-04 OVMax= 3.03D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.64D-03 CP: 9.43D-01
E= -723.413371494748 Delta-E= -0.000105408452 Rises=F Damp=F
DIIS: error= 2.22D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -723.413371494748 IErMin= 2 ErrMin= 2.22D-04
ErrMax= 2.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-05 BMatP= 1.78D-04
IDIUse=3 WtCom= 9.98D-01 WtEn= 2.22D-03
Coeff-Com: 0.876D-01 0.912D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.874D-01 0.913D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.35D-04 MaxDP=1.78D-02 DE=-1.05D-04 OVMax= 2.31D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.79D-04 CP: 9.58D-01 1.08D+00
E= -723.413352845784 Delta-E= 0.000018648964 Rises=F Damp=F
DIIS: error= 3.11D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413371494748 IErMin= 2 ErrMin= 2.22D-04
ErrMax= 3.11D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.20D-05 BMatP= 1.48D-05
IDIUse=3 WtCom= 3.62D-01 WtEn= 6.38D-01
Coeff-Com: -0.198D-01 0.606D+00 0.414D+00
Coeff-En: 0.000D+00 0.651D+00 0.349D+00
Coeff: -0.718D-02 0.635D+00 0.372D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=7.81D-05 MaxDP=3.34D-03 DE= 1.86D-05 OVMax= 1.78D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.92D-05 CP: 9.61D-01 1.10D+00 1.18D+00
E= -723.413388549031 Delta-E= -0.000035703247 Rises=F Damp=F
DIIS: error= 2.19D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413388549031 IErMin= 4 ErrMin= 2.19D-05
ErrMax= 2.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.58D-07 BMatP= 1.48D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.108D-01 0.247D+00 0.123D+00 0.640D+00
Coeff: -0.108D-01 0.247D+00 0.123D+00 0.640D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.45D-05 MaxDP=1.99D-03 DE=-3.57D-05 OVMax= 2.66D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 6.85D-06 CP: 9.63D-01 1.10D+00 1.29D+00 1.32D+00
E= -723.413389025892 Delta-E= -0.000000476861 Rises=F Damp=F
DIIS: error= 1.23D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413389025892 IErMin= 5 ErrMin= 1.23D-05
ErrMax= 1.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.08D-08 BMatP= 3.58D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.455D-02-0.146D+00-0.105D+00 0.834D-01 0.116D+01
Coeff: 0.455D-02-0.146D+00-0.105D+00 0.834D-01 0.116D+01
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.55D-05 MaxDP=2.05D-03 DE=-4.77D-07 OVMax= 4.59D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 2.44D-06 CP: 9.65D-01 1.11D+00 1.41D+00 1.67D+00 2.27D+00

E= -723.413389218191 Delta-E= -0.000000192299 Rises=F Damp=F
DIIS: error= 7.24D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413389218191 IErMin= 6 ErrMin= 7.24D-06
ErrMax= 7.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.72D-09 BMatP= 3.08D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.143D-02-0.367D-01-0.211D-01-0.433D-01 0.952D-01 0.100D+01
Coeff: 0.143D-02-0.367D-01-0.211D-01-0.433D-01 0.952D-01 0.100D+01
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.35D-06 MaxDP=2.12D-04 DE=-1.92D-07 OVMax= 1.83D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.21D-06 CP: 9.65D-01 1.11D+00 1.42D+00 1.73D+00 2.57D+00
CP: 1.21D+00
E= -723.413389256053 Delta-E= -0.000000037862 Rises=F Damp=F
DIIS: error= 6.01D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413389256053 IErMin= 7 ErrMin= 6.01D-06
ErrMax= 6.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.53D-09 BMatP= 4.72D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.990D-03 0.369D-01 0.294D-01-0.510D-01-0.410D+00 0.566D+00
Coeff-Com: 0.829D+00
Coeff: -0.990D-03 0.369D-01 0.294D-01-0.510D-01-0.410D+00 0.566D+00
Coeff: 0.829D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=1.48D-06 MaxDP=4.73D-05 DE=-3.79D-08 OVMax= 1.49D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 3.75D-07 CP: 9.65D-01 1.11D+00 1.42D+00 1.75D+00 2.70D+00
CP: 1.35D+00 1.73D+00
E= -723.413389272865 Delta-E= -0.000000016812 Rises=F Damp=F
DIIS: error= 2.81D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413389272865 IErMin= 8 ErrMin= 2.81D-06
ErrMax= 2.81D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.35D-10 BMatP= 2.53D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.821D-03 0.266D-01 0.190D-01-0.106D-01-0.223D+00-0.191D-03
Coeff-Com: 0.452D+00 0.737D+00
Coeff: -0.821D-03 0.266D-01 0.190D-01-0.106D-01-0.223D+00-0.191D-03
Coeff: 0.452D+00 0.737D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.73D-07 MaxDP=1.66D-05 DE=-1.68D-08 OVMax= 7.14D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.98D-07 CP: 9.65D-01 1.11D+00 1.42D+00 1.75D+00 2.70D+00
CP: 1.37D+00 1.99D+00 1.43D+00
E= -723.413389276748 Delta-E= -0.000000003883 Rises=F Damp=F
DIIS: error= 1.31D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413389276748 IErMin= 9 ErrMin= 1.31D-06
ErrMax= 1.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-10 BMatP= 8.35D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.586D-04 0.290D-03-0.726D-03 0.133D-01 0.286D-01-0.205D+00
Coeff-Com: -0.391D-01 0.321D+00 0.882D+00
Coeff: -0.586D-04 0.290D-03-0.726D-03 0.133D-01 0.286D-01-0.205D+00
Coeff: -0.391D-01 0.321D+00 0.882D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=3.24D-07 MaxDP=1.15D-05 DE=-3.88D-09 OVMax= 3.79D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.05D-07 CP: 9.65D-01 1.11D+00 1.42D+00 1.74D+00 2.68D+00
CP: 1.34D+00 2.07D+00 1.74D+00 1.92D+00
E= -723.413389277768 Delta-E= -0.000000001020 Rises=F Damp=F
DIIS: error= 2.96D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413389277768 IErMin=10 ErrMin= 2.96D-07
ErrMax= 2.96D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.16D-11 BMatP= 1.73D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.172D-03-0.627D-02-0.491D-02 0.875D-02 0.659D-01-0.910D-01
Coeff-Com: -0.118D+00-0.301D-01 0.384D+00 0.791D+00
Coeff: 0.172D-03-0.627D-02-0.491D-02 0.875D-02 0.659D-01-0.910D-01
Coeff: -0.118D+00-0.301D-01 0.384D+00 0.791D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=1.99D-07 MaxDP=8.61D-06 DE=-1.02D-09 OVMax= 1.39D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 5.45D-08 CP: 9.65D-01 1.11D+00 1.42D+00 1.74D+00 2.67D+00
CP: 1.31D+00 2.02D+00 1.89D+00 2.31D+00 1.63D+00
E= -723.413389277911 Delta-E= -0.000000000142 Rises=F Damp=F
DIIS: error= 2.11D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413389277911 IErMin=11 ErrMin= 2.11D-07
ErrMax= 2.11D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.48D-12 BMatP= 3.16D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.430D-04-0.134D-02-0.907D-03 0.165D-03 0.990D-02 0.800D-02
Coeff-Com: -0.199D-01-0.475D-01-0.403D-01 0.190D+00 0.902D+00
Coeff: 0.430D-04-0.134D-02-0.907D-03 0.165D-03 0.990D-02 0.800D-02
Coeff: -0.199D-01-0.475D-01-0.403D-01 0.190D+00 0.902D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=9.71D-08 MaxDP=4.65D-06 DE=-1.42D-10 OVMax= 3.36D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 2.51D-08 CP: 9.65D-01 1.11D+00 1.42D+00 1.74D+00 2.66D+00
CP: 1.31D+00 1.98D+00 1.92D+00 2.41D+00 1.93D+00
CP: 1.58D+00
E= -723.413389277937 Delta-E= -0.000000000026 Rises=F Damp=F
DIIS: error= 5.25D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413389277937 IErMin=12 ErrMin= 5.25D-08
ErrMax= 5.25D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-12 BMatP= 3.48D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.130D-04 0.600D-03 0.556D-03-0.183D-02-0.867D-02 0.240D-01
Coeff-Com: 0.134D-01-0.216D-01-0.106D+00-0.689D-01 0.488D+00 0.680D+00

Coeff: -0.130D-04 0.600D-03 0.556D-03-0.183D-02-0.867D-02 0.240D-01
Coeff: 0.134D-01-0.216D-01-0.106D+00-0.689D-01 0.488D+00 0.680D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.86D-08 MaxDP=2.61D-06 DE=-2.59D-11 OVMax= 1.52D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 6.97D-09 CP: 9.65D-01 1.11D+00 1.42D+00 1.74D+00 2.66D+00
CP: 1.30D+00 1.97D+00 1.94D+00 2.44D+00 2.04D+00
CP: 1.88D+00 1.38D+00
E= -723.413389277929 Delta-E= 0.000000000008 Rises=F Damp=F
DIIS: error= 3.38D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=12 EnMin= -723.413389277937 IErMin=13 ErrMin= 3.38D-08
ErrMax= 3.38D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-13 BMatP= 1.45D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.100D-04 0.390D-03 0.322D-03-0.734D-03-0.448D-02 0.879D-02
Coeff-Com: 0.760D-02-0.280D-02-0.366D-01-0.504D-01 0.874D-01 0.273D+00
Coeff-Com: 0.718D+00
Coeff: -0.100D-04 0.390D-03 0.322D-03-0.734D-03-0.448D-02 0.879D-02
Coeff: 0.760D-02-0.280D-02-0.366D-01-0.504D-01 0.874D-01 0.273D+00
Coeff: 0.718D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=2.38D-08 MaxDP=1.32D-06 DE= 7.73D-12 OVMax= 3.03D-07

Cycle 17 Pass 1 IDiag 1:
RMSU= 2.92D-09 CP: 9.65D-01 1.11D+00 1.42D+00 1.74D+00 2.66D+00
CP: 1.30D+00 1.96D+00 1.94D+00 2.43D+00 2.05D+00
CP: 1.97D+00 1.55D+00 1.22D+00
E= -723.413389277924 Delta-E= 0.000000000005 Rises=F Damp=F
DIIS: error= 1.45D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=12 EnMin= -723.413389277937 IErMin=14 ErrMin= 1.45D-08
ErrMax= 1.45D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.64D-14 BMatP= 1.44D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.595D-06-0.702D-06-0.139D-04 0.160D-03 0.438D-03-0.249D-02
Coeff-Com: -0.693D-03 0.452D-02 0.124D-01-0.304D-02-0.897D-01-0.546D-01
Coeff-Com: 0.282D+00 0.851D+00
Coeff: -0.595D-06-0.702D-06-0.139D-04 0.160D-03 0.438D-03-0.249D-02
Coeff: -0.693D-03 0.452D-02 0.124D-01-0.304D-02-0.897D-01-0.546D-01
Coeff: 0.282D+00 0.851D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=1.09D-08 MaxDP=6.43D-07 DE= 5.23D-12 OVMax= 2.43D-07

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.12D-09 CP: 9.65D-01 1.11D+00 1.42D+00 1.74D+00 2.66D+00
CP: 1.30D+00 1.96D+00 1.94D+00 2.42D+00 2.05D+00
CP: 2.01D+00 1.65D+00 1.38D+00 1.74D+00
E= -723.413389277938 Delta-E= -0.000000000015 Rises=F Damp=F
DIIS: error= 1.03D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.413389277938 IErMin=15 ErrMin= 1.03D-08

Supporting Information file

ErrMax= 1.03D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-14 BMatP= 3.64D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.287D-05-0.123D-03-0.107D-03 0.305D-03 0.161D-02-0.398D-02
Coeff-Com: -0.290D-02 0.323D-02 0.178D-01 0.144D-01-0.724D-01-0.109D+00
Coeff-Com: -0.968D-01 0.408D+00 0.841D+00
Coeff: 0.287D-05-0.123D-03-0.107D-03 0.305D-03 0.161D-02-0.398D-02
Coeff: -0.290D-02 0.323D-02 0.178D-01 0.144D-01-0.724D-01-0.109D+00
Coeff: -0.968D-01 0.408D+00 0.841D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=2.33D-09 MaxDP=1.35D-07 DE=-1.46D-11 OVMax= 1.64D-07

SCF Done: E(RwB97XD) = -723.413389278 A.U. after 18 cycles
NFock= 18 Conv=0.23D-08 -V/T= 2.0047
KE= 7.200275150764D+02 PE=-3.699413871316D+03 EE= 1.246809184567D+03
Leave Link 502 at Sat Sep 26 04:31:50 2026, MaxMem= 805306368 cpu: 8147.4 elap: 1358.2
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23232 LenP2D= 51916.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 04:31:51 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 04:31:51 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 04:44:16 2026, MaxMem= 805306368 cpu: 4469.1 elap: 745.0
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.49011197D+00 1.72286729D-02 1.90761443D-02
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)

Supporting Information file

Number	Number	X	Y	Z
1	6	0.000787971	-0.001692603	-0.000389775
2	6	-0.001575100	0.000975336	0.000330016
3	6	0.000782077	0.001689241	0.000393166
4	6	0.001768600	0.000189841	-0.000153119
5	6	-0.001560472	-0.000965075	-0.000330499
6	6	-0.001539884	-0.000450071	0.000221743
7	6	0.001747259	-0.000200133	0.000160801
8	6	0.000284113	0.000085421	-0.000103387
9	6	-0.001516836	0.000481179	-0.000264945
10	6	0.000083402	-0.000196492	-0.000488174
11	6	0.000184789	-0.000131889	0.000059333
12	6	-0.000704868	0.003235926	0.001544514
13	6	-0.000024141	-0.000075474	0.000614112
14	6	-0.000262198	-0.004581262	-0.001554343
15	6	-0.001417705	0.000508725	-0.002152118
16	6	-0.002544076	0.000224891	0.002025238
17	7	0.002495238	0.001219766	0.000102484
18	7	0.003942756	-0.000486135	0.000043146
19	1	-0.001016198	-0.000545241	0.000774939
20	1	0.000492242	-0.001165993	0.000252397
21	1	-0.001029040	0.000465382	-0.000723309
22	1	0.000534721	0.001362773	-0.000230569
23	1	-0.000171065	-0.000968622	-0.000343689
24	1	0.000291065	-0.000867218	0.000446905
25	1	0.000126577	0.000932249	-0.000552599
26	1	-0.000159224	0.000955481	0.000317732

Cartesian Forces: Max 0.004581262 RMS 0.001221753
Leave Link 716 at Sat Sep 26 04:44:16 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.004559077 RMS 0.001033462
Search for a local minimum.
Step number 18 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .10335D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 14 15 16 17 18
DE= -1.55D-04 DEPred=-1.29D-04 R= 1.20D+00
TightC=F SS= 1.41D+00 RLast= 1.94D-01 DXNew= 1.2000D+00 5.8321D-01
Trust test= 1.20D+00 RLast= 1.94D-01 DXMaxT set to 7.14D-01

Supporting Information file

ITU= 1 1 1 1 -1 1 1 1 1 1 1 1 1 0 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00224	0.00446	0.01114	0.01478	0.01684
Eigenvalues ---	0.01758	0.02414	0.02669	0.02799	0.02924
Eigenvalues ---	0.03114	0.03386	0.03641	0.03791	0.04361
Eigenvalues ---	0.04439	0.04467	0.05026	0.06630	0.07163
Eigenvalues ---	0.09965	0.10441	0.10995	0.11225	0.11517
Eigenvalues ---	0.11709	0.13826	0.15199	0.15392	0.15881
Eigenvalues ---	0.16000	0.16000	0.16007	0.16112	0.17344
Eigenvalues ---	0.22346	0.23022	0.24409	0.24993	0.24996
Eigenvalues ---	0.24997	0.25000	0.25000	0.25032	0.29287
Eigenvalues ---	0.29801	0.35698	0.37236	0.38384	0.45163
Eigenvalues ---	0.45807	0.46348	0.47545	0.47634	0.47688
Eigenvalues ---	0.47689	0.48043	0.48314	0.50785	0.54807
Eigenvalues ---	0.55255	0.55337	0.55659	0.55686	0.84423
Eigenvalues ---	0.93722	0.95028	0.95195	0.97266	0.97717
Eigenvalues ---	1.05325	1.37278			

RFO step: Lambda=-2.20829473D-04 EMin= 2.24462698D-03
Quartic linear search produced a step of 0.99234.
Iteration 1 RMS(Cart)= 0.05113215 RMS(Int)= 0.00276144
Iteration 2 RMS(Cart)= 0.00288093 RMS(Int)= 0.00001143
Iteration 3 RMS(Cart)= 0.00000733 RMS(Int)= 0.00001006
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001006
ITry= 1 IFail=0 DXMaxC= 1.90D-01 DCOld= 1.00D+10 DXMaxT= 7.14D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.32124	0.00122	-0.00124	0.00029	-0.00096	2.32028
R2	2.53669	-0.00077	0.00225	0.00001	0.00226	2.53895
R3	2.53414	-0.00073	0.00167	-0.00023	0.00144	2.53558
R4	2.32120	0.00121	-0.00126	0.00030	-0.00096	2.32024
R5	2.31799	0.00098	-0.00101	0.00032	-0.00069	2.31730
R6	2.53427	-0.00072	0.00169	-0.00021	0.00148	2.53575
R7	2.53578	-0.00059	0.00102	-0.00031	0.00071	2.53649
R8	2.31787	0.00096	-0.00103	0.00034	-0.00069	2.31718
R9	2.31840	-0.00030	-0.00058	-0.00010	-0.00068	2.31773
R10	2.53601	-0.00059	0.00103	-0.00030	0.00073	2.53674
R11	2.62856	-0.00034	0.00109	0.00014	0.00122	2.62979
R12	2.31816	-0.00037	-0.00064	-0.00004	-0.00068	2.31748
R13	2.68498	0.00110	-0.00379	0.00122	-0.00257	2.68242
R14	2.70000	-0.00155	0.00168	-0.00077	0.00092	2.70091
R15	2.62926	-0.00038	0.00125	0.00002	0.00128	2.63054
R16	2.69907	-0.00252	0.00162	-0.00073	0.00089	2.69996
R17	2.82198	-0.00134	0.00435	-0.00153	0.00281	2.82479
R18	2.05353	-0.00019	0.00047	-0.00049	-0.00001	2.05352
R19	2.82148	-0.00199	0.00424	-0.00158	0.00266	2.82414
R20	2.05301	-0.00010	0.00046	-0.00034	0.00012	2.05314
R21	1.95009	-0.00126	-0.00030	-0.00123	-0.00153	1.94856

R22	1.91930	-0.00096	-0.00004	-0.00059	-0.00063	1.91867
R23	1.92803	-0.00072	0.00105	0.00003	0.00108	1.92911
R24	1.95002	-0.00121	-0.00029	-0.00122	-0.00151	1.94851
R25	1.91940	-0.00108	-0.00003	-0.00062	-0.00065	1.91875
R26	1.92808	-0.00069	0.00106	0.00002	0.00108	1.92916
A1	2.56028	-0.00003	-0.00210	-0.00124	-0.00334	2.55694
A2	2.61005	0.00031	0.00273	0.00223	0.00495	2.61500
A3	2.56151	-0.00004	-0.00182	-0.00105	-0.00287	2.55864
A4	2.72037	-0.00046	-0.00403	-0.00336	-0.00739	2.71297
A5	2.60898	0.00028	0.00244	0.00216	0.00460	2.61357
A6	2.84120	0.00016	0.00553	0.00316	0.00870	2.84989
A7	2.72119	-0.00050	-0.00388	-0.00317	-0.00704	2.71415
A8	2.84070	0.00013	0.00537	0.00320	0.00857	2.84927
A9	2.09003	-0.00028	-0.00029	-0.00112	-0.00142	2.08862
A10	2.10219	0.00023	-0.00097	0.00082	-0.00017	2.10203
A11	2.09041	0.00006	0.00098	0.00055	0.00152	2.09193
A12	2.08938	0.00024	-0.00054	-0.00081	-0.00137	2.08801
A13	2.09083	0.00000	0.00097	0.00049	0.00144	2.09227
A14	2.10237	-0.00023	-0.00074	0.00072	-0.00005	2.10232
A15	2.04155	0.00053	-0.00313	0.00271	-0.00042	2.04113
A16	1.90555	0.00227	-0.00890	0.00466	-0.00424	1.90131
A17	2.04159	0.00142	-0.00360	0.00357	-0.00004	2.04156
A18	1.90460	0.00314	-0.00942	0.00526	-0.00417	1.90043
A19	2.00917	0.00007	0.00349	0.00106	0.00454	2.01371
A20	1.92092	-0.00103	0.00222	-0.00077	0.00144	1.92236
A21	1.91189	-0.00068	-0.00453	-0.00425	-0.00878	1.90311
A22	1.89757	0.00042	-0.00023	0.00038	0.00013	1.89770
A23	1.84040	0.00065	-0.00233	0.00150	-0.00083	1.83957
A24	1.87835	0.00070	0.00111	0.00231	0.00342	1.88177
A25	2.00868	0.00024	0.00337	0.00132	0.00469	2.01337
A26	1.92129	-0.00130	0.00222	-0.00107	0.00114	1.92243
A27	1.91219	-0.00065	-0.00438	-0.00412	-0.00850	1.90370
A28	1.89753	0.00043	-0.00013	0.00035	0.00020	1.89773
A29	1.84035	0.00066	-0.00238	0.00153	-0.00084	1.83951
A30	1.87824	0.00076	0.00102	0.00220	0.00322	1.88145
A31	2.90509	0.00003	-0.00189	-0.00094	-0.00283	2.90226
A32	3.12258	0.00008	0.00001	0.00128	0.00129	3.12387
A33	2.90613	-0.00006	-0.00190	-0.00076	-0.00265	2.90348
A34	3.12140	0.00014	0.00037	0.00043	0.00080	3.12219
A35	3.94710	0.00280	-0.01202	0.00736	-0.00466	3.94244
A36	3.94619	0.00456	-0.01303	0.00882	-0.00420	3.94199
A37	3.14707	-0.00036	-0.00050	-0.00168	-0.00217	3.14491
A38	3.14414	-0.00047	-0.00016	0.00154	0.00137	3.14551
A39	3.14707	-0.00034	-0.00032	-0.00159	-0.00188	3.14520
A40	3.14619	-0.00064	0.00181	-0.00640	-0.00460	3.14158
A41	4.04763	0.00069	0.01346	-0.01215	0.00131	4.04894
A42	4.03117	0.00355	0.01143	-0.00387	0.00757	4.03873
D1	0.02551	-0.00025	0.00052	-0.00141	-0.00089	0.02463

D2	-0.02094	-0.00021	-0.00067	0.00056	-0.00011	-0.02105
D3	-0.01559	-0.00006	-0.00029	0.00101	0.00071	-0.01488
D4	0.02562	-0.00028	0.00062	-0.00193	-0.00131	0.02431
D5	0.00708	-0.00001	-0.00085	-0.00038	-0.00125	0.00583
D6	-0.01537	-0.00010	-0.00007	-0.00022	-0.00030	-0.01567
D7	-0.00555	0.00011	0.00114	-0.00276	-0.00164	-0.00718
D8	3.10115	-0.00003	-0.01004	0.00640	-0.00366	3.09749
D9	0.00751	-0.00006	-0.00063	-0.00105	-0.00170	0.00581
D10	-0.00431	0.00007	0.00274	-0.00778	-0.00508	-0.00939
D11	3.10240	-0.00005	-0.00822	-0.00069	-0.00893	3.09347
D12	0.00460	0.00020	-0.00271	0.00804	0.00530	0.00989
D13	-3.10005	-0.00020	0.00888	-0.00415	0.00471	-3.09534
D14	-3.10153	-0.00008	0.00757	-0.00027	0.00728	-3.09425
D15	0.07701	-0.00048	0.01916	-0.01246	0.00669	0.08370
D16	2.49231	-0.00053	-0.00091	0.00402	0.00312	2.49542
D17	-0.68500	-0.00025	-0.01125	0.01235	0.00109	-0.68391
D18	-0.68384	0.00002	-0.01408	0.01772	0.00363	-0.68021
D19	2.49498	-0.00040	-0.00240	0.00547	0.00307	2.49805
D20	-1.34774	0.00072	0.07352	0.03166	0.10517	-1.24258
D21	0.80373	0.00051	0.07755	0.03234	0.10990	0.91363
D22	2.86564	0.00034	0.07750	0.03213	0.10964	2.97527
D23	-1.35162	0.00079	0.07400	0.03244	0.10642	-1.24520
D24	0.79975	0.00050	0.07808	0.03303	0.11112	0.91087
D25	2.86192	0.00026	0.07801	0.03258	0.11060	2.97252

Item	Value	Threshold	Converged?
Maximum Force	0.004559	0.000450	NO
RMS Force	0.001033	0.000300	NO
Maximum Displacement	0.190245	0.001800	NO
RMS Displacement	0.051402	0.001200	NO

Predicted change in Energy=-1.532348D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 04:44:16 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.023060	0.673380	0.049074
2	6	0	3.345331	1.694847	0.118948
3	6	0	4.023196	-0.666409	-0.051477
4	6	0	2.142771	2.287961	0.168069
5	6	0	3.347437	-1.689192	-0.120736
6	6	0	0.917103	2.325411	0.175723
7	6	0	2.145073	-2.283021	-0.168441

8	6	0	-0.379749	1.979760	0.157264
9	6	0	0.919529	-2.322628	-0.174236
10	6	0	-1.456027	1.393086	0.115906
11	6	0	-0.377818	-1.978450	-0.153392
12	6	0	-2.665206	0.706350	0.062082
13	6	0	-1.455305	-1.394433	-0.109782
14	6	0	-2.665220	-0.707991	-0.058523
15	6	0	-3.903675	1.411012	0.173595
16	6	0	-3.902972	-1.412694	-0.171257
17	7	0	-3.730829	2.878737	-0.050866
18	7	0	-3.740633	-2.882019	0.048233
19	1	0	-3.348656	3.143026	-0.971371
20	1	0	-4.614499	3.359760	0.085574
21	1	0	-3.363918	-3.151949	0.969319
22	1	0	-4.626884	-3.356815	-0.093465
23	1	0	-3.067250	3.244401	0.633288
24	1	0	-4.729201	1.055650	-0.437216
25	1	0	-4.730329	-1.055720	0.435763
26	1	0	-3.076818	-3.249982	-0.634503

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.227841	0.000000			
3	C	1.343557	2.462534	0.000000		
4	C	2.481234	1.341771	3.508918	0.000000	
5	C	2.463138	3.392517	1.227816	4.165619	0.000000
6	C	3.520258	2.509407	4.318613	1.226263	4.702281
7	C	3.509196	4.164930	2.480819	4.583353	1.341860
8	C	4.593807	3.736157	5.141178	2.541301	5.237405
9	C	4.319472	4.702188	3.520068	4.782366	2.509749
10	C	5.526558	4.810832	5.855888	3.708756	5.712242
11	C	5.142074	5.237281	4.593557	4.965780	3.736612
12	C	6.688360	6.091544	6.828769	5.062545	6.474869
13	C	5.857779	5.713324	5.526970	5.155907	4.811792
14	C	6.830290	6.475480	6.688549	5.669554	6.092510
15	C	7.961956	7.254766	8.197660	6.109711	7.891548
16	C	8.198917	7.891700	7.962125	7.096548	7.255855
17	N	8.062033	7.176522	8.526017	5.907294	8.424531
18	N	8.539075	8.435851	8.074399	7.833103	7.189724
19	H	7.841087	6.935090	8.348784	5.673202	8.301299
20	H	9.045739	8.132155	9.530928	6.842240	9.430107
21	H	8.369435	8.320371	7.860623	7.781918	6.954866
22	H	9.543810	9.440371	9.058914	8.818170	8.146871
23	H	7.564652	6.617164	8.126363	5.317473	8.127553
24	H	8.774091	8.118864	8.928535	7.007778	8.536182
25	H	8.930909	8.537111	8.775715	7.647964	8.121655
26	H	8.140536	8.140210	7.577927	7.652258	6.631070

Supporting Information file

		6	7	8	9	10
6	C	0.000000				
7	C	4.781632	0.000000			
8	C	1.342252	4.965090	0.000000		
9	C	4.661195	1.226198	4.506502	0.000000	
10	C	2.550403	5.153886	1.226487	4.419727	0.000000
11	C	4.506479	2.541254	3.970382	1.342387	3.549973
12	C	3.932837	5.668180	2.618004	4.699030	1.391624
13	C	4.421207	3.708875	3.551523	2.550596	2.796640
14	C	4.699940	5.062779	3.534677	3.933303	2.430452
15	C	4.906733	7.095790	3.569565	6.109366	2.448393
16	C	6.109579	6.110346	4.902017	4.907597	3.733953
17	N	4.686234	7.822008	3.475804	6.978198	2.722075
18	N	6.987710	5.920075	5.911373	4.698885	4.847734
19	H	4.492329	7.763230	3.382515	6.980415	2.797589
20	H	5.628199	8.808934	4.454508	7.936151	3.720842
21	H	6.997028	5.691969	5.991588	4.510367	5.002570
22	H	7.943295	6.856971	6.824958	5.642585	5.714869
23	H	4.114484	7.639600	3.008085	6.894804	2.508205
24	H	5.819685	7.646869	4.486102	6.587114	3.336686
25	H	6.587348	7.010170	5.312178	5.822203	4.101220
26	H	6.906003	5.331077	5.937279	4.128272	4.974752

		11	12	13	14	15
11	C	0.000000				
12	C	3.533655	0.000000			
13	C	1.226359	2.430367	0.000000		
14	C	2.618258	1.419473	1.392022	0.000000	
15	C	4.901738	1.429262	3.734346	2.465324	0.000000
16	C	3.570309	2.465129	2.448507	1.428757	2.844687
17	N	5.903004	2.422308	4.841638	3.741684	1.494816
18	N	3.487924	3.746082	2.731411	2.427820	4.297955
19	H	5.976996	2.733591	4.991557	4.016304	2.149154
20	H	6.819314	3.292549	5.711481	4.512986	2.076207
21	H	3.399172	4.024643	2.810004	2.741819	4.663168
22	H	4.467442	4.514608	3.729627	3.296303	4.829754
23	H	5.927064	2.632417	4.966820	4.032571	2.066940
24	H	5.312329	2.152065	4.102257	2.741140	1.086676
25	H	4.488082	2.740303	3.337383	2.151722	2.614738
26	H	3.022063	4.038220	2.519464	2.638729	4.802248

		16	17	18	19	20
16	C	0.000000				
17	N	4.296570	0.000000			
18	N	1.494472	5.761617	0.000000		
19	H	4.658544	1.031132	6.123268	0.000000	
20	H	4.832034	1.015318	6.302765	1.663270	0.000000
21	H	2.148604	6.127363	1.031105	6.587353	6.689343
22	H	2.075982	6.299749	1.015357	6.682253	6.718972
23	H	4.799403	1.020840	6.191023	1.632298	1.645381

```
  24  H    2.616507   2.114157   4.088785   2.558978   2.365458
  25  H    1.086473   4.088491   2.113066   4.638805   4.430859
  26  H    2.067064   6.191088   1.020870   6.407646   6.824343
                21         22         23         24         25
  21  H    0.000000
  22  H    1.663299   0.000000
  23  H    6.412038   6.821780   0.000000
  24  H    4.641791   4.427016   2.949355   0.000000
  25  H    2.558503   2.363434   4.614747   2.284726   0.000000
  26  H    1.632263   1.645247   6.616979   4.616032   2.948619
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=3 Diff= 6.98D-04
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.528382   -0.667556   -0.023707
    2          6           0        3.852145   -1.691937   -0.054355
    3          6           0        4.526562    0.675097    0.025541
    4          6           0        2.650451   -2.288255   -0.080553
    5          6           0        3.849311    1.698791    0.055759
    6          6           0        1.424839   -2.327763   -0.086557
    7          6           0        2.646082    2.292250    0.080930
    8          6           0        0.127482   -1.983556   -0.081105
    9          6           0        1.420481    2.330257    0.085419
   10          6           0       -0.949651   -1.397305   -0.062023
   11          6           0        0.123638    1.983636    0.077975
   12          6           0       -2.159830   -0.710782   -0.034288
   13          6           0       -0.952995    1.396803    0.056914
   14          6           0       -2.161907    0.707134    0.032150
   15          6           0       -3.397276   -1.421004   -0.118561
   16          6           0       -3.400679    1.413822    0.118070
   17          7           0       -3.222249   -2.878818    0.161827
   18          7           0       -3.240523    2.873916   -0.157470
   19          1           0       -2.839581   -3.107157    1.091698
   20          1           0       -4.105228   -3.365998    0.044032
   21          1           0       -2.864312    3.108979   -1.088269
   22          1           0       -4.127454    3.352485   -0.033877
   23          1           0       -2.558214   -3.269404   -0.507960
   24          1           0       -4.223252   -1.043753    0.478358
```

```
    25        1        0      -4.227582    1.032688   -0.474714
    26        1        0      -2.577170    3.268686    0.510582
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6015164           0.2702208           0.1871604
 Leave Link  202 at Sat Sep 26 04:44:16 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1009.1800686368 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0154319003 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1009.1646367366 Hartrees.
 Leave Link  301 at Sat Sep 26 04:44:16 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23229 LenP2D=   51907.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.87D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=           5 IRanWt=          -1 IRanGd=           0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=           0 NUsed=           0 NTot=          32
 NSgBfM=   683   683   683   683   683 MxSgAt=    26 MxSgA2=    26.
 Leave Link  302 at Sat Sep 26 04:44:17 2026, MaxMem=    805306368 cpu:                  5.8 elap:
1.0
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
```

Supporting Information file

```
 Leave Link  303 at Sat Sep 26 04:44:17 2026, MaxMem=    805306368 cpu:                  0.7 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=    -0.000000   -0.000000    0.000000
       Rot=    1.000000   -0.000100    0.000002    0.000217 Ang=  -0.03 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Generating alternative initial guess.
 ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn=          5 AccDes=
0.00D+00
 Harris functional with IExCor= 4639 and IRadAn=       5 diagonalized for initial guess.
 HarFok:  IExCor= 4639 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Petite list used in FoFCou.
 Harris En= -691.983410796122
 Leave Link  401 at Sat Sep 26 04:44:25 2026, MaxMem=    805306368 cpu:                 47.9 elap:
8.0
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.407698241592
 DIIS: error= 3.49D-03 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -723.407698241592     IErMin= 1 ErrMin= 3.49D-03
 ErrMax= 3.49D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.61D-03 BMatP= 4.61D-03
 IDIUse=3 WtCom= 9.65D-01 WtEn= 3.49D-02
 Coeff-Com:  0.100D+01
```

Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.707 Goal= None Shift= 0.000
GapD= 0.707 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=8.60D-03 MaxDP=3.38D-01 OVMax= 1.83D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 7.28D-03 CP: 1.45D+00
E= -723.413376399919 Delta-E= -0.005678158327 Rises=F Damp=F
DIIS: error= 7.56D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413376399919 IErMin= 2 ErrMin= 7.56D-04
ErrMax= 7.56D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-04 BMatP= 4.61D-03
IDIUse=3 WtCom= 9.92D-01 WtEn= 7.56D-03
Coeff-Com: -0.922D-01 0.109D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.915D-01 0.109D+01
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=9.60D-03 MaxDP=3.38D-01 DE=-5.68D-03 OVMax= 4.98D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 4.29D-03 CP: 8.88D-01 1.21D-01
E= -723.413629447666 Delta-E= -0.000253047747 Rises=F Damp=F
DIIS: error= 3.99D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.413629447666 IErMin= 2 ErrMin= 7.56D-04
ErrMax= 3.99D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.03D-04 BMatP= 2.42D-04
IDIUse=3 WtCom= 1.37D-01 WtEn= 8.63D-01
Coeff-Com: -0.946D-01 0.752D+00 0.342D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.129D-01 0.103D+00 0.910D+00
Gap= 0.182 Goal= None Shift= 0.000
RMSDP=7.67D+02 MaxDP=3.11D+04 DE=-2.53D-04 OVMax= 9.59D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.413459759264 Delta-E= 0.000169688402 Rises=F Damp=F
DIIS: error= 8.71D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413459759264 IErMin= 1 ErrMin= 8.71D-04
ErrMax= 8.71D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-04 BMatP= 2.08D-04
IDIUse=3 WtCom= 9.91D-01 WtEn= 8.71D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.182 Goal= None Shift= 0.000
RMSDP=4.27D-03 MaxDP=1.12D-01 DE= 1.70D-04 OVMax= 3.14D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.16D-03 CP: 9.06D-01

E= -723.413588194231 Delta-E= -0.000128434968 Rises=F Damp=F
DIIS: error= 2.30D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413588194231 IErMin= 2 ErrMin= 2.30D-04
ErrMax= 2.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.67D-05 BMatP= 2.08D-04
IDIUse=3 WtCom= 9.98D-01 WtEn= 2.30D-03
Coeff-Com: 0.832D-01 0.917D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.830D-01 0.917D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.92D-04 MaxDP=2.18D-02 DE=-1.28D-04 OVMax= 2.55D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.20D-04 CP: 9.21D-01 1.08D+00
E= -723.413566654661 Delta-E= 0.000021539571 Rises=F Damp=F
DIIS: error= 3.34D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413588194231 IErMin= 2 ErrMin= 2.30D-04
ErrMax= 3.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.67D-05 BMatP= 1.67D-05
IDIUse=3 WtCom= 3.54D-01 WtEn= 6.46D-01
Coeff-Com: -0.207D-01 0.609D+00 0.412D+00
Coeff-En: 0.000D+00 0.652D+00 0.348D+00
Coeff: -0.733D-02 0.637D+00 0.371D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=8.13D-05 MaxDP=3.83D-03 DE= 2.15D-05 OVMax= 1.81D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.07D-05 CP: 9.24D-01 1.09D+00 1.17D+00
E= -723.413607999010 Delta-E= -0.000041344350 Rises=F Damp=F
DIIS: error= 2.53D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413607999010 IErMin= 4 ErrMin= 2.53D-05
ErrMax= 2.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-07 BMatP= 1.67D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.108D-01 0.231D+00 0.109D+00 0.671D+00
Coeff: -0.108D-01 0.231D+00 0.109D+00 0.671D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=5.01D-05 MaxDP=2.49D-03 DE=-4.13D-05 OVMax= 2.66D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 8.72D-06 CP: 9.26D-01 1.10D+00 1.28D+00 1.34D+00
E= -723.413608530105 Delta-E= -0.000000531094 Rises=F Damp=F
DIIS: error= 1.20D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413608530105 IErMin= 5 ErrMin= 1.20D-05
ErrMax= 1.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.06D-08 BMatP= 3.98D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.355D-02-0.122D+00-0.932D-01 0.151D+00 0.106D+01
Coeff: 0.355D-02-0.122D+00-0.932D-01 0.151D+00 0.106D+01
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.48D-05 MaxDP=2.24D-03 DE=-5.31D-07 OVMax= 4.19D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 2.90D-06 CP: 9.28D-01 1.11D+00 1.37D+00 1.69D+00 2.12D+00
E= -723.413608718160 Delta-E= -0.000000188055 Rises=F Damp=F
DIIS: error= 7.46D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413608718160 IErMin= 6 ErrMin= 7.46D-06
ErrMax= 7.46D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.18D-09 BMatP= 4.06D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.251D-02-0.732D-01-0.493D-01 0.175D-02 0.450D+00 0.668D+00
Coeff: 0.251D-02-0.732D-01-0.493D-01 0.175D-02 0.450D+00 0.668D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=5.30D-06 MaxDP=2.79D-04 DE=-1.88D-07 OVMax= 1.22D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 8.43D-07 CP: 9.28D-01 1.11D+00 1.39D+00 1.75D+00 2.36D+00
CP: 1.14D+00
E= -723.413608750662 Delta-E= -0.000000032502 Rises=F Damp=F
DIIS: error= 5.22D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413608750662 IErMin= 7 ErrMin= 5.22D-06
ErrMax= 5.22D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.68D-09 BMatP= 9.18D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.155D-03 0.115D-01 0.121D-01-0.561D-01-0.182D+00 0.274D+00
Coeff-Com: 0.940D+00
Coeff: -0.155D-03 0.115D-01 0.121D-01-0.561D-01-0.182D+00 0.274D+00
Coeff: 0.940D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=2.08D-06 MaxDP=7.68D-05 DE=-3.25D-08 OVMax= 1.39D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 4.12D-07 CP: 9.28D-01 1.11D+00 1.39D+00 1.78D+00 2.50D+00
CP: 1.32D+00 2.11D+00
E= -723.413608769783 Delta-E= -0.000000019121 Rises=F Damp=F
DIIS: error= 2.85D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413608769783 IErMin= 8 ErrMin= 2.85D-06
ErrMax= 2.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.76D-10 BMatP= 2.68D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.834D-03 0.275D-01 0.204D-01-0.250D-01-0.216D+00-0.108D+00
Coeff-Com: 0.461D+00 0.842D+00
Coeff: -0.834D-03 0.275D-01 0.204D-01-0.250D-01-0.216D+00-0.108D+00
Coeff: 0.461D+00 0.842D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=7.24D-07 MaxDP=2.26D-05 DE=-1.91D-08 OVMax= 9.27D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 2.19D-07 CP: 9.28D-01 1.11D+00 1.39D+00 1.79D+00 2.54D+00
CP: 1.38D+00 2.65D+00 1.53D+00
E= -723.413608775970 Delta-E= -0.000000006188 Rises=F Damp=F
DIIS: error= 1.58D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413608775970 IErMin= 9 ErrMin= 1.58D-06

ErrMax= 1.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D-10 BMatP= 9.76D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.306D-03 0.845D-02 0.544D-02 0.394D-02-0.415D-01-0.127D+00
Coeff-Com: -0.324D-01 0.334D+00 0.849D+00
Coeff: -0.306D-03 0.845D-02 0.544D-02 0.394D-02-0.415D-01-0.127D+00
Coeff: -0.324D-01 0.334D+00 0.849D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=3.21D-07 MaxDP=9.53D-06 DE=-6.19D-09 OVMax= 4.05D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.27D-07   CP: 9.28D-01 1.11D+00 1.39D+00 1.79D+00 2.53D+00
               CP: 1.36D+00 2.75D+00 1.74D+00 1.72D+00
E= -723.413608777392   Delta-E=   -0.000000001422 Rises=F Damp=F
DIIS: error= 6.26D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413608777392   IErMin=10 ErrMin= 6.26D-07
ErrMax= 6.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.91D-11 BMatP= 2.20D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.154D-03-0.581D-02-0.470D-02 0.105D-01 0.577D-01-0.250D-01
Coeff-Com: -0.172D+00-0.141D+00 0.388D+00 0.892D+00
Coeff: 0.154D-03-0.581D-02-0.470D-02 0.105D-01 0.577D-01-0.250D-01
Coeff: -0.172D+00-0.141D+00 0.388D+00 0.892D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=3.18D-07 MaxDP=1.22D-05 DE=-1.42D-09 OVMax= 2.52D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 7.14D-08   CP: 9.28D-01 1.11D+00 1.39D+00 1.79D+00 2.52D+00
               CP: 1.34D+00 2.70D+00 1.85D+00 2.20D+00 1.92D+00
E= -723.413608777766   Delta-E=   -0.000000000374 Rises=F Damp=F
DIIS: error= 3.54D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413608777766   IErMin=11 ErrMin= 3.54D-07
ErrMax= 3.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-11 BMatP= 5.91D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.115D-03-0.392D-02-0.299D-02 0.459D-02 0.336D-01 0.459D-02
Coeff-Com: -0.773D-01-0.113D+00 0.722D-01 0.452D+00 0.630D+00
Coeff: 0.115D-03-0.392D-02-0.299D-02 0.459D-02 0.336D-01 0.459D-02
Coeff: -0.773D-01-0.113D+00 0.722D-01 0.452D+00 0.630D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=7.66D-08 MaxDP=3.23D-06 DE=-3.74D-10 OVMax= 4.71D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 2.47D-08   CP: 9.28D-01 1.11D+00 1.39D+00 1.79D+00 2.52D+00
               CP: 1.34D+00 2.67D+00 1.87D+00 2.27D+00 2.21D+00
               CP: 1.33D+00
E= -723.413608777793   Delta-E=   -0.000000000027 Rises=F Damp=F
DIIS: error= 7.85D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413608777793   IErMin=12 ErrMin= 7.85D-08
ErrMax= 7.85D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-12 BMatP= 1.40D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.589D-05-0.424D-04 0.603D-04-0.111D-02-0.207D-02 0.942D-02
Coeff-Com: 0.157D-01-0.994D-02-0.881D-01-0.637D-01 0.280D+00 0.860D+00
Coeff: 0.589D-05-0.424D-04 0.603D-04-0.111D-02-0.207D-02 0.942D-02
Coeff: 0.157D-01-0.994D-02-0.881D-01-0.637D-01 0.280D+00 0.860D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=7.38D-08 MaxDP=4.17D-06 DE=-2.66D-11 OVMax= 2.89D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 1.11D-08   CP: 9.28D-01 1.11D+00 1.39D+00 1.79D+00 2.52D+00
               CP: 1.34D+00 2.64D+00 1.88D+00 2.30D+00 2.38D+00
               CP: 1.62D+00 1.83D+00
E= -723.413608777806   Delta-E=   -0.000000000013 Rises=F Damp=F
DIIS: error= 5.04D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.413608777806   IErMin=13 ErrMin= 5.04D-08
ErrMax= 5.04D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.19D-13 BMatP= 2.41D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.108D-04 0.444D-03 0.386D-03-0.109D-02-0.494D-02 0.428D-02
Coeff-Com: 0.167D-01 0.847D-02-0.509D-01-0.857D-01 0.581D-01 0.421D+00
Coeff-Com: 0.634D+00
Coeff: -0.108D-04 0.444D-03 0.386D-03-0.109D-02-0.494D-02 0.428D-02
Coeff: 0.167D-01 0.847D-02-0.509D-01-0.857D-01 0.581D-01 0.421D+00
Coeff: 0.634D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=3.05D-08 MaxDP=1.86D-06 DE=-1.30D-11 OVMax= 5.96D-07

Cycle 17 Pass 1 IDiag 1:
RMSU= 3.38D-09   CP: 9.28D-01 1.11D+00 1.39D+00 1.79D+00 2.52D+00
               CP: 1.34D+00 2.63D+00 1.89D+00 2.30D+00 2.41D+00
               CP: 1.71D+00 2.06D+00 1.28D+00
E= -723.413608777803   Delta-E=   0.000000000003 Rises=F Damp=F
DIIS: error= 1.75D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.413608777806   IErMin=14 ErrMin= 1.75D-08
ErrMax= 1.75D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.52D-14 BMatP= 4.19D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.459D-05 0.156D-03 0.120D-03-0.188D-03-0.133D-02 0.412D-04
Coeff-Com: 0.297D-02 0.462D-02-0.181D-02-0.192D-01-0.294D-01 0.879D-02
Coeff-Com: 0.221D+00 0.815D+00
Coeff: -0.459D-05 0.156D-03 0.120D-03-0.188D-03-0.133D-02 0.412D-04
Coeff: 0.297D-02 0.462D-02-0.181D-02-0.192D-01-0.294D-01 0.879D-02
Coeff: 0.221D+00 0.815D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=1.57D-08 MaxDP=1.00D-06 DE= 2.50D-12 OVMax= 2.94D-07

Cycle 18 Pass 1 IDiag 1:
RMSU= 2.38D-09   CP: 9.28D-01 1.11D+00 1.39D+00 1.79D+00 2.52D+00
               CP: 1.34D+00 2.63D+00 1.89D+00 2.29D+00 2.41D+00
               CP: 1.73D+00 2.20D+00 1.42D+00 1.64D+00
E= -723.413608777802   Delta-E=   0.000000000001 Rises=F Damp=F

Supporting Information file

DIIS: error= 9.28D-09 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=13 EnMin= -723.413608777806 IErMin=15 ErrMin= 9.28D-09
ErrMax= 9.28D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-14 BMatP= 5.52D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.235D-05-0.105D-03-0.936D-04 0.305D-03 0.124D-02-0.129D-02
Coeff-Com: -0.489D-02-0.168D-02 0.162D-01 0.221D-01-0.291D-01-0.126D+00
Coeff-Com: -0.146D+00 0.197D+00 0.107D+01
Coeff: 0.235D-05-0.105D-03-0.936D-04 0.305D-03 0.124D-02-0.129D-02
Coeff: -0.489D-02-0.168D-02 0.162D-01 0.221D-01-0.291D-01-0.126D+00
Coeff: -0.146D+00 0.197D+00 0.107D+01
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=5.90D-09 MaxDP=4.50D-07 DE= 1.36D-12 OVMax= 2.79D-07

SCF Done: E(RwB97XD) = -723.413608778 A.U. after 18 cycles
NFock= 18 Conv=0.59D-08 -V/T= 2.0047
KE= 7.200289176953D+02 PE=-3.699395564530D+03 EE= 1.246788401320D+03
Leave Link 502 at Sat Sep 26 05:05:09 2026, MaxMem= 805306368 cpu: 7463.3 elap: 1244.1
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23229 LenP2D= 51907.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 05:05:10 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 05:05:10 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 05:17:33 2026, MaxMem= 805306368 cpu: 4458.2 elap: 743.2
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.46347944D+00 8.57465773D-03 9.24584684D-03
***** Axes restored to original set *****

Supporting Information file

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000693786	-0.002047077	-0.000467570
2	6	-0.001488675	0.001338315	0.000386545
3	6	0.000692588	0.002044853	0.000461312
4	6	0.001841003	-0.000369869	-0.000248079
5	6	-0.001498009	-0.001336011	-0.000393902
6	6	-0.001633761	0.000100424	0.000267589
7	6	0.001855646	0.000368667	0.000256626
8	6	0.000533546	-0.000009034	-0.000019612
9	6	-0.001666610	-0.000075355	-0.000220446
10	6	-0.000256112	-0.000388713	-0.000527773
11	6	0.000519257	-0.000070740	0.000074150
12	6	-0.000252487	0.003969362	0.001231986
13	6	-0.000407739	0.000310568	0.000269282
14	6	0.000107767	-0.004803435	-0.000988341
15	6	-0.001769218	0.001156923	-0.002202802
16	6	-0.002470753	-0.000706599	0.002102230
17	7	0.002923477	0.000207101	0.000220615
18	7	0.003809283	0.000141474	-0.000193844
19	1	-0.000854805	-0.000545999	0.000696490
20	1	0.000365623	-0.000998325	0.000080995
21	1	-0.000863648	0.000502502	-0.000654062
22	1	0.000389460	0.001099613	-0.000061855
23	1	-0.000398373	-0.000847861	-0.000108470
24	1	0.000151895	-0.001075433	0.000616986
25	1	0.000058696	0.001165009	-0.000667547
26	1	-0.000381837	0.000869640	0.000089496

Cartesian Forces: Max 0.004803435 RMS 0.001280393
Leave Link 716 at Sat Sep 26 05:17:33 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.004222643 RMS 0.001034759
Search for a local minimum.
Step number 19 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .10348D-02 SwitMx=.10000D-02 MixMth= 1
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 16 17 18 19
DE= -2.19D-04 DEPred=-1.53D-04 R= 1.43D+00

Supporting Information file

TightC=F SS= 1.41D+00 RLast= 2.69D-01 DXNew= 1.2000D+00 8.0583D-01
Trust test= 1.43D+00 RLast= 2.69D-01 DXMaxT set to 8.06D-01
ITU= 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 0 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00223	0.00445	0.01096	0.01416	0.01687
Eigenvalues ---	0.01764	0.02451	0.02673	0.02799	0.02910
Eigenvalues ---	0.03107	0.03331	0.03642	0.03790	0.04359
Eigenvalues ---	0.04439	0.04468	0.05026	0.06272	0.07158
Eigenvalues ---	0.09963	0.10316	0.11010	0.11204	0.11506
Eigenvalues ---	0.11737	0.13801	0.15233	0.15527	0.15879
Eigenvalues ---	0.16000	0.16001	0.16010	0.16118	0.17607
Eigenvalues ---	0.22345	0.23096	0.24136	0.24990	0.24995
Eigenvalues ---	0.24999	0.25000	0.25000	0.25014	0.29202
Eigenvalues ---	0.29703	0.36036	0.37236	0.38371	0.45256
Eigenvalues ---	0.45800	0.46304	0.47568	0.47614	0.47688
Eigenvalues ---	0.47688	0.47953	0.48324	0.50985	0.54805
Eigenvalues ---	0.55320	0.55463	0.55659	0.55742	0.83020
Eigenvalues ---	0.93713	0.95029	0.95163	0.97703	0.98006
Eigenvalues ---	1.02912	1.37146			

RFO step: Lambda=-1.48966066D-04 EMin= 2.23198665D-03
Quartic linear search produced a step of 0.55717.
Iteration 1 RMS(Cart)= 0.03299741 RMS(Int)= 0.00112423
Iteration 2 RMS(Cart)= 0.00116828 RMS(Int)= 0.00000794
Iteration 3 RMS(Cart)= 0.00000114 RMS(Int)= 0.00000789
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000789
ITry= 1 IFail=0 DXMaxC= 1.30D-01 DCOld= 1.00D+10 DXMaxT= 8.06D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.32028	0.00129	-0.00053	0.00084	0.00031	2.32060
R2	2.53895	-0.00099	0.00126	-0.00114	0.00012	2.53908
R3	2.53558	-0.00083	0.00080	-0.00111	-0.00031	2.53527
R4	2.32024	0.00128	-0.00053	0.00083	0.00030	2.32054
R5	2.31730	0.00105	-0.00039	0.00082	0.00043	2.31773
R6	2.53575	-0.00085	0.00082	-0.00116	-0.00034	2.53541
R7	2.53649	-0.00056	0.00040	-0.00092	-0.00052	2.53597
R8	2.31718	0.00105	-0.00039	0.00081	0.00042	2.31760
R9	2.31773	-0.00005	-0.00038	0.00047	0.00009	2.31782
R10	2.53674	-0.00060	0.00041	-0.00101	-0.00061	2.53614
R11	2.62979	-0.00048	0.00068	-0.00082	-0.00014	2.62965
R12	2.31748	-0.00007	-0.00038	0.00046	0.00008	2.31756
R13	2.68242	0.00147	-0.00143	0.00252	0.00109	2.68351
R14	2.70091	-0.00145	0.00051	-0.00246	-0.00195	2.69896
R15	2.63054	-0.00058	0.00071	-0.00098	-0.00027	2.63027
R16	2.69996	-0.00203	0.00050	-0.00269	-0.00220	2.69776
R17	2.82479	-0.00204	0.00157	-0.00233	-0.00077	2.82403
R18	2.05352	-0.00011	-0.00001	-0.00102	-0.00103	2.05249
R19	2.82414	-0.00237	0.00148	-0.00234	-0.00085	2.82329

R20	2.05314	-0.00003	0.00007	-0.00097	-0.00090	2.05223
R21	1.94856	-0.00108	-0.00085	-0.00121	-0.00206	1.94649
R22	1.91867	-0.00078	-0.00035	-0.00043	-0.00078	1.91789
R23	1.92911	-0.00064	0.00060	-0.00003	0.00057	1.92968
R24	1.94851	-0.00103	-0.00084	-0.00116	-0.00201	1.94650
R25	1.91875	-0.00085	-0.00036	-0.00043	-0.00079	1.91795
R26	1.92916	-0.00062	0.00060	-0.00004	0.00057	1.92973
A1	2.55694	0.00016	-0.00186	-0.00012	-0.00198	2.55496
A2	2.61500	0.00012	0.00276	0.00080	0.00356	2.61856
A3	2.55864	0.00015	-0.00160	-0.00016	-0.00176	2.55688
A4	2.71297	-0.00015	-0.00412	-0.00108	-0.00520	2.70777
A5	2.61357	0.00011	0.00256	0.00067	0.00323	2.61680
A6	2.84989	-0.00033	0.00484	0.00026	0.00510	2.85499
A7	2.71415	-0.00018	-0.00392	-0.00126	-0.00519	2.70896
A8	2.84927	-0.00035	0.00478	0.00006	0.00483	2.85410
A9	2.08862	-0.00016	-0.00079	-0.00085	-0.00164	2.08698
A10	2.10203	0.00032	-0.00009	0.00132	0.00123	2.10326
A11	2.09193	-0.00015	0.00085	-0.00043	0.00042	2.09235
A12	2.08801	0.00020	-0.00076	-0.00064	-0.00141	2.08660
A13	2.09227	-0.00018	0.00080	-0.00047	0.00033	2.09260
A14	2.10232	-0.00001	-0.00003	0.00093	0.00091	2.10323
A15	2.04113	0.00033	-0.00023	0.00463	0.00440	2.04553
A16	1.90131	0.00276	-0.00236	0.00719	0.00483	1.90614
A17	2.04156	0.00081	-0.00002	0.00507	0.00505	2.04661
A18	1.90043	0.00341	-0.00232	0.00882	0.00650	1.90693
A19	2.01371	-0.00001	0.00253	-0.00193	0.00060	2.01430
A20	1.92236	-0.00092	0.00080	0.00029	0.00109	1.92344
A21	1.90311	-0.00063	-0.00489	-0.00167	-0.00657	1.89655
A22	1.89770	0.00035	0.00007	0.00044	0.00051	1.89821
A23	1.83957	0.00077	-0.00046	0.00179	0.00133	1.84090
A24	1.88177	0.00055	0.00191	0.00134	0.00325	1.88501
A25	2.01337	0.00007	0.00261	-0.00205	0.00056	2.01393
A26	1.92243	-0.00105	0.00064	0.00042	0.00106	1.92349
A27	1.90370	-0.00064	-0.00473	-0.00190	-0.00664	1.89706
A28	1.89773	0.00035	0.00011	0.00046	0.00056	1.89830
A29	1.83951	0.00079	-0.00047	0.00186	0.00139	1.84090
A30	1.88145	0.00060	0.00179	0.00149	0.00328	1.88473
A31	2.90226	0.00008	-0.00158	0.00130	-0.00028	2.90198
A32	3.12387	0.00013	0.00072	-0.00077	-0.00005	3.12382
A33	2.90348	0.00001	-0.00148	0.00025	-0.00123	2.90225
A34	3.12219	0.00021	0.00044	0.00162	0.00206	3.12425
A35	3.94244	0.00309	-0.00259	0.01182	0.00923	3.95167
A36	3.94199	0.00422	-0.00234	0.01390	0.01156	3.95354
A37	3.14491	-0.00018	-0.00121	0.00110	-0.00007	3.14483
A38	3.14551	-0.00044	0.00076	-0.01076	-0.01001	3.13550
A39	3.14520	-0.00023	-0.00105	0.00064	-0.00040	3.14480
A40	3.14158	-0.00024	-0.00257	0.00781	0.00522	3.14681
A41	4.04894	0.00161	0.00073	-0.01133	-0.01060	4.03834

A42	4.03873	0.00324	0.00422	-0.00837	-0.00415	4.03458
D1	0.02463	-0.00021	-0.00050	-0.00247	-0.00297	0.02166
D2	-0.02105	-0.00010	-0.00006	0.00169	0.00163	-0.01942
D3	-0.01488	-0.00006	0.00040	-0.00083	-0.00044	-0.01532
D4	0.02431	-0.00017	-0.00073	-0.00114	-0.00187	0.02244
D5	0.00583	-0.00005	-0.00069	-0.00134	-0.00206	0.00377
D6	-0.01567	0.00000	-0.00017	0.00223	0.00205	-0.01362
D7	-0.00718	0.00006	-0.00091	-0.00060	-0.00154	-0.00872
D8	3.09749	-0.00001	-0.00204	-0.00656	-0.00861	3.08887
D9	0.00581	0.00000	-0.00095	0.00023	-0.00073	0.00509
D10	-0.00939	0.00005	-0.00283	0.01087	0.00804	-0.00134
D11	3.09347	0.00005	-0.00498	0.01180	0.00680	3.10026
D12	0.00989	0.00011	0.00295	-0.00450	-0.00157	0.00832
D13	-3.09534	-0.00011	0.00263	0.00112	0.00373	-3.09161
D14	-3.09425	-0.00018	0.00406	-0.00594	-0.00190	-3.09615
D15	0.08370	-0.00040	0.00373	-0.00032	0.00340	0.08710
D16	2.49542	-0.00046	0.00174	0.00671	0.00845	2.50387
D17	-0.68391	-0.00018	0.00061	0.00811	0.00872	-0.67519
D18	-0.68021	-0.00017	0.00202	-0.00184	0.00018	-0.68003
D19	2.49805	-0.00039	0.00171	0.00386	0.00558	2.50363
D20	-1.24258	0.00055	0.05860	0.00101	0.05960	-1.18298
D21	0.91363	0.00026	0.06123	0.00038	0.06162	0.97525
D22	2.97527	0.00001	0.06109	0.00118	0.06226	3.03753
D23	-1.24520	0.00059	0.05929	0.00120	0.06049	-1.18471
D24	0.91087	0.00026	0.06191	0.00061	0.06253	0.97339
D25	2.97252	-0.00001	0.06162	0.00153	0.06315	3.03567

Item	Value	Threshold	Converged?
Maximum Force	0.004223	0.000450	NO
RMS Force	0.001035	0.000300	NO
Maximum Displacement	0.130016	0.001800	NO
RMS Displacement	0.033080	0.001200	NO

Predicted change in Energy=-1.115428D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 05:17:33 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.023512	0.669413	0.052862
2	6	0	3.344395	1.690187	0.122286
3	6	0	4.022695	-0.670458	-0.047454
4	6	0	2.143329	2.286142	0.169086
5	6	0	3.344308	-1.691625	-0.117688

6	6	0	0.917318	2.320287	0.172868
7	6	0	2.142555	-2.286209	-0.166304
8	6	0	-0.380035	1.977907	0.149307
9	6	0	0.916626	-2.320286	-0.173150
10	6	0	-1.457467	1.393564	0.103765
11	6	0	-0.380537	-1.976570	-0.153975
12	6	0	-2.667837	0.708448	0.058670
13	6	0	-1.457565	-1.391481	-0.112213
14	6	0	-2.668186	-0.706946	-0.056227
15	6	0	-3.904707	1.413411	0.172759
16	6	0	-3.904921	-1.411746	-0.164725
17	7	0	-3.734178	2.880798	-0.052981
18	7	0	-3.733578	-2.880504	0.048554
19	1	0	-3.417457	3.149107	-0.995680
20	1	0	-4.599476	3.369899	0.152134
21	1	0	-3.410553	-3.155781	0.987099
22	1	0	-4.600519	-3.367710	-0.154273
23	1	0	-3.016396	3.228303	0.584796
24	1	0	-4.737757	1.054314	-0.424534
25	1	0	-4.734602	-1.056462	0.439252
26	1	0	-3.020453	-3.223924	-0.596662

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.228006	0.000000			
3	C	1.343622	2.462021	0.000000		
4	C	2.482420	1.341609	3.510042	0.000000	
5	C	2.462703	3.390316	1.227975	4.164999	0.000000
6	C	3.519691	2.508045	4.316997	1.226492	4.697886
7	C	3.510233	4.164064	2.481875	4.584635	1.341679
8	C	4.594854	3.735625	5.141652	2.542196	5.235215
9	C	4.317653	4.697366	3.519290	4.779237	2.508372
10	C	5.528844	4.811051	5.857920	3.710349	5.711783
11	C	5.141951	5.234172	4.594097	4.964371	3.735904
12	C	6.691466	6.092192	6.831974	5.064447	6.475904
13	C	5.858049	5.710560	5.527867	5.154655	4.811247
14	C	6.832649	6.475281	6.690987	5.670980	6.092902
15	C	7.963955	7.254560	8.199678	6.110680	7.891377
16	C	8.199916	7.890308	7.963063	7.096980	7.254782
17	N	8.067415	7.180144	8.531151	5.911684	8.427111
18	N	8.530790	8.425815	8.065562	7.826032	7.178965
19	H	7.913049	7.007207	8.416893	5.746628	8.362118
20	H	9.036504	8.119570	9.523978	6.829365	9.423138
21	H	8.412505	8.358268	7.905714	7.818521	6.999461
22	H	9.524452	9.422340	9.035840	8.806253	8.119783
23	H	7.509406	6.560441	8.071486	5.261487	8.072034
24	H	8.782705	8.125549	8.936585	7.015635	8.541318

25	H	8.934904	8.539014	8.779302	7.651923	8.122955
26	H	8.074491	8.073207	7.511841	7.590246	6.564110

		6	7	8	9	10
6	C	0.000000				
7	C	4.778708	0.000000			
8	C	1.341977	4.964449	0.000000		
9	C	4.653456	1.226422	4.501086	0.000000	
10	C	2.550136	5.154981	1.226536	4.416524	0.000000
11	C	4.500471	2.542051	3.966090	1.342066	3.547395
12	C	3.932481	5.670843	2.617973	4.698441	1.391552
13	C	4.415718	3.710031	3.547146	2.550132	2.793407
14	C	4.698135	5.064526	3.533599	3.932863	2.429730
15	C	4.906562	7.097291	3.569667	6.107815	2.448294
16	C	6.107048	6.110373	4.900326	4.906407	3.732545
17	N	4.690586	7.826033	3.479427	6.978230	2.723940
18	N	6.978145	5.910016	5.904284	4.689071	4.842664
19	H	4.565383	7.819480	3.450890	7.026742	2.851714
20	H	5.615793	8.806131	4.443122	7.931670	3.712204
21	H	7.027145	5.737900	6.020024	4.557269	5.029053
22	H	7.931385	6.829264	6.817645	5.615723	5.710963
23	H	4.058114	7.588727	2.950177	6.843244	2.455182
24	H	5.825758	7.652743	4.491332	6.589626	3.339835
25	H	6.589203	7.012437	5.315423	5.823115	4.105460
26	H	6.843720	5.265090	5.881100	4.061590	4.924909

		11	12	13	14	15
11	C	0.000000				
12	C	3.533593	0.000000			
13	C	1.226402	2.429745	0.000000		
14	C	2.618174	1.420050	1.391879	0.000000	
15	C	4.900868	1.428229	3.733248	2.465225	0.000000
16	C	3.569373	2.464854	2.448004	1.427595	2.845244
17	N	5.903484	2.422531	4.841368	3.742761	1.494410
18	N	3.478649	3.743859	2.724568	2.422889	4.299118
19	H	6.016969	2.762319	5.023807	4.038952	2.148326
20	H	6.817469	3.289877	5.710712	4.515968	2.076288
21	H	3.445807	4.043003	2.852263	2.763409	4.667425
22	H	4.443368	4.516156	3.712872	3.289861	4.842544
23	H	5.880837	2.597686	4.925260	4.002293	2.062208
24	H	5.314586	2.153527	4.103550	2.742410	1.086132
25	H	4.489588	2.744315	3.339959	2.153540	2.619164
26	H	2.953137	4.002168	2.456656	2.598334	4.783178

		16	17	18	19	20
16	C	0.000000				
17	N	4.297391	0.000000			
18	N	1.494020	5.762196	0.000000		
19	H	4.661490	1.030040	6.127526	0.000000	
20	H	4.842204	1.014905	6.310946	1.662346	0.000000
21	H	2.147733	6.134068	1.030043	6.609318	6.685448

22	H	2.075997	6.309094	1.014937	6.676565	6.744573
23	H	4.783442	1.021142	6.174093	1.632491	1.647236
24	H	2.615831	2.116900	4.088396	2.541173	2.390314
25	H	1.085995	4.092085	2.117032	4.634729	4.437721
26	H	2.062242	6.170302	1.021170	6.397840	6.821474

		21	22	23	24	25
21	H	0.000000				
22	H	1.662428	0.000000			
23	H	6.408880	6.823713	0.000000		
24	H	4.634553	4.432401	2.950942	0.000000	
25	H	2.541729	2.390004	4.618726	2.280682	0.000000
26	H	1.632519	1.647116	6.559504	4.613251	2.951155

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=0 Diff= 2.70D-03
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.528566	-0.671573	-0.026415
2	6	0	3.849264	-1.694100	-0.057808
3	6	0	4.527991	0.671113	0.023735
4	6	0	2.648090	-2.291159	-0.082615
5	6	0	3.849790	1.694320	0.055557
6	6	0	1.422074	-2.325188	-0.085448
7	6	0	2.648144	2.290535	0.081586
8	6	0	0.124783	-1.981921	-0.075054
9	6	0	1.422219	2.325077	0.086823
10	6	0	-0.952544	-1.396079	-0.051680
11	6	0	0.124993	1.981131	0.080164
12	6	0	-2.162789	-0.709525	-0.032558
13	6	0	-0.952141	1.395095	0.060018
14	6	0	-2.162885	0.709176	0.029340
15	6	0	-3.399770	-1.418026	-0.120542
16	6	0	-3.399507	1.417774	0.111078
17	7	0	-3.229593	-2.875979	0.159950
18	7	0	-3.227814	2.877498	-0.156921
19	1	0	-2.913173	-3.108915	1.112106
20	1	0	-4.094935	-3.372242	-0.026968
21	1	0	-2.904488	3.117431	-1.105015
22	1	0	-4.094711	3.372112	0.027316

```
    23        1        0     -2.511714   -3.247223   -0.464196
    24        1        0     -4.232904   -1.036689    0.462684
    25        1        0     -4.229101    1.040315   -0.479416
    26        1        0     -2.514790    3.244667    0.475195
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6020579           0.2702826           0.1872367
 Leave Link  202 at Sat Sep 26 05:17:33 2026, MaxMem=    805306368 cpu:                  0.0 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1009.4597028448 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0154142796 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1009.4442885652 Hartrees.
 Leave Link  301 at Sat Sep 26 05:17:33 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23215 LenP2D=   51906.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.89D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=           5 IRanWt=          -1 IRanGd=           0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=           0 NUsed=           0 NTot=          32
 NSgBfM=   683   683   683   683   683 MxSgAt=    26 MxSgA2=    26.
 Leave Link  302 at Sat Sep 26 05:17:34 2026, MaxMem=    805306368 cpu:                  5.6 elap:
0.9
 (Enter /home/user/gauss16/g16/l303.exe)
```

Supporting Information file

```
 DipDrv:  MaxL=1.
 Leave Link  303 at Sat Sep 26 05:17:34 2026, MaxMem=    805306368 cpu:                  0.7 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=    -0.000000    0.000000   -0.000000
       Rot=    1.000000   -0.000091    0.000044    0.000646 Ang=  -0.07 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Generating alternative initial guess.
 ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn=          5 AccDes=
0.00D+00
 Harris functional with IExCor= 4639 and IRadAn=       5 diagonalized for initial guess.
 HarFok:  IExCor= 4639 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Petite list used in FoFCou.
 Harris En= -691.982977034946
 Leave Link  401 at Sat Sep 26 05:17:43 2026, MaxMem=    805306368 cpu:                 51.2 elap:
8.5
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.411231960468
 DIIS: error= 2.33D-03 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -723.411231960468     IErMin= 1 ErrMin= 2.33D-03
 ErrMax= 2.33D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-03 BMatP= 2.23D-03
 IDIUse=3 WtCom= 9.77D-01 WtEn= 2.33D-02
```

Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.706 Goal=   None   Shift=   0.000
GapD=   0.706 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=9.89D-03 MaxDP=3.78D-01   OVMax= 1.20D-02

Cycle   2 Pass 0 IDiag 1:
RMSU= 8.29D-03   CP: 1.52D+00
E= -723.413699304542   Delta-E=   -0.002467344074 Rises=F Damp=F
DIIS: error= 7.61D-04 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.413699304542   IErMin= 2 ErrMin= 7.61D-04
ErrMax= 7.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-04 BMatP= 2.23D-03
IDIUse=3 WtCom= 9.92D-01 WtEn= 7.61D-03
Coeff-Com: -0.252D-01 0.103D+01
Coeff-En: 0.000D+00 0.100D+01
Coeff: -0.251D-01 0.103D+01
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=8.98D-03 MaxDP=3.38D-01 DE=-2.47D-03 OVMax= 3.08D-03

Cycle   3 Pass 0 IDiag 1:
RMSU= 4.14D-03   CP: 1.00D+00 2.92D-01
E= -723.413825843349   Delta-E=   -0.000126538807 Rises=F Damp=F
DIIS: error= 4.94D-03 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -723.413825843349   IErMin= 2 ErrMin= 7.61D-04
ErrMax= 4.94D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.48D-04 BMatP= 1.70D-04
IDIUse=3 WtCom= 1.25D-01 WtEn= 8.75D-01
Coeff-Com: -0.602D-01 0.780D+00 0.280D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.750D-02 0.972D-01 0.910D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=7.65D+02 MaxDP=3.02D+04 DE=-1.27D-04 OVMax= 9.89D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle   4 Pass 1 IDiag 1:
E= -723.413619268080   Delta-E=   0.000206575269 Rises=F Damp=F
DIIS: error= 1.10D-03 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -723.413619268080   IErMin= 1 ErrMin= 1.10D-03
ErrMax= 1.10D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.07D-04 BMatP= 2.07D-04
IDIUse=3 WtCom= 9.89D-01 WtEn= 1.10D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.181 Goal=   None   Shift=   0.000
GapD=   0.181 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=4.61D-03 MaxDP=1.18D-01 DE= 2.07D-04 OVMax= 2.23D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.08D-03 CP: 8.13D-01
E= -723.413749107239 Delta-E= -0.000129839159 Rises=F Damp=F
DIIS: error= 1.80D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413749107239 IErMin= 2 ErrMin= 1.80D-04
ErrMax= 1.80D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-05 BMatP= 2.07D-04
IDIUse=3 WtCom= 9.98D-01 WtEn= 1.80D-03
Coeff-Com: 0.420D-01 0.958D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.419D-01 0.958D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.69D-04 MaxDP=2.16D-02 DE=-1.30D-04 OVMax= 2.57D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.47D-04 CP: 8.28D-01 1.07D+00
E= -723.413729951293 Delta-E= 0.000019155947 Rises=F Damp=F
DIIS: error= 3.13D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413749107239 IErMin= 2 ErrMin= 1.80D-04
ErrMax= 3.13D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-05 BMatP= 1.04D-05
IDIUse=3 WtCom= 3.61D-01 WtEn= 6.39D-01
Coeff-Com: -0.215D-01 0.632D+00 0.389D+00
Coeff-En: 0.000D+00 0.685D+00 0.315D+00
Coeff: -0.775D-02 0.666D+00 0.342D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.75D-05 MaxDP=2.28D-03 DE= 1.92D-05 OVMax= 1.44D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.59D-05 CP: 8.29D-01 1.07D+00 1.10D+00
E= -723.413761570492 Delta-E= -0.000031619199 Rises=F Damp=F
DIIS: error= 3.37D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413761570492 IErMin= 4 ErrMin= 3.37D-05
ErrMax= 3.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.29D-07 BMatP= 1.04D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.804D-02 0.190D+00 0.422D-01 0.776D+00
Coeff: -0.804D-02 0.190D+00 0.422D-01 0.776D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.21D-05 MaxDP=2.17D-03 DE=-3.16D-05 OVMax= 2.25D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 7.57D-06 CP: 8.31D-01 1.07D+00 1.19D+00 1.34D+00
E= -723.413761977911 Delta-E= -0.000000407419 Rises=F Damp=F
DIIS: error= 6.34D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413761977911 IErMin= 5 ErrMin= 6.34D-06
ErrMax= 6.34D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.09D-08 BMatP= 3.29D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.203D-02-0.814D-01-0.829D-01 0.352D+00 0.810D+00
Coeff: 0.203D-02-0.814D-01-0.829D-01 0.352D+00 0.810D+00
Gap= 0.181 Goal= None Shift= 0.000

RMSDP=2.55D-05 MaxDP=1.36D-03 DE=-4.07D-07 OVMax= 1.50D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 2.27D-06 CP: 8.32D-01 1.08D+00 1.24D+00 1.54D+00 1.76D+00
E= -723.413762036874 Delta-E= -0.000000058963 Rises=F Damp=F
DIIS: error= 2.38D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413762036874 IErMin= 6 ErrMin= 2.38D-06
ErrMax= 2.38D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.79D-09 BMatP= 3.09D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.186D-02-0.601D-01-0.444D-01 0.873D-01 0.381D+00 0.634D+00
Coeff: 0.186D-02-0.601D-01-0.444D-01 0.873D-01 0.381D+00 0.634D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=4.09D-06 MaxDP=2.29D-04 DE=-5.90D-08 OVMax= 5.95D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 6.39D-07 CP: 8.32D-01 1.08D+00 1.25D+00 1.58D+00 1.96D+00
CP: 1.26D+00
E= -723.413762046323 Delta-E= -0.000000009449 Rises=F Damp=F
DIIS: error= 1.16D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413762046323 IErMin= 7 ErrMin= 1.16D-06
ErrMax= 1.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.17D-10 BMatP= 4.79D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.322D-03-0.704D-02-0.388D-03-0.378D-01-0.217D-01 0.258D+00
Coeff-Com: 0.808D+00
Coeff: 0.322D-03-0.704D-02-0.388D-03-0.378D-01-0.217D-01 0.258D+00
Coeff: 0.808D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=1.02D-06 MaxDP=3.93D-05 DE=-9.45D-09 OVMax= 4.63D-05

Cycle 11 Pass 1 IDiag 1:
RMSU= 2.62D-07 CP: 8.32D-01 1.08D+00 1.25D+00 1.60D+00 2.03D+00
CP: 1.45D+00 1.89D+00
E= -723.413762049222 Delta-E= -0.000000002899 Rises=F Damp=F
DIIS: error= 7.99D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413762049222 IErMin= 8 ErrMin= 7.99D-07
ErrMax= 7.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D-10 BMatP= 8.17D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.308D-03 0.115D-01 0.108D-01-0.391D-01-0.107D+00-0.317D-01
Coeff-Com: 0.385D+00 0.771D+00
Coeff: -0.308D-03 0.115D-01 0.108D-01-0.391D-01-0.107D+00-0.317D-01
Coeff: 0.385D+00 0.771D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=6.68D-07 MaxDP=3.21D-05 DE=-2.90D-09 OVMax= 3.01D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.09D-07 CP: 8.32D-01 1.08D+00 1.25D+00 1.61D+00 2.05D+00
CP: 1.53D+00 2.38D+00 1.71D+00
E= -723.413762050170 Delta-E= -0.000000000947 Rises=F Damp=F

DIIS: error= 4.52D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413762050170 IErMin= 9 ErrMin= 4.52D-07
ErrMax= 4.52D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.65D-11 BMatP= 2.20D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.189D-03 0.620D-02 0.483D-02-0.107D-01-0.432D-01-0.533D-01
Coeff-Com: 0.373D-01 0.326D+00 0.733D+00
Coeff: -0.189D-03 0.620D-02 0.483D-02-0.107D-01-0.432D-01-0.533D-01
Coeff: 0.373D-01 0.326D+00 0.733D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=2.81D-07 MaxDP=1.22D-05 DE=-9.47D-10 OVMax= 1.60D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 6.65D-08 CP: 8.32D-01 1.08D+00 1.25D+00 1.61D+00 2.04D+00
CP: 1.54D+00 2.54D+00 1.96D+00 1.60D+00
E= -723.413762050434 Delta-E= -0.000000000265 Rises=F Damp=F
DIIS: error= 3.96D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413762050434 IErMin=10 ErrMin= 3.96D-07
ErrMax= 3.96D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-11 BMatP= 4.65D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.474D-04-0.210D-02-0.236D-02 0.113D-01 0.243D-01-0.706D-02
Coeff-Com: -0.138D+00-0.188D+00 0.306D+00 0.996D+00
Coeff: 0.474D-04-0.210D-02-0.236D-02 0.113D-01 0.243D-01-0.706D-02
Coeff: -0.138D+00-0.188D+00 0.306D+00 0.996D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=2.21D-07 MaxDP=1.01D-05 DE=-2.65D-10 OVMax= 1.67D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 3.79D-08 CP: 8.32D-01 1.08D+00 1.25D+00 1.61D+00 2.03D+00
CP: 1.53D+00 2.63D+00 2.12D+00 2.29D+00 2.25D+00
E= -723.413762050582 Delta-E= -0.000000000147 Rises=F Damp=F
DIIS: error= 1.76D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413762050582 IErMin=11 ErrMin= 1.76D-07
ErrMax= 1.76D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.52D-12 BMatP= 1.54D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.672D-04-0.248D-02-0.231D-02 0.814D-02 0.217D-01 0.985D-02
Coeff-Com: -0.779D-01-0.180D+00-0.257D-01 0.519D+00 0.730D+00
Coeff: 0.672D-04-0.248D-02-0.231D-02 0.814D-02 0.217D-01 0.985D-02
Coeff: -0.779D-01-0.180D+00-0.257D-01 0.519D+00 0.730D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=8.36D-08 MaxDP=4.58D-06 DE=-1.47D-10 OVMax= 8.04D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.67D-08 CP: 8.32D-01 1.08D+00 1.25D+00 1.61D+00 2.03D+00
CP: 1.52D+00 2.65D+00 2.14D+00 2.58D+00 2.91D+00
CP: 1.47D+00
E= -723.413762050621 Delta-E= -0.000000000040 Rises=F Damp=F
DIIS: error= 1.13D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413762050621 IErMin=12 ErrMin= 1.13D-07

ErrMax= 1.13D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-12 BMatP= 5.52D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.475D-06 0.131D-03 0.291D-03-0.230D-02-0.389D-02 0.687D-02
Coeff-Com: 0.368D-01 0.226D-01-0.145D+00-0.254D+00 0.211D+00 0.113D+01
Coeff: 0.475D-06 0.131D-03 0.291D-03-0.230D-02-0.389D-02 0.687D-02
Coeff: 0.368D-01 0.226D-01-0.145D+00-0.254D+00 0.211D+00 0.113D+01
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=6.90D-08 MaxDP=4.35D-06 DE=-3.96D-11 OVMax= 6.73D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 3.15D-08   CP: 8.32D-01 1.08D+00 1.25D+00 1.61D+00 2.03D+00
               CP: 1.51D+00 2.65D+00 2.11D+00 2.77D+00 3.00D+00
               CP: 1.97D+00 2.41D+00
E= -723.413762050642   Delta-E=   -0.000000000021 Rises=F Damp=F
DIIS: error= 4.04D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.413762050642   IErMin=13 ErrMin= 4.04D-08
ErrMax= 4.04D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.76D-13 BMatP= 1.17D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.130D-04 0.557D-03 0.611D-03-0.281D-02-0.630D-02 0.192D-02
Coeff-Com: 0.353D-01 0.475D-01-0.712D-01-0.233D+00-0.362D-01 0.596D+00
Coeff-Com: 0.668D+00
Coeff: -0.130D-04 0.557D-03 0.611D-03-0.281D-02-0.630D-02 0.192D-02
Coeff: 0.353D-01 0.475D-01-0.712D-01-0.233D+00-0.362D-01 0.596D+00
Coeff: 0.668D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=2.00D-08 MaxDP=1.33D-06 DE=-2.11D-11 OVMax= 1.96D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 4.00D-09   CP: 8.32D-01 1.08D+00 1.25D+00 1.61D+00 2.03D+00
               CP: 1.51D+00 2.65D+00 2.10D+00 2.80D+00 3.00D+00
               CP: 2.14D+00 2.94D+00 1.28D+00
E= -723.413762050634   Delta-E=   0.000000000008 Rises=F Damp=F
DIIS: error= 1.71D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.413762050642   IErMin=14 ErrMin= 1.71D-08
ErrMax= 1.71D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.50D-14 BMatP= 3.76D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.388D-05 0.136D-03 0.119D-03-0.377D-03-0.108D-02-0.805D-03
Coeff-Com: 0.283D-02 0.887D-02 0.869D-02-0.161D-01-0.520D-01-0.499D-01
Coeff-Com: 0.200D+00 0.900D+00
Coeff: -0.388D-05 0.136D-03 0.119D-03-0.377D-03-0.108D-02-0.805D-03
Coeff: 0.283D-02 0.887D-02 0.869D-02-0.161D-01-0.520D-01-0.499D-01
Coeff: 0.200D+00 0.900D+00
Gap=   0.181 Goal=   None   Shift=   0.000
RMSDP=8.38D-09 MaxDP=2.87D-07 DE= 8.19D-12 OVMax= 8.37D-07

SCF Done: E(RwB97XD) = -723.413762051   A.U. after   17 cycles
         NFock= 17 Conv=0.84D-08   -V/T= 2.0047
KE= 7.200382779897D+02 PE=-3.699952251138D+03 EE= 1.247055922533D+03

Supporting Information file

Leave Link 502 at Sat Sep 26 05:39:30 2026, MaxMem= 805306368 cpu: 7844.3 elap: 1307.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23215 LenP2D= 51906.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 05:39:31 2026, MaxMem= 805306368 cpu: 3.8 elap: 0.6
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 05:39:31 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 05:49:37 2026, MaxMem= 805306368 cpu: 3634.5 elap: 605.8
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.48325007D+00 8.46938272D-03 9.76937858D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000438748	-0.001777603	-0.000403801
2	6	-0.001025895	0.001276055	0.000362606
3	6	0.000430438	0.001792131	0.000421448
4	6	0.001419861	-0.000737815	-0.000278183
5	6	-0.001016905	-0.001296082	-0.000349812
6	6	-0.001334686	0.000511780	0.000127725
7	6	0.001439335	0.000742053	0.000274381
8	6	0.000555790	-0.000039903	-0.000150021
9	6	-0.001338376	-0.000501004	-0.000299861
10	6	-0.000326154	-0.000485740	0.000157941
11	6	0.000642038	0.000028231	-0.000018027
12	6	0.000054320	0.003746392	0.000735124

13	6	-0.000587505	0.000440807	0.000587307
14	6	0.000494035	-0.003645232	-0.001284075
15	6	-0.001621118	0.001280999	-0.001579702
16	6	-0.001869833	-0.001298680	0.001523074
17	7	0.002563874	-0.000781020	0.000249663
18	7	0.002632726	0.000725222	-0.000078726
19	1	-0.000566468	-0.000295679	0.000361834
20	1	0.000168672	-0.000628696	0.000018956
21	1	-0.000574561	0.000242558	-0.000384955
22	1	0.000169561	0.000654734	0.000018581
23	1	-0.000382902	-0.000579370	0.000085642
24	1	0.000028604	-0.000929878	0.000446492
25	1	-0.000030358	0.000931009	-0.000481963
26	1	-0.000363241	0.000624731	-0.000061647

Cartesian Forces: Max 0.003746392 RMS 0.001063003
Leave Link 716 at Sat Sep 26 05:49:37 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002699608 RMS 0.000806997
Search for a local minimum.
Step number 20 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .80700D-03 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 18 19 20
DE= -1.53D-04 DEPred=-1.12D-04 R= 1.37D+00
TightC=F SS= 1.41D+00 RLast= 1.55D-01 DXNew= 1.3552D+00 4.6550D-01
Trust test= 1.37D+00 RLast= 1.55D-01 DXMaxT set to 8.06D-01
ITU= 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 0 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00233	0.00467	0.01061	0.01305	0.01696
Eigenvalues ---	0.01794	0.02657	0.02722	0.02800	0.02957
Eigenvalues ---	0.03132	0.03377	0.03662	0.03790	0.04360
Eigenvalues ---	0.04448	0.04475	0.05026	0.05783	0.07165
Eigenvalues ---	0.09959	0.10172	0.11050	0.11204	0.11526
Eigenvalues ---	0.11760	0.13806	0.15261	0.15563	0.15886
Eigenvalues ---	0.16000	0.16002	0.16042	0.16118	0.17245
Eigenvalues ---	0.22306	0.22666	0.24400	0.24991	0.24995
Eigenvalues ---	0.24998	0.25000	0.25003	0.25005	0.28962
Eigenvalues ---	0.29891	0.36056	0.37237	0.38543	0.44948
Eigenvalues ---	0.45813	0.46593	0.47310	0.47627	0.47688
Eigenvalues ---	0.47689	0.47900	0.48342	0.51434	0.54805

```
    Eigenvalues ---    0.55225   0.55602   0.55659   0.56032   0.62166
    Eigenvalues ---    0.93656   0.93773   0.95031   0.95555   0.97728
    Eigenvalues ---    0.98748   1.37226
 RFO step:  Lambda=-1.73425022D-04 EMin= 2.33124367D-03
 Quartic linear search produced a step of  0.91097.
 Iteration  1 RMS(Cart)=  0.04518721 RMS(Int)=  0.00198704
 Iteration  2 RMS(Cart)=  0.00212377 RMS(Int)=  0.00002359
 Iteration  3 RMS(Cart)=  0.00000405 RMS(Int)=  0.00002338
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00002338
  ITry=  1 IFail=0 DXMaxC= 1.72D-01 DCOld= 1.00D+10 DXMaxT= 8.06D-01 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)   (Quad)   (Total)
    R1        2.32060   0.00100   0.00028   0.00067   0.00096   2.32156
    R2        2.53908  -0.00089   0.00011  -0.00100  -0.00088   2.53819
    R3        2.53527  -0.00070  -0.00028  -0.00101  -0.00128   2.53399
    R4        2.32054   0.00101   0.00027   0.00070   0.00098   2.32152
    R5        2.31773   0.00084   0.00039   0.00070   0.00109   2.31883
    R6        2.53541  -0.00070  -0.00031  -0.00094  -0.00124   2.53416
    R7        2.53597  -0.00045  -0.00047  -0.00089  -0.00137   2.53460
    R8        2.31760   0.00087   0.00039   0.00076   0.00114   2.31874
    R9        2.31782   0.00009   0.00008   0.00038   0.00046   2.31828
   R10        2.53614  -0.00043  -0.00055  -0.00074  -0.00130   2.53484
   R11        2.62965  -0.00042  -0.00012  -0.00079  -0.00092   2.62873
   R12        2.31756   0.00020   0.00007   0.00056   0.00063   2.31819
   R13        2.68351   0.00146   0.00099   0.00279   0.00377   2.68728
   R14        2.69896  -0.00115  -0.00178  -0.00233  -0.00410   2.69486
   R15        2.63027  -0.00055  -0.00025  -0.00101  -0.00126   2.62901
   R16        2.69776  -0.00094  -0.00200  -0.00081  -0.00281   2.69495
   R17        2.82403  -0.00215  -0.00070  -0.00318  -0.00388   2.82015
   R18        2.05249   0.00004  -0.00094  -0.00057  -0.00151   2.05098
   R19        2.82329  -0.00207  -0.00078  -0.00301  -0.00379   2.81950
   R20        2.05223   0.00006  -0.00082  -0.00063  -0.00145   2.05078
   R21        1.94649  -0.00058  -0.00188  -0.00104  -0.00292   1.94357
   R22        1.91789  -0.00044  -0.00071  -0.00029  -0.00100   1.91689
   R23        1.92968  -0.00041   0.00052   0.00015   0.00067   1.93035
   R24        1.94650  -0.00060  -0.00183  -0.00114  -0.00297   1.94353
   R25        1.91795  -0.00046  -0.00072  -0.00029  -0.00102   1.91694
   R26        1.92973  -0.00042   0.00052   0.00010   0.00062   1.93035
    A1        2.55496   0.00026  -0.00180  -0.00010  -0.00189   2.55307
    A2        2.61856  -0.00006   0.00324   0.00081   0.00405   2.62262
    A3        2.55688   0.00027  -0.00160   0.00020  -0.00140   2.55548
    A4        2.70777   0.00015  -0.00474  -0.00141  -0.00617   2.70160
    A5        2.61680  -0.00007   0.00294   0.00090   0.00385   2.62065
    A6        2.85499  -0.00064   0.00465  -0.00040   0.00420   2.85919
    A7        2.70896   0.00016  -0.00473  -0.00093  -0.00567   2.70329
    A8        2.85410  -0.00063   0.00440  -0.00003   0.00433   2.85843
    A9        2.08698   0.00001  -0.00150  -0.00091  -0.00248   2.08449
```

A10	2.10326	0.00030	0.00112	0.00176	0.00290	2.10616
A11	2.09235	-0.00031	0.00038	-0.00116	-0.00076	2.09159
A12	2.08660	0.00009	-0.00129	-0.00081	-0.00219	2.08441
A13	2.09260	-0.00029	0.00030	-0.00074	-0.00043	2.09216
A14	2.10323	0.00022	0.00082	0.00216	0.00299	2.10622
A15	2.04553	0.00021	0.00401	0.00386	0.00787	2.05340
A16	1.90614	0.00247	0.00440	0.00950	0.01390	1.92004
A17	2.04661	0.00035	0.00460	0.00249	0.00709	2.05370
A18	1.90693	0.00235	0.00592	0.00453	0.01045	1.91738
A19	2.01430	0.00008	0.00054	-0.00003	0.00051	2.01482
A20	1.92344	-0.00065	0.00099	0.00038	0.00136	1.92481
A21	1.89655	-0.00049	-0.00598	-0.00373	-0.00972	1.88683
A22	1.89821	0.00018	0.00046	-0.00002	0.00044	1.89865
A23	1.84090	0.00064	0.00121	0.00238	0.00358	1.84448
A24	1.88501	0.00032	0.00296	0.00116	0.00412	1.88913
A25	2.01393	0.00017	0.00051	0.00065	0.00116	2.01508
A26	1.92349	-0.00068	0.00096	0.00051	0.00147	1.92497
A27	1.89706	-0.00055	-0.00605	-0.00432	-0.01037	1.88669
A28	1.89830	0.00015	0.00051	-0.00026	0.00025	1.89854
A29	1.84090	0.00062	0.00127	0.00198	0.00324	1.84414
A30	1.88473	0.00037	0.00299	0.00155	0.00454	1.88927
A31	2.90198	0.00006	-0.00025	-0.00101	-0.00132	2.90066
A32	3.12382	0.00021	-0.00005	0.00394	0.00381	3.12763
A33	2.90225	0.00006	-0.00112	0.00115	-0.00003	2.90222
A34	3.12425	0.00014	0.00187	-0.00111	0.00068	3.12494
A35	3.95167	0.00268	0.00841	0.01336	0.02177	3.97344
A36	3.95354	0.00270	0.01053	0.00702	0.01754	3.97109
A37	3.14483	-0.00017	-0.00007	-0.00127	-0.00137	3.14346
A38	3.13550	0.00022	-0.00912	0.03271	0.02357	3.15908
A39	3.14480	-0.00003	-0.00036	0.00070	0.00039	3.14519
A40	3.14681	-0.00044	0.00476	-0.03366	-0.02888	3.11792
A41	4.03834	0.00181	-0.00966	-0.00458	-0.01424	4.02410
A42	4.03458	0.00223	-0.00378	-0.00504	-0.00882	4.02576
D1	0.02166	-0.00003	-0.00270	0.00027	-0.00244	0.01922
D2	-0.01942	-0.00001	0.00149	0.00223	0.00371	-0.01571
D3	-0.01532	0.00011	-0.00040	0.00716	0.00677	-0.00855
D4	0.02244	-0.00017	-0.00170	-0.00473	-0.00646	0.01598
D5	0.00377	0.00006	-0.00188	0.00191	0.00004	0.00381
D6	-0.01362	-0.00009	0.00187	-0.00435	-0.00250	-0.01612
D7	-0.00872	-0.00003	-0.00140	0.02017	0.01880	0.01007
D8	3.08887	0.00016	-0.00785	0.03512	0.02726	3.11613
D9	0.00509	-0.00011	-0.00066	-0.00414	-0.00483	0.00026
D10	-0.00134	-0.00008	0.00732	-0.02016	-0.01287	-0.01421
D11	3.10026	0.00003	0.00619	-0.02829	-0.02210	3.07816
D12	0.00832	0.00011	-0.00143	0.00059	-0.00085	0.00747
D13	-3.09161	-0.00032	0.00339	-0.01623	-0.01283	-3.10444
D14	-3.09615	0.00003	-0.00173	0.01010	0.00834	-3.08781
D15	0.08710	-0.00041	0.00310	-0.00673	-0.00363	0.08346

D16	2.50387	-0.00033	0.00770	-0.00102	0.00668	2.51055
D17	-0.67519	-0.00025	0.00794	-0.01068	-0.00275	-0.67794
D18	-0.68003	0.00014	0.00016	0.02345	0.02362	-0.65641
D19	2.50363	-0.00029	0.00508	0.00654	0.01161	2.51524
D20	-1.18298	0.00036	0.05429	0.02301	0.07731	-1.10567
D21	0.97525	0.00012	0.05613	0.02328	0.07941	1.05466
D22	3.03753	-0.00016	0.05672	0.02268	0.07939	3.11692
D23	-1.18471	0.00035	0.05511	0.02288	0.07799	-1.10672
D24	0.97339	0.00012	0.05696	0.02345	0.08041	1.05380
D25	3.03567	-0.00016	0.05753	0.02304	0.08056	3.11623

Item	Value	Threshold	Converged?
Maximum Force	0.002700	0.000450	NO
RMS Force	0.000807	0.000300	NO
Maximum Displacement	0.171977	0.001800	NO
RMS Displacement	0.045436	0.001200	NO

Predicted change in Energy=-1.170710D-04
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 05:49:37 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.020094	0.673422	0.042685
2	6	0	3.337969	1.692688	0.113767
3	6	0	4.020294	-0.666046	-0.056757
4	6	0	2.138350	2.289846	0.162846
5	6	0	3.340965	-1.687251	-0.126439
6	6	0	0.911628	2.317767	0.171541
7	6	0	2.141690	-2.285679	-0.170736
8	6	0	-0.384795	1.974261	0.155600
9	6	0	0.915072	-2.317293	-0.169694
10	6	0	-1.461311	1.387149	0.118175
11	6	0	-0.382062	-1.977012	-0.138848
12	6	0	-2.672535	0.706349	0.051014
13	6	0	-1.460409	-1.394488	-0.086798
14	6	0	-2.672096	-0.711507	-0.058094
15	6	0	-3.909032	1.410192	0.147545
16	6	0	-3.907009	-1.415411	-0.173392
17	7	0	-3.725219	2.878298	-0.047415
18	7	0	-3.732387	-2.879038	0.057716
19	1	0	-3.469755	3.168875	-1.000359
20	1	0	-4.562361	3.377808	0.233015
21	1	0	-3.501559	-3.149754	1.022697

22	1	0	-4.563613	-3.382707	-0.232780
23	1	0	-2.955229	3.183979	0.550190
24	1	0	-4.738509	1.056328	-0.456357
25	1	0	-4.751259	-1.049492	0.401992
26	1	0	-2.948411	-3.199206	-0.513540

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.228516	0.000000			
3	C	1.343154	2.461356	0.000000		
4	C	2.483592	1.340930	3.511017	0.000000	
5	C	2.462234	3.388465	1.228496	4.165006	0.000000
6	C	3.518954	2.506230	4.314982	1.227070	4.693681
7	C	3.511442	4.164064	2.483013	4.587670	1.341021
8	C	4.594342	3.733632	5.140149	2.542815	5.231396
9	C	4.316323	4.693690	3.518775	4.778360	2.506747
10	C	5.528191	4.808998	5.856125	3.711390	5.707330
11	C	5.141666	5.231553	4.594139	4.964834	3.734307
12	C	6.692715	6.091220	6.832938	5.066022	6.474796
13	C	5.859089	5.709230	5.528981	5.156326	4.810454
14	C	6.834733	6.475381	6.692544	5.674268	6.092097
15	C	7.963972	7.252583	8.199190	6.111043	7.888705
16	C	8.200540	7.888754	7.963497	7.098474	7.253222
17	N	8.053537	7.163817	8.517948	5.896772	8.413170
18	N	8.527670	8.419843	8.063157	7.822657	7.175415
19	H	7.963232	7.054467	8.467458	5.794529	8.410208
20	H	9.000470	8.078927	9.492034	6.788822	9.393966
21	H	8.494254	8.429386	7.994517	7.882713	7.090808
22	H	9.497793	9.397591	9.005259	8.789236	8.085062
23	H	7.430719	6.482188	7.990557	5.185948	7.989291
24	H	8.781160	8.121545	8.935484	7.013997	8.538968
25	H	8.946181	8.546240	8.791906	7.659965	8.134498
26	H	7.991664	7.990164	7.428890	7.514142	6.480132

		6	7	8	9	10
6	C	0.000000				
7	C	4.777230	0.000000			
8	C	1.341255	4.963539	0.000000		
9	C	4.647605	1.227027	4.495876	0.000000	
10	C	2.549458	5.153130	1.226779	4.410550	0.000000
11	C	4.496121	2.542758	3.962230	1.341379	3.542374
12	C	3.931593	5.672580	2.617688	4.697024	1.391065
13	C	4.412951	3.711656	3.544597	2.549774	2.789178
14	C	4.698118	5.065890	3.534226	3.931764	2.429285
15	C	4.905408	7.097324	3.569101	6.104650	2.448006
16	C	6.105314	6.110985	4.899397	4.905697	3.731057
17	N	4.675734	7.816808	3.466544	6.967166	2.715921
18	N	6.970410	5.908388	5.896649	4.686805	4.833404

19	H	4.614569	7.869482	3.504328	7.072110	2.908524
20	H	5.576022	8.785352	4.407720	7.911929	3.686791
21	H	7.077745	5.832424	6.059835	4.649883	5.056111
22	H	7.914363	6.794734	6.805179	5.581673	5.700787
23	H	3.980739	7.511024	2.868144	6.764721	2.376348
24	H	5.823189	7.654262	4.491315	6.589876	3.343584
25	H	6.592407	7.026302	5.316934	5.834504	4.103843
26	H	6.768030	5.182777	5.812455	3.977751	4.862631

		11	12	13	14	15
11	C	0.000000				
12	C	3.533092	0.000000			
13	C	1.226734	2.429353	0.000000		
14	C	2.617686	1.422048	1.391212	0.000000	
15	C	4.898437	1.426057	3.730536	2.464529	0.000000
16	C	3.569571	2.464984	2.448221	1.426108	2.843771
17	N	5.895684	2.415615	4.836074	3.741107	1.492358
18	N	3.475193	3.738761	2.717841	2.415745	4.293806
19	H	6.062689	2.793739	5.069156	4.072037	2.145603
20	H	6.803476	3.277387	5.700807	4.514460	2.075008
21	H	3.529273	4.062139	2.911741	2.793057	4.661012
22	H	4.412501	4.514099	3.688387	3.277752	4.852319
23	H	5.807908	2.543176	4.858250	3.952845	2.053822
24	H	5.317950	2.155959	4.109624	2.748439	1.085334
25	H	4.499187	2.743584	3.344791	2.156115	2.612304
26	H	2.867107	3.955779	2.377660	2.544096	4.754616

		16	17	18	19	20
16	C	0.000000				
17	N	4.299401	0.000000			
18	N	1.492015	5.758300	0.000000		
19	H	4.678754	1.028493	6.145384	0.000000	
20	H	4.854854	1.014376	6.314089	1.660919	0.000000
21	H	2.145452	6.126383	1.028473	6.634669	6.660178
22	H	2.074828	6.319608	1.014399	6.686473	6.776543
23	H	4.752246	1.021498	6.132429	1.633759	1.649559
24	H	2.623157	2.124515	4.094345	2.523594	2.428072
25	H	1.085229	4.084391	2.122231	4.626387	4.434549
26	H	2.053420	6.144652	1.021498	6.407904	6.813171

		21	22	23	24	25
21	H	0.000000				
22	H	1.660857	0.000000			
23	H	6.374787	6.805975	0.000000		
24	H	4.626961	4.448101	2.952985	0.000000	
25	H	2.521533	2.425291	4.601082	2.274071	0.000000
26	H	1.633536	1.649659	6.471214	4.617064	2.951225

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]

Supporting Information file

Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=1 Diff= 2.83D-03
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.527942	-0.669295	-0.021151
2	6	0	3.847012	-1.691278	-0.054869
3	6	0	4.526575	0.672895	0.029710
4	6	0	2.648090	-2.291249	-0.081584
5	6	0	3.846048	1.695145	0.062754
6	6	0	1.421399	-2.320926	-0.088545
7	6	0	2.646074	2.293357	0.086049
8	6	0	0.124570	-1.978611	-0.084297
9	6	0	1.419417	2.323453	0.084580
10	6	0	-0.952635	-1.391810	-0.067532
11	6	0	0.122680	1.980735	0.066839
12	6	0	-2.164646	-0.710466	-0.024366
13	6	0	-0.954989	1.395425	0.036553
14	6	0	-2.165864	0.710411	0.033315
15	6	0	-3.400342	-1.418814	-0.094616
16	6	0	-3.401565	1.416559	0.123765
17	7	0	-3.214647	-2.878675	0.153284
18	7	0	-3.228840	2.871062	-0.160307
19	1	0	-2.958315	-3.134241	1.115978
20	1	0	-4.051336	-3.389012	-0.108379
21	1	0	-2.998863	3.106922	-1.134595
22	1	0	-4.060518	3.383933	0.112241
23	1	0	-2.444612	-3.204885	-0.433308
24	1	0	-4.229919	-1.044296	0.496558
25	1	0	-4.245683	1.029035	-0.437494
26	1	0	-2.444943	3.212644	0.398518

Rotational constants (GHZ): 0.6028419 0.2705958 0.1874567
Leave Link 202 at Sat Sep 26 05:49:37 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.0899698303 Hartrees.

Supporting Information file

IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0153778077 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.0745920226 Hartrees.
Leave Link 301 at Sat Sep 26 05:49:37 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23221 LenP2D= 51929.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.92D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 05:49:38 2026, MaxMem= 805306368 cpu: 6.4 elap: 1.1
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 05:49:39 2026, MaxMem= 805306368 cpu: 0.8 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000104 -0.000077 -0.000461 Ang= -0.05 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

Supporting Information file

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.981784764914
Leave Link 401 at Sat Sep 26 05:49:47 2026, MaxMem= 805306368 cpu: 51.9 elap: 8.7
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.408474762242
DIIS: error= 2.94D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.408474762242 IErMin= 1 ErrMin= 2.94D-03
ErrMax= 2.94D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.83D-03 BMatP= 5.83D-03
IDIUse=3 WtCom= 9.71D-01 WtEn= 2.94D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.704 Goal= None Shift= 0.000
GapD= 0.704 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=9.35D-03 MaxDP=3.53D-01 OVMax= 1.53D-02

Cycle 2 Pass 0 IDiag 1:
RMSU= 7.88D-03 CP: 1.48D+00
E= -723.413613863902 Delta-E= -0.005139101661 Rises=F Damp=F
DIIS: error= 7.27D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413613863902 IErMin= 2 ErrMin= 7.27D-04
ErrMax= 7.27D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-04 BMatP= 5.83D-03
IDIUse=3 WtCom= 9.93D-01 WtEn= 7.27D-03
Coeff-Com: -0.539D-01 0.105D+01
Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.535D-01 0.105D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=6.82D-03 MaxDP=2.36D-01 DE=-5.14D-03 OVMax= 4.21D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 4.69D-03 CP: 1.15D+00 5.44D-01
E= -723.413857256691 Delta-E= -0.000243392789 Rises=F Damp=F
DIIS: error= 4.75D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.413857256691 IErMin= 2 ErrMin= 7.27D-04
ErrMax= 4.75D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.21D-04 BMatP= 2.22D-04
IDIUse=3 WtCom= 1.27D-01 WtEn= 8.73D-01
Coeff-Com: -0.526D-01 0.768D+00 0.284D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: -0.667D-02 0.974D-01 0.909D+00
Gap= 0.181 Goal= None Shift= 0.000
RMSDP=7.37D+02 MaxDP=2.90D+04 DE=-2.43D-04 OVMax= 9.93D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.413652077515 Delta-E= 0.000205179176 Rises=F Damp=F
DIIS: error= 1.15D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413652077515 IErMin= 1 ErrMin= 1.15D-03
ErrMax= 1.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-04 BMatP= 2.26D-04
IDIUse=3 WtCom= 9.89D-01 WtEn= 1.15D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.181 Goal= None Shift= 0.000
GapD= 0.181 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=6.32D-03 MaxDP=1.60D-01 DE= 2.05D-04 OVMax= 2.86D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.64D-03 CP: 6.87D-01
E= -723.413785062930 Delta-E= -0.000132985415 Rises=F Damp=F
DIIS: error= 3.47D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413785062930 IErMin= 2 ErrMin= 3.47D-04
ErrMax= 3.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.04D-05 BMatP= 2.26D-04
IDIUse=3 WtCom= 9.97D-01 WtEn= 3.47D-03
Coeff-Com: 0.147D+00 0.853D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.146D+00 0.854D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.22D-04 MaxDP=1.57D-02 DE=-1.33D-04 OVMax= 3.98D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.56D-04 CP: 6.92D-01 1.04D+00
E= -723.413758226758 Delta-E= 0.000026836171 Rises=F Damp=F

DIIS: error= 4.90D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413785062930 IErMin= 2 ErrMin= 3.47D-04
ErrMax= 4.90D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.37D-05 BMatP= 3.04D-05
IDIUse=3 WtCom= 3.11D-01 WtEn= 6.89D-01
Coeff-Com: -0.176D-01 0.578D+00 0.439D+00
Coeff-En: 0.000D+00 0.612D+00 0.388D+00
Coeff: -0.547D-02 0.602D+00 0.404D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=7.19D-05 MaxDP=3.75D-03 DE= 2.68D-05 OVMax= 2.04D-03

Cycle 7 Pass 1 IDiag 1:
RMSU= 2.78D-05 CP: 6.93D-01 1.05D+00 1.21D+00
E= -723.413821331513 Delta-E= -0.000063104755 Rises=F Damp=F
DIIS: error= 3.74D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413821331513 IErMin= 4 ErrMin= 3.74D-05
ErrMax= 3.74D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.28D-07 BMatP= 3.04D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.116D-01 0.236D+00 0.146D+00 0.630D+00
Coeff: -0.116D-01 0.236D+00 0.146D+00 0.630D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.67D-05 MaxDP=1.75D-03 DE=-6.31D-05 OVMax= 3.09D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 8.29D-06 CP: 6.94D-01 1.05D+00 1.29D+00 1.17D+00
E= -723.413821989682 Delta-E= -0.000000658169 Rises=F Damp=F
DIIS: error= 1.02D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413821989682 IErMin= 5 ErrMin= 1.02D-05
ErrMax= 1.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.19D-08 BMatP= 5.28D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.480D-04-0.347D-01-0.338D-01 0.170D+00 0.899D+00
Coeff: -0.480D-04-0.347D-01-0.338D-01 0.170D+00 0.899D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.88D-05 MaxDP=1.32D-03 DE=-6.58D-07 OVMax= 2.97D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 3.95D-06 CP: 6.94D-01 1.05D+00 1.34D+00 1.28D+00 1.88D+00
E= -723.413822152302 Delta-E= -0.000000162619 Rises=F Damp=F
DIIS: error= 6.40D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413822152302 IErMin= 6 ErrMin= 6.40D-06
ErrMax= 6.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-08 BMatP= 5.19D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.252D-02-0.711D-01-0.504D-01-0.379D-01 0.477D+00 0.680D+00
Coeff: 0.252D-02-0.711D-01-0.504D-01-0.379D-01 0.477D+00 0.680D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=6.54D-06 MaxDP=4.83D-04 DE=-1.63D-07 OVMax= 2.10D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.25D-06 CP: 6.94D-01 1.05D+00 1.36D+00 1.31D+00 2.31D+00

CP: 1.51D+00
E= -723.413822213489 Delta-E= -0.000000061187 Rises=F Damp=F
DIIS: error= 4.20D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413822213489 IErMin= 7 ErrMin= 4.20D-06
ErrMax= 4.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-09 BMatP= 2.03D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.104D-02-0.230D-01-0.146D-01-0.429D-01 0.186D-01 0.297D+00
Coeff-Com: 0.763D+00
Coeff: 0.104D-02-0.230D-01-0.146D-01-0.429D-01 0.186D-01 0.297D+00
Coeff: 0.763D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.12D-06 MaxDP=1.09D-04 DE=-6.12D-08 OVMax= 1.34D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 5.95D-07 CP: 6.94D-01 1.05D+00 1.35D+00 1.32D+00 2.44D+00
CP: 1.81D+00 1.83D+00
E= -723.413822233479 Delta-E= -0.000000019990 Rises=F Damp=F
DIIS: error= 2.45D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413822233479 IErMin= 8 ErrMin= 2.45D-06
ErrMax= 2.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-09 BMatP= 3.96D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.689D-03 0.217D-01 0.160D-01 0.324D-02-0.208D+00-0.159D+00
Coeff-Com: 0.275D+00 0.105D+01
Coeff: -0.689D-03 0.217D-01 0.160D-01 0.324D-02-0.208D+00-0.159D+00
Coeff: 0.275D+00 0.105D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.45D-06 MaxDP=1.33D-04 DE=-2.00D-08 OVMax= 1.39D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 3.32D-07 CP: 6.94D-01 1.05D+00 1.35D+00 1.32D+00 2.50D+00
CP: 2.02D+00 2.67D+00 2.24D+00
E= -723.413822244270 Delta-E= -0.000000010791 Rises=F Damp=F
DIIS: error= 1.40D-06 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413822244270 IErMin= 9 ErrMin= 1.40D-06
ErrMax= 1.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-10 BMatP= 1.13D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.560D-03 0.156D-01 0.111D-01 0.111D-01-0.109D+00-0.132D+00
Coeff-Com: -0.873D-02 0.503D+00 0.709D+00
Coeff: -0.560D-03 0.156D-01 0.111D-01 0.111D-01-0.109D+00-0.132D+00
Coeff: -0.873D-02 0.503D+00 0.709D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.08D-07 MaxDP=3.80D-05 DE=-1.08D-08 OVMax= 5.52D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.73D-07 CP: 6.94D-01 1.05D+00 1.35D+00 1.31D+00 2.49D+00
CP: 2.04D+00 2.92D+00 2.66D+00 1.59D+00
E= -723.413822246373 Delta-E= -0.000000002103 Rises=F Damp=F
DIIS: error= 8.50D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -723.413822246373 IErMin=10 ErrMin= 8.50D-07
ErrMax= 8.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.00D-10 BMatP= 3.39D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.251D-04-0.163D-02-0.143D-02 0.376D-02 0.295D-01 0.914D-02
Coeff-Com: -0.101D+00-0.204D+00 0.314D+00 0.951D+00
Coeff: 0.251D-04-0.163D-02-0.143D-02 0.376D-02 0.295D-01 0.914D-02
Coeff: -0.101D+00-0.204D+00 0.314D+00 0.951D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=5.29D-07 MaxDP=2.93D-05 DE=-2.10D-09 OVMax= 4.23D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 1.03D-07 CP: 6.94D-01 1.05D+00 1.35D+00 1.31D+00 2.47D+00
CP: 2.02D+00 3.00D+00 2.86D+00 2.19D+00 2.32D+00
E= -723.413822247239 Delta-E= -0.000000000867 Rises=F Damp=F
DIIS: error= 3.68D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413822247239 IErMin=11 ErrMin= 3.68D-07
ErrMax= 3.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.40D-11 BMatP= 1.00D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.152D-03-0.472D-02-0.353D-02-0.808D-03 0.414D-01 0.386D-01
Coeff-Com: -0.515D-01-0.248D+00-0.148D-01 0.521D+00 0.722D+00
Coeff: 0.152D-03-0.472D-02-0.353D-02-0.808D-03 0.414D-01 0.386D-01
Coeff: -0.515D-01-0.248D+00-0.148D-01 0.521D+00 0.722D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.14D-07 MaxDP=1.37D-05 DE=-8.67D-10 OVMax= 2.01D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 4.49D-08 CP: 6.94D-01 1.05D+00 1.35D+00 1.31D+00 2.46D+00
CP: 2.01D+00 3.00D+00 2.91D+00 2.46D+00 2.97D+00
CP: 1.60D+00
E= -723.413822247433 Delta-E= -0.000000000194 Rises=F Damp=F
DIIS: error= 1.92D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413822247433 IErMin=12 ErrMin= 1.92D-07
ErrMax= 1.92D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.01D-12 BMatP= 3.40D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.233D-04-0.520D-03-0.350D-03-0.989D-03 0.807D-03 0.617D-02
Coeff-Com: 0.167D-01-0.649D-03-0.834D-01-0.125D+00 0.142D+00 0.105D+01
Coeff: 0.233D-04-0.520D-03-0.350D-03-0.989D-03 0.807D-03 0.617D-02
Coeff: 0.167D-01-0.649D-03-0.834D-01-0.125D+00 0.142D+00 0.105D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.17D-07 MaxDP=8.73D-06 DE=-1.94D-10 OVMax= 9.56D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 6.48D-08 CP: 6.94D-01 1.05D+00 1.35D+00 1.31D+00 2.46D+00
CP: 2.00D+00 3.00D+00 2.88D+00 2.55D+00 3.00D+00
CP: 1.85D+00 2.01D+00
E= -723.413822247472 Delta-E= -0.000000000039 Rises=F Damp=F
DIIS: error= 8.94D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.413822247472 IErMin=13 ErrMin= 8.94D-08

ErrMax= 8.94D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-12 BMatP= 4.01D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.217D-04 0.772D-03 0.596D-03-0.345D-03-0.862D-02-0.535D-02
Coeff-Com: 0.199D-01 0.530D-01-0.387D-01-0.170D+00-0.801D-01 0.496D+00
Coeff-Com: 0.733D+00
Coeff: -0.217D-04 0.772D-03 0.596D-03-0.345D-03-0.862D-02-0.535D-02
Coeff: 0.199D-01 0.530D-01-0.387D-01-0.170D+00-0.801D-01 0.496D+00
Coeff: 0.733D+00
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=4.60D-08 MaxDP=2.85D-06 DE=-3.89D-11 OVMax= 3.42D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 1.06D-08   CP: 6.94D-01 1.05D+00 1.35D+00 1.31D+00 2.46D+00
                CP: 2.00D+00 3.00D+00 2.85D+00 2.56D+00 3.00D+00
                CP: 1.94D+00 2.56D+00 1.40D+00
E= -723.413822247470   Delta-E=   0.000000000002 Rises=F Damp=F
DIIS: error= 4.15D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=13 EnMin= -723.413822247472   IErMin=14 ErrMin= 4.15D-08
ErrMax= 4.15D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.30D-13 BMatP= 1.37D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.144D-04 0.448D-03 0.335D-03 0.208D-04-0.388D-02-0.369D-02
Coeff-Com: 0.524D-02 0.230D-01 0.437D-03-0.463D-01-0.578D-01-0.137D-01
Coeff-Com: 0.306D+00 0.790D+00
Coeff: -0.144D-04 0.448D-03 0.335D-03 0.208D-04-0.388D-02-0.369D-02
Coeff: 0.524D-02 0.230D-01 0.437D-03-0.463D-01-0.578D-01-0.137D-01
Coeff: 0.306D+00 0.790D+00
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=2.67D-08 MaxDP=1.70D-06 DE= 2.05D-12 OVMax= 1.61D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 4.76D-09   CP: 6.94D-01 1.05D+00 1.35D+00 1.31D+00 2.46D+00
                CP: 2.00D+00 3.00D+00 2.84D+00 2.55D+00 3.00D+00
                CP: 1.97D+00 2.87D+00 1.54D+00 1.86D+00
E= -723.413822247462   Delta-E=   0.000000000009 Rises=F Damp=F
DIIS: error= 2.94D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=13 EnMin= -723.413822247472   IErMin=15 ErrMin= 2.94D-08
ErrMax= 2.94D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-13 BMatP= 3.30D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.304D-05-0.135D-03-0.109D-03 0.130D-03 0.205D-02 0.651D-03
Coeff-Com: -0.601D-02-0.125D-01 0.159D-01 0.510D-01 0.134D-01-0.220D+00
Coeff-Com: -0.188D+00 0.339D+00 0.100D+01
Coeff: 0.304D-05-0.135D-03-0.109D-03 0.130D-03 0.205D-02 0.651D-03
Coeff: -0.601D-02-0.125D-01 0.159D-01 0.510D-01 0.134D-01-0.220D+00
Coeff: -0.188D+00 0.339D+00 0.100D+01
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=2.67D-08 MaxDP=1.67D-06 DE= 8.64D-12 OVMax= 1.40D-06

Cycle 19 Pass 1 IDiag 1:

Supporting Information file

RMSU= 5.77D-09 CP: 6.94D-01 1.05D+00 1.35D+00 1.31D+00 2.46D+00
CP: 2.00D+00 3.00D+00 2.82D+00 2.55D+00 3.00D+00
CP: 1.99D+00 3.00D+00 1.65D+00 2.71D+00 2.02D+00
E= -723.413822247474 Delta-E= -0.000000000012 Rises=F Damp=F
DIIS: error= 8.83D-09 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.413822247474 IErMin=16 ErrMin= 8.83D-09
ErrMax= 8.83D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-14 BMatP= 1.04D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.386D-05-0.136D-03-0.104D-03 0.329D-04 0.155D-02 0.905D-03
Coeff-Com: -0.345D-02-0.937D-02 0.583D-02 0.297D-01 0.182D-01-0.879D-01
Coeff-Com: -0.137D+00-0.143D-01 0.412D+00 0.784D+00
Coeff: 0.386D-05-0.136D-03-0.104D-03 0.329D-04 0.155D-02 0.905D-03
Coeff: -0.345D-02-0.937D-02 0.583D-02 0.297D-01 0.182D-01-0.879D-01
Coeff: -0.137D+00-0.143D-01 0.412D+00 0.784D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=9.69D-09 MaxDP=5.56D-07 DE=-1.23D-11 OVMax= 5.37D-07

SCF Done: E(RwB97XD) = -723.413822247 A.U. after 19 cycles
NFock= 19 Conv=0.97D-08 -V/T= 2.0047
KE= 7.200567496870D+02 PE=-3.701208598876D+03 EE= 1.247663434919D+03
Leave Link 502 at Sat Sep 26 06:12:06 2026, MaxMem= 805306368 cpu: 8030.1 elap: 1338.8
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23221 LenP2D= 51929.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 06:12:07 2026, MaxMem= 805306368 cpu: 2.9 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 06:12:07 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.

Supporting Information file

Leave Link 703 at Sat Sep 26 06:23:04 2026, MaxMem= 805306368 cpu: 3945.1 elap: 657.6
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.51309243D+00-1.88086569D-02-2.27680221D-02
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000009636	-0.001145148	-0.000333890
2	6	-0.000170991	0.001054933	0.000253102
3	6	0.000031370	0.001131487	0.000262680
4	6	0.000562598	-0.001162034	-0.000276220
5	6	-0.000235279	-0.001025659	-0.000310116
6	6	-0.000605457	0.001001091	0.000471828
7	6	0.000625589	0.001144790	0.000318134
8	6	0.000582189	-0.000246819	0.000269604
9	6	-0.000740039	-0.000997797	0.000116572
10	6	-0.000580211	-0.000291102	-0.001322443
11	6	0.000647355	0.000063890	0.000372432
12	6	0.000677751	0.001410711	0.001394975
13	6	-0.000499390	0.000616831	-0.001386178
14	6	0.000390399	-0.001889647	0.000618376
15	6	-0.000643360	0.001456955	-0.000577036
16	6	-0.000564732	-0.001231074	0.000611838
17	7	0.000562175	-0.001340599	-0.000124084
18	7	0.000815559	0.001150815	-0.000519334
19	1	-0.000118191	0.000100788	-0.000035383
20	1	-0.000100223	0.000057922	-0.000084818
21	1	-0.000144175	0.000009428	0.000159661
22	1	-0.000048700	-0.000089330	0.000051191
23	1	-0.000104757	-0.000065541	0.000246580
24	1	-0.000122549	-0.000368633	0.000252806
25	1	-0.000090342	0.000650124	-0.000111080
26	1	-0.000116952	0.000003618	-0.000319199

Cartesian Forces: Max 0.001889647 RMS 0.000684588
Leave Link 716 at Sat Sep 26 06:23:04 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001369343 RMS 0.000453872
Search for a local minimum.
Step number 21 out of a maximum of 103

Supporting Information file

All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .45387D-03 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 19 20 21
DE= -6.02D-05 DEPred=-1.17D-04 R= 5.14D-01
TightC=F SS= 1.41D+00 RLast= 2.10D-01 DXNew= 1.3552D+00 6.2885D-01
Trust test= 5.14D-01 RLast= 2.10D-01 DXMaxT set to 8.06D-01
ITU= 1 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 0 0 1
ITU= 0
Eigenvalues --- 0.00275 0.00485 0.01008 0.01231 0.01700
Eigenvalues --- 0.01829 0.02673 0.02794 0.02928 0.03038
Eigenvalues --- 0.03301 0.03661 0.03781 0.03915 0.04363
Eigenvalues --- 0.04458 0.04555 0.05026 0.05604 0.07453
Eigenvalues --- 0.09948 0.10106 0.11083 0.11205 0.11554
Eigenvalues --- 0.11795 0.13838 0.15282 0.15538 0.15875
Eigenvalues --- 0.16000 0.16002 0.16086 0.16190 0.16720
Eigenvalues --- 0.21979 0.22501 0.24872 0.24988 0.24991
Eigenvalues --- 0.25000 0.25001 0.25003 0.25191 0.28718
Eigenvalues --- 0.30010 0.35748 0.37237 0.38742 0.43526
Eigenvalues --- 0.45810 0.46168 0.47095 0.47627 0.47688
Eigenvalues --- 0.47690 0.47825 0.48351 0.51712 0.53308
Eigenvalues --- 0.54807 0.55555 0.55641 0.55660 0.56721
Eigenvalues --- 0.92887 0.93710 0.95031 0.95422 0.97725
Eigenvalues --- 0.98898 1.37234
En-DIIS/RFO-DIIS/Sim-DIIS IScMMF= -3 using points: 21 20
RFO step: Lambda=-1.98255500D-04.
NNeg= 0 NGDIIS= 2 SimSw= 2.50D-01 Rises=F DC= -6.02D-05 SmlDif= 1.00D-05
NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj= 3.0
RMS Error= 0.9431283302D-02 NUsed= 2 OKEnD=T EnDIS=F
InvSVX: RCond= 4.36D-02 Info= 0 Equed=N FErr= 1.42D-15 BErr= 5.55D-17
DidBck=T Rises=F RFO-DIIS coefs: 0.73764 0.26236
Iteration 1 RMS(Cart)= 0.02243956 RMS(Int)= 0.00028854
Iteration 2 RMS(Cart)= 0.00040677 RMS(Int)= 0.00002471
Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00002471
ITry= 1 IFail=0 DXMaxC= 8.15D-02 DCOld= 1.00D+10 DXMaxT= 8.06D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.32156	0.00046	-0.00025	0.00114	0.00089	2.32245
R2	2.53819	-0.00061	0.00023	-0.00173	-0.00149	2.53670
R3	2.53399	-0.00038	0.00034	-0.00154	-0.00120	2.53279
R4	2.32152	0.00046	-0.00026	0.00113	0.00088	2.32240
R5	2.31883	0.00041	-0.00029	0.00110	0.00082	2.31964
R6	2.53416	-0.00042	0.00033	-0.00159	-0.00126	2.53290
R7	2.53460	-0.00011	0.00036	-0.00118	-0.00082	2.53378
R8	2.31874	0.00042	-0.00030	0.00111	0.00081	2.31955
R9	2.31828	0.00039	-0.00012	0.00069	0.00056	2.31884

R10	2.53484	-0.00024	0.00034	-0.00130	-0.00097	2.53387
R11	2.62873	-0.00031	0.00024	-0.00120	-0.00097	2.62777
R12	2.31819	0.00039	-0.00016	0.00072	0.00055	2.31874
R13	2.68728	0.00108	-0.00099	0.00407	0.00307	2.69035
R14	2.69486	0.00036	0.00108	-0.00250	-0.00142	2.69344
R15	2.62901	-0.00031	0.00033	-0.00135	-0.00103	2.62798
R16	2.69495	-0.00010	0.00074	-0.00305	-0.00232	2.69264
R17	2.82015	-0.00120	0.00102	-0.00452	-0.00351	2.81664
R18	2.05098	0.00007	0.00040	-0.00116	-0.00077	2.05022
R19	2.81950	-0.00109	0.00099	-0.00449	-0.00349	2.81601
R20	2.05078	0.00023	0.00038	-0.00089	-0.00051	2.05028
R21	1.94357	0.00003	0.00077	-0.00121	-0.00044	1.94313
R22	1.91689	0.00009	0.00026	-0.00034	-0.00008	1.91681
R23	1.93035	0.00005	-0.00018	0.00013	-0.00005	1.93030
R24	1.94353	0.00011	0.00078	-0.00111	-0.00033	1.94320
R25	1.91694	0.00007	0.00027	-0.00042	-0.00015	1.91678
R26	1.93035	0.00009	-0.00016	0.00018	0.00001	1.93036
A1	2.55307	0.00036	0.00050	0.00053	0.00104	2.55411
A2	2.62262	-0.00035	-0.00106	0.00021	-0.00085	2.62177
A3	2.55548	0.00032	0.00037	0.00044	0.00082	2.55630
A4	2.70160	0.00063	0.00162	-0.00000	0.00160	2.70320
A5	2.62065	-0.00033	-0.00101	0.00007	-0.00094	2.61971
A6	2.85919	-0.00088	-0.00110	-0.00156	-0.00270	2.85649
A7	2.70329	0.00057	0.00149	-0.00027	0.00119	2.70448
A8	2.85843	-0.00091	-0.00114	-0.00180	-0.00299	2.85544
A9	2.08449	0.00001	0.00065	-0.00103	-0.00049	2.08400
A10	2.10616	0.00029	-0.00076	0.00235	0.00158	2.10775
A11	2.09159	-0.00027	0.00020	-0.00074	-0.00054	2.09105
A12	2.08441	0.00011	0.00057	-0.00068	-0.00019	2.08422
A13	2.09216	-0.00041	0.00011	-0.00123	-0.00108	2.09108
A14	2.10622	0.00029	-0.00079	0.00177	0.00102	2.10724
A15	2.05340	-0.00013	-0.00206	0.00530	0.00324	2.05664
A16	1.92004	0.00044	-0.00365	0.00856	0.00492	1.92496
A17	2.05370	-0.00049	-0.00186	0.00618	0.00432	2.05803
A18	1.91738	0.00137	-0.00274	0.01305	0.01031	1.92769
A19	2.01482	0.00018	-0.00013	-0.00064	-0.00077	2.01405
A20	1.92481	-0.00005	-0.00036	0.00036	-0.00000	1.92481
A21	1.88683	-0.00016	0.00255	-0.00274	-0.00019	1.88664
A22	1.89865	-0.00014	-0.00012	-0.00037	-0.00049	1.89816
A23	1.84448	0.00019	-0.00094	0.00234	0.00140	1.84588
A24	1.88913	-0.00003	-0.00108	0.00124	0.00016	1.88929
A25	2.01508	-0.00003	-0.00030	-0.00095	-0.00125	2.01383
A26	1.92497	0.00003	-0.00039	0.00037	-0.00001	1.92495
A27	1.88669	-0.00008	0.00272	-0.00272	-0.00000	1.88669
A28	1.89854	-0.00010	-0.00006	-0.00034	-0.00041	1.89814
A29	1.84414	0.00028	-0.00085	0.00261	0.00176	1.84590
A30	1.88927	-0.00010	-0.00119	0.00125	0.00005	1.88933
A31	2.90066	0.00015	0.00035	0.00202	0.00230	2.90295

A32	3.12763	0.00002	-0.00100	-0.00046	-0.00155	3.12608
A33	2.90222	0.00010	0.00001	0.00043	0.00037	2.90259
A34	3.12494	0.00023	-0.00018	0.00289	0.00262	3.12756
A35	3.97344	0.00031	-0.00571	0.01387	0.00816	3.98159
A36	3.97109	0.00087	-0.00460	0.01923	0.01463	3.98572
A37	3.14346	0.00033	0.00036	0.00107	0.00140	3.14487
A38	3.15908	-0.00106	-0.00618	-0.02649	-0.03268	3.12640
A39	3.14519	-0.00022	-0.00010	-0.00064	-0.00072	3.14447
A40	3.11792	0.00133	0.00758	0.02380	0.03139	3.14931
A41	4.02410	0.00088	0.00374	-0.01538	-0.01164	4.01246
A42	4.02576	0.00019	0.00232	-0.01218	-0.00987	4.01589
D1	0.01922	-0.00024	0.00064	-0.00483	-0.00419	0.01503
D2	-0.01571	0.00010	-0.00097	0.00283	0.00186	-0.01385
D3	-0.00855	-0.00030	-0.00178	-0.00257	-0.00433	-0.01288
D4	0.01598	0.00025	0.00169	-0.00102	0.00067	0.01665
D5	0.00381	-0.00032	-0.00001	-0.00331	-0.00330	0.00051
D6	-0.01612	0.00041	0.00066	0.00596	0.00660	-0.00951
D7	0.01007	-0.00018	-0.00493	-0.01390	-0.01882	-0.00874
D8	3.11613	-0.00012	-0.00715	-0.01881	-0.02596	3.09017
D9	0.00026	0.00029	0.00127	0.00095	0.00221	0.00246
D10	-0.01421	-0.00002	0.00338	0.01712	0.02048	0.00627
D11	3.07816	0.00037	0.00580	0.02999	0.03579	3.11396
D12	0.00747	0.00005	0.00022	-0.00048	-0.00025	0.00722
D13	-3.10444	0.00052	0.00337	0.00483	0.00819	-3.09625
D14	-3.08781	-0.00067	-0.00219	-0.01471	-0.01689	-3.10470
D15	0.08346	-0.00020	0.00095	-0.00941	-0.00845	0.07501
D16	2.51055	-0.00004	-0.00175	0.00913	0.00736	2.51791
D17	-0.67794	0.00068	0.00072	0.02345	0.02418	-0.65376
D18	-0.65641	-0.00061	-0.00620	-0.00226	-0.00846	-0.66487
D19	2.51524	-0.00013	-0.00305	0.00315	0.00011	2.51535
D20	-1.10567	-0.00002	-0.02028	0.00415	-0.01614	-1.12181
D21	1.05466	-0.00012	-0.02083	0.00345	-0.01738	1.03728
D22	3.11692	-0.00027	-0.02083	0.00353	-0.01730	3.09962
D23	-1.10672	0.00001	-0.02046	0.00443	-0.01603	-1.12275
D24	1.05380	-0.00011	-0.02110	0.00355	-0.01754	1.03626
D25	3.11623	-0.00027	-0.02114	0.00365	-0.01749	3.09875

Item	Value	Threshold	Converged?
Maximum Force	0.001369	0.000450	NO
RMS Force	0.000454	0.000300	NO
Maximum Displacement	0.081457	0.001800	NO
RMS Displacement	0.022449	0.001200	NO

Predicted change in Energy=-9.991569D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 06:23:04 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Supporting Information file

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.019226	0.665356	0.055078
2	6	0	3.339327	1.686827	0.123987
3	6	0	4.017565	-0.673428	-0.042888
4	6	0	2.141198	2.285976	0.167591
5	6	0	3.337380	-1.694526	-0.113995
6	6	0	0.914125	2.318413	0.167857
7	6	0	2.137812	-2.290547	-0.162388
8	6	0	-0.382066	1.976517	0.139598
9	6	0	0.910761	-2.321149	-0.169920
10	6	0	-1.460454	1.393099	0.090423
11	6	0	-0.384733	-1.975786	-0.151435
12	6	0	-2.672075	0.711726	0.053733
13	6	0	-1.461642	-1.389081	-0.110977
14	6	0	-2.672694	-0.707900	-0.053509
15	6	0	-3.907415	1.414867	0.158727
16	6	0	-3.908661	-1.410611	-0.147717
17	7	0	-3.732095	2.879625	-0.054212
18	7	0	-3.722097	-2.875879	0.049215
19	1	0	-3.486218	3.159622	-1.012578
20	1	0	-4.569423	3.378490	0.226659
21	1	0	-3.459437	-3.162807	1.001097
22	1	0	-4.561046	-3.376978	-0.222646
23	1	0	-2.959089	3.195493	0.534085
24	1	0	-4.749433	1.048761	-0.419236
25	1	0	-4.743479	-1.051741	0.445097
26	1	0	-2.956824	-3.182261	-0.554075

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.228989	0.000000			
3	C	1.342364	2.461434	0.000000		
4	C	2.483155	1.340296	3.510431	0.000000	
5	C	2.462223	3.389718	1.228963	4.165878	0.000000
6	C	3.519513	2.506478	4.315886	1.227502	4.696306
7	C	3.510608	4.164751	2.482504	4.588405	1.340353
8	C	4.593218	3.732683	5.139286	2.542323	5.232126
9	C	4.316525	4.695549	3.518999	4.780532	2.506843
10	C	5.527907	4.808877	5.856364	3.711480	5.709153
11	C	5.139371	5.230604	4.592184	4.964345	3.732913
12	C	6.691462	6.090379	6.832224	5.065454	6.475472
13	C	5.855612	5.706638	5.526166	5.154037	4.808734
14	C	6.832233	6.473841	6.690357	5.673248	6.090820

15	C	7.962672	7.251926	8.197983	6.111025	7.888584
16	C	8.197692	7.886778	7.961124	7.096828	7.251680
17	N	8.062127	7.173529	8.525347	5.907384	8.420446
18	N	8.512841	8.407591	8.047462	7.812617	7.159501
19	H	7.980785	7.074529	8.481706	5.815829	8.422096
20	H	9.008630	8.088299	9.498793	6.799228	9.400483
21	H	8.454595	8.397110	7.949369	7.858185	7.042443
22	H	9.488870	9.390322	8.996336	8.783018	8.076359
23	H	7.438274	6.489553	7.998447	5.193695	7.998614
24	H	8.789844	8.132051	8.942474	7.025373	8.544902
25	H	8.937870	8.540176	8.782775	7.656118	8.125641
26	H	7.990025	7.988072	7.429513	7.510809	6.482595

		6	7	8	9	10
6	C	0.000000				
7	C	4.780061	0.000000			
8	C	1.340821	4.964756	0.000000		
9	C	4.651843	1.227455	4.498570	0.000000	
10	C	2.549672	5.155645	1.227076	4.414304	0.000000
11	C	4.497680	2.542131	3.963005	1.340867	3.544722
12	C	3.931323	5.674096	2.617482	4.699476	1.390554
13	C	4.412202	3.710977	3.543376	2.549613	2.789460
14	C	4.698175	5.065332	3.534171	3.931574	2.429905
15	C	4.905479	7.097744	3.569860	6.105788	2.448011
16	C	6.104463	6.110183	4.898169	4.904733	3.729774
17	N	4.685256	7.822926	3.475034	6.972629	2.718645
18	N	6.963426	5.892871	5.891496	4.671095	4.831242
19	H	4.632934	7.877618	3.516107	7.076888	2.905329
20	H	5.585384	8.790696	4.416681	7.916791	3.691345
21	H	7.061594	5.783055	6.051863	4.601989	5.057819
22	H	7.909960	6.786653	6.801103	5.572991	5.697834
23	H	3.988130	7.520645	2.877946	6.775301	2.385659
24	H	5.833745	7.658400	4.499658	6.592136	3.345998
25	H	6.591151	7.018250	5.318420	5.827527	4.108684
26	H	6.764824	5.186896	5.807198	3.980868	4.856791

		11	12	13	14	15
11	C	0.000000				
12	C	3.535074	0.000000			
13	C	1.227026	2.430158	0.000000		
14	C	2.617611	1.423672	1.390667	0.000000	
15	C	4.899185	1.425305	3.730505	2.464898	0.000000
16	C	3.568964	2.464557	2.447389	1.424883	2.842047
17	N	5.898245	2.415591	4.835290	3.740678	1.490502
18	N	3.462431	3.738111	2.710330	2.410794	4.296141
19	H	6.060791	2.791423	5.059890	4.066862	2.143253
20	H	6.806090	3.277417	5.701055	4.513830	2.073328
21	H	3.491582	4.065642	2.893786	2.785269	4.676042
22	H	4.405677	4.512438	3.683817	3.273905	4.851232
23	H	5.817162	2.546019	4.865878	3.957748	2.052034

```
  24  H    5.316974   2.157014   4.104591   2.744533   1.084928
  25  H    4.495372   2.748398   3.345664   2.157541   2.620146
  26  H    2.869382   3.951411   2.376426   2.540424   4.748188
                16         17         18         19         20
  16  C    0.000000
  17  N    4.294886   0.000000
  18  N    1.490167   5.756442   0.000000
  19  H    4.670489   1.028261   6.132725   0.000000
  20  H    4.848944   1.014334   6.313999   1.660405   0.000000
  21  H    2.142841   6.139952   1.028299   6.635414   6.679850
  22  H    2.073118   6.313526   1.014319   6.671311   6.770399
  23  H    4.752129   1.021471   6.138309   1.634417   1.649598
  24  H    2.613260   2.126096   4.083829   2.530515   2.424299
  25  H    1.084959   4.089969   2.127774   4.630453   4.439027
  26  H    2.051796   6.131669   1.021505   6.380436   6.800991
                21         22         23         24         25
  21  H    0.000000
  22  H    1.660409   0.000000
  23  H    6.395032   6.807076   0.000000
  24  H    4.628039   4.434107   2.953407   0.000000
  25  H    2.532687   2.426085   4.607706   2.271390   0.000000
  26  H    1.634490   1.649632   6.469918   4.597083   2.954589
                26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=0 Diff= 4.47D-03
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.525407   -0.674638   -0.028382
    2          6           0        3.843832   -1.696786   -0.061273
    3          6           0        4.525939    0.666789    0.021777
    4          6           0        2.644724   -2.295120   -0.084283
    5          6           0        3.847430    1.690901    0.055970
    6          6           0        1.417598   -2.325510   -0.084210
    7          6           0        2.648836    2.290258    0.082275
    8          6           0        0.121968   -1.980672   -0.069028
    9          6           0        1.421835    2.323146    0.087891
   10          6           0       -0.955467   -1.394083   -0.041411
   11          6           0        0.125772    1.979495    0.080869
   12          6           0       -2.165963   -0.709825   -0.029853
```

13	6	0	-0.952097	1.393507	0.060641
14	6	0	-2.164258	0.712722	0.026694
15	6	0	-3.402419	-1.414212	-0.110529
16	6	0	-3.399098	1.420395	0.094955
17	7	0	-3.229693	-2.870733	0.154628
18	7	0	-3.209950	2.877396	-0.153981
19	1	0	-2.984871	-3.116781	1.122534
20	1	0	-4.067688	-3.377908	-0.108833
21	1	0	-2.946228	3.129758	-1.115315
22	1	0	-4.048219	3.389264	0.099275
23	1	0	-2.456863	-3.208663	-0.421514
24	1	0	-4.244172	-1.026330	0.453447
25	1	0	-4.234158	1.041998	-0.485241
26	1	0	-2.444530	3.203828	0.438510

Rotational constants (GHZ): 0.6027584 0.2707562 0.1875145
Leave Link 202 at Sat Sep 26 06:23:04 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.2432956741 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0153780413 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.2279176327 Hartrees.
Leave Link 301 at Sat Sep 26 06:23:04 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23222 LenP2D= 51945.

Supporting Information file

LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.90D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 06:23:05 2026, MaxMem= 805306368 cpu: 5.6 elap: 0.9
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 06:23:05 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 0.999999 -0.000003 0.000115 0.001039 Ang= -0.12 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.982004943443
Leave Link 401 at Sat Sep 26 06:23:13 2026, MaxMem= 805306368 cpu: 43.8 elap: 7.3
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.

Supporting Information file

```
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
      NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
      wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
      NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
Symmetry not used in FoFCou.
E= -723.411675113169
DIIS: error= 2.37D-03 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -723.411675113169     IErMin= 1 ErrMin= 2.37D-03
ErrMax= 2.37D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.39D-03 BMatP= 4.39D-03
IDIUse=3 WtCom= 9.76D-01 WtEn= 2.37D-02
Coeff-Com:  0.100D+01
Coeff-En:   0.100D+01
Coeff:      0.100D+01
Gap=     0.704 Goal=   None    Shift=    0.000
GapD=    0.704 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=8.58D-03 MaxDP=3.20D-01              OVMax= 8.73D-03

Cycle   2  Pass 0  IDiag  1:
RMSU=  7.25D-03    CP:  1.43D+00
E= -723.413863349286     Delta-E=       -0.002188236118 Rises=F Damp=F
DIIS: error= 7.34D-04 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.413863349286     IErMin= 2 ErrMin= 7.34D-04
ErrMax= 7.34D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-04 BMatP= 4.39D-03
IDIUse=3 WtCom= 9.93D-01 WtEn= 7.34D-03
Coeff-Com:  0.453D-03 0.100D+01
Coeff-En:   0.000D+00 0.100D+01
Coeff:      0.450D-03 0.100D+01
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=6.77D-03 MaxDP=2.31D-01 DE=-2.19D-03 OVMax= 2.93D-03

Cycle   3  Pass 0  IDiag  1:
RMSU=  4.01D-03    CP:  1.08D+00  4.54D-01
E= -723.413957337360     Delta-E=       -0.000093988073 Rises=F Damp=F
DIIS: error= 4.79D-03 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -723.413957337360     IErMin= 2 ErrMin= 7.34D-04
ErrMax= 4.79D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 6.55D-04 BMatP= 1.48D-04
IDIUse=3 WtCom= 1.26D-01 WtEn= 8.74D-01
Coeff-Com: -0.124D-01 0.780D+00 0.233D+00
Coeff-En:   0.000D+00 0.000D+00 0.100D+01
Coeff:     -0.157D-02 0.985D-01 0.903D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=7.56D+02 MaxDP=2.98D+04 DE=-9.40D-05 OVMax= 9.91D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle   4  Pass 1  IDiag  1:
E= -723.413754460512     Delta-E=        0.000202876847 Rises=F Damp=F
DIIS: error= 1.09D-03 at cycle   1 NSaved=   1.
```

NSaved= 1 IEnMin= 1 EnMin= -723.413754460512 IErMin= 1 ErrMin= 1.09D-03
ErrMax= 1.09D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-04 BMatP= 1.96D-04
IDIUse=3 WtCom= 9.89D-01 WtEn= 1.09D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.180 Goal= None Shift= 0.000
GapD= 0.180 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=5.04D-03 MaxDP=1.36D-01 DE= 2.03D-04 OVMax= 2.27D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.12D-03 CP: 7.70D-01
E= -723.413883228437 Delta-E= -0.000128767924 Rises=F Damp=F
DIIS: error= 1.21D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413883228437 IErMin= 2 ErrMin= 1.21D-04
ErrMax= 1.21D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.98D-06 BMatP= 1.96D-04
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.21D-03
Coeff-Com: 0.194D-01 0.981D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.193D-01 0.981D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.71D-04 MaxDP=1.64D-02 DE=-1.29D-04 OVMax= 1.09D-03

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.85D-04 CP: 7.80D-01 1.05D+00
E= -723.413879814119 Delta-E= 0.000003414317 Rises=F Damp=F
DIIS: error= 1.76D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413883228437 IErMin= 2 ErrMin= 1.21D-04
ErrMax= 1.76D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-05 BMatP= 5.98D-06
IDIUse=3 WtCom= 4.30D-01 WtEn= 5.70D-01
Coeff-Com: -0.176D-01 0.579D+00 0.438D+00
Coeff-En: 0.000D+00 0.601D+00 0.399D+00
Coeff: -0.756D-02 0.592D+00 0.416D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.31D-05 MaxDP=1.58D-03 DE= 3.41D-06 OVMax= 8.24D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 9.78D-06 CP: 7.81D-01 1.05D+00 1.09D+00
E= -723.413889954476 Delta-E= -0.000010140357 Rises=F Damp=F
DIIS: error= 2.46D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413889954476 IErMin= 4 ErrMin= 2.46D-05
ErrMax= 2.46D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-07 BMatP= 5.98D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.923D-02 0.220D+00 0.183D+00 0.606D+00
Coeff: -0.923D-02 0.220D+00 0.183D+00 0.606D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.21D-05 MaxDP=1.28D-03 DE=-1.01D-05 OVMax= 2.14D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 5.67D-06 CP: 7.81D-01 1.06D+00 1.15D+00 1.39D+00
E= -723.413890268945 Delta-E= -0.000000314469 Rises=F Damp=F
DIIS: error= 1.08D-05 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413890268945 IErMin= 5 ErrMin= 1.08D-05
ErrMax= 1.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.44D-08 BMatP= 2.01D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.462D-03-0.409D-01-0.258D-01 0.197D+00 0.869D+00
Coeff: 0.462D-03-0.409D-01-0.258D-01 0.197D+00 0.869D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.58D-05 MaxDP=1.00D-03 DE=-3.14D-07 OVMax= 3.74D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 2.73D-06 CP: 7.82D-01 1.06D+00 1.19D+00 1.86D+00 2.03D+00
E= -723.413890407272 Delta-E= -0.000000138326 Rises=F Damp=F
DIIS: error= 9.64D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413890407272 IErMin= 6 ErrMin= 9.64D-06
ErrMax= 9.64D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-08 BMatP= 3.44D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.270D-02-0.827D-01-0.638D-01-0.407D-01 0.521D+00 0.663D+00
Coeff: 0.270D-02-0.827D-01-0.638D-01-0.407D-01 0.521D+00 0.663D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=5.83D-06 MaxDP=3.86D-04 DE=-1.38D-07 OVMax= 2.11D-04

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.20D-06 CP: 7.82D-01 1.06D+00 1.20D+00 2.06D+00 2.63D+00
CP: 1.69D+00
E= -723.413890474380 Delta-E= -0.000000067108 Rises=F Damp=F
DIIS: error= 4.66D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413890474380 IErMin= 7 ErrMin= 4.66D-06
ErrMax= 4.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-09 BMatP= 1.73D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.811D-03-0.177D-01-0.150D-01-0.698D-01-0.598D-01 0.226D+00
Coeff-Com: 0.936D+00
Coeff: 0.811D-03-0.177D-01-0.150D-01-0.698D-01-0.598D-01 0.226D+00
Coeff: 0.936D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.51D-06 MaxDP=2.12D-04 DE=-6.71D-08 OVMax= 2.04D-04

Cycle 11 Pass 1 IDiag 1:
RMSU= 7.00D-07 CP: 7.82D-01 1.06D+00 1.19D+00 2.14D+00 2.94D+00
CP: 2.28D+00 2.09D+00
E= -723.413890502931 Delta-E= -0.000000028552 Rises=F Damp=F
DIIS: error= 2.73D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413890502931 IErMin= 8 ErrMin= 2.73D-06
ErrMax= 2.73D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-09 BMatP= 3.13D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.890D-03 0.302D-01 0.228D-01-0.121D-01-0.261D+00-0.195D+00

Coeff-Com: 0.412D+00 0.100D+01
Coeff: -0.890D-03 0.302D-01 0.228D-01-0.121D-01-0.261D+00-0.195D+00
Coeff: 0.412D+00 0.100D+01
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=3.54D-06 MaxDP=1.85D-04 DE=-2.86D-08 OVMax= 1.71D-04

Cycle 12 Pass 1 IDiag 1:
RMSU= 5.63D-07   CP: 7.82D-01 1.06D+00 1.19D+00 2.15D+00 3.00D+00
               CP: 2.63D+00 3.00D+00 2.07D+00
E= -723.413890514713   Delta-E=   -0.000000011782 Rises=F Damp=F
DIIS: error= 9.61D-07 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.413890514713   IErMin= 9 ErrMin= 9.61D-07
ErrMax= 9.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.64D-10 BMatP= 1.12D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.548D-03 0.171D-01 0.131D-01 0.351D-02-0.115D+00-0.124D+00
Coeff-Com: 0.597D-01 0.450D+00 0.696D+00
Coeff: -0.548D-03 0.171D-01 0.131D-01 0.351D-02-0.115D+00-0.124D+00
Coeff: 0.597D-01 0.450D+00 0.696D+00
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=6.73D-07 MaxDP=4.37D-05 DE=-1.18D-08 OVMax= 5.07D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 3.93D-07   CP: 7.82D-01 1.06D+00 1.18D+00 2.15D+00 3.00D+00
               CP: 2.65D+00 3.00D+00 2.29D+00 1.04D+00
E= -723.413890516276   Delta-E=   -0.000000001563 Rises=F Damp=F
DIIS: error= 8.50D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413890516276   IErMin=10 ErrMin= 8.50D-07
ErrMax= 8.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.59D-11 BMatP= 2.64D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.116D-03-0.477D-02-0.348D-02 0.670D-02 0.591D-01 0.256D-01
Coeff-Com: -0.156D+00-0.245D+00 0.398D+00 0.920D+00
Coeff: 0.116D-03-0.477D-02-0.348D-02 0.670D-02 0.591D-01 0.256D-01
Coeff: -0.156D+00-0.245D+00 0.398D+00 0.920D+00
Gap=   0.180 Goal=   None   Shift=   0.000
RMSDP=5.54D-07 MaxDP=3.69D-05 DE=-1.56D-09 OVMax= 4.19D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 2.23D-07   CP: 7.82D-01 1.06D+00 1.18D+00 2.13D+00 3.00D+00
               CP: 2.61D+00 3.00D+00 2.37D+00 8.79D-01 2.12D+00
E= -723.413890516973   Delta-E=   -0.000000000697 Rises=F Damp=F
DIIS: error= 2.72D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413890516973   IErMin=11 ErrMin= 2.72D-07
ErrMax= 2.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-11 BMatP= 9.59D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.111D-03-0.387D-02-0.290D-02 0.170D-02 0.356D-01 0.266D-01
Coeff-Com: -0.608D-01-0.151D+00 0.473D-01 0.328D+00 0.779D+00
Coeff: 0.111D-03-0.387D-02-0.290D-02 0.170D-02 0.356D-01 0.266D-01
Coeff: -0.608D-01-0.151D+00 0.473D-01 0.328D+00 0.779D+00

Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.25D-07 MaxDP=1.87D-05 DE=-6.97D-10 OVMax= 1.14D-05

Cycle 15 Pass 1 IDiag 1:
RMSU= 6.85D-08 CP: 7.82D-01 1.06D+00 1.18D+00 2.13D+00 2.98D+00
CP: 2.59D+00 3.00D+00 2.33D+00 9.61D-01 2.30D+00
CP: 1.47D+00
E= -723.413890517044 Delta-E= -0.000000000071 Rises=F Damp=F
DIIS: error= 1.72D-07 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413890517044 IErMin=12 ErrMin= 1.72D-07
ErrMax= 1.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.55D-12 BMatP= 1.26D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.126D-04 0.711D-03 0.485D-03-0.225D-02-0.123D-01-0.176D-02
Coeff-Com: 0.428D-01 0.439D-01-0.139D+00-0.239D+00 0.236D+00 0.107D+01
Coeff: -0.126D-04 0.711D-03 0.485D-03-0.225D-02-0.123D-01-0.176D-02
Coeff: 0.428D-01 0.439D-01-0.139D+00-0.239D+00 0.236D+00 0.107D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.86D-07 MaxDP=1.56D-05 DE=-7.12D-11 OVMax= 9.33D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 2.67D-08 CP: 7.82D-01 1.06D+00 1.18D+00 2.13D+00 2.96D+00
CP: 2.57D+00 3.00D+00 2.27D+00 1.02D+00 2.44D+00
CP: 1.87D+00 2.02D+00
E= -723.413890517071 Delta-E= -0.000000000027 Rises=F Damp=F
DIIS: error= 6.25D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.413890517071 IErMin=13 ErrMin= 6.25D-08
ErrMax= 6.25D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-12 BMatP= 3.55D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.279D-04 0.110D-02 0.801D-03-0.147D-02-0.130D-01-0.576D-02
Coeff-Com: 0.338D-01 0.505D-01-0.804D-01-0.179D+00-0.233D-01 0.527D+00
Coeff-Com: 0.689D+00
Coeff: -0.279D-04 0.110D-02 0.801D-03-0.147D-02-0.130D-01-0.576D-02
Coeff: 0.338D-01 0.505D-01-0.804D-01-0.179D+00-0.233D-01 0.527D+00
Coeff: 0.689D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.27D-08 MaxDP=3.22D-06 DE=-2.68D-11 OVMax= 2.71D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 9.69D-09 CP: 7.82D-01 1.06D+00 1.18D+00 2.13D+00 2.96D+00
CP: 2.57D+00 3.00D+00 2.26D+00 1.03D+00 2.47D+00
CP: 1.96D+00 2.31D+00 1.41D+00
E= -723.413890517081 Delta-E= -0.000000000011 Rises=F Damp=F
DIIS: error= 3.51D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.413890517081 IErMin=14 ErrMin= 3.51D-08
ErrMax= 3.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.72D-13 BMatP= 1.06D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.452D-05 0.119D-03 0.929D-04 0.179D-03-0.284D-03-0.102D-02
Coeff-Com: -0.222D-02 0.169D-02 0.160D-01 0.180D-01-0.719D-01-0.153D+00

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Coeff-Com: 0.147D+00 0.105D+01
Coeff: -0.452D-05 0.119D-03 0.929D-04 0.179D-03-0.284D-03-0.102D-02
Coeff: -0.222D-02 0.169D-02 0.160D-01 0.180D-01-0.719D-01-0.153D+00
Coeff: 0.147D+00 0.105D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.96D-08 MaxDP=8.74D-07 DE=-1.07D-11 OVMax= 1.82D-06

Cycle 18 Pass 1 IDiag 1:
RMSU= 4.45D-09 CP: 7.82D-01 1.06D+00 1.18D+00 2.13D+00 2.96D+00
CP: 2.58D+00 3.00D+00 2.25D+00 1.04D+00 2.48D+00
CP: 1.96D+00 2.43D+00 1.80D+00 2.00D+00
E= -723.413890517085 Delta-E= -0.000000000004 Rises=F Damp=F
DIIS: error= 1.63D-08 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=15 EnMin= -723.413890517085 IErMin=15 ErrMin= 1.63D-08
ErrMax= 1.63D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.33D-14 BMatP= 1.72D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.484D-05-0.213D-03-0.152D-03 0.393D-03 0.288D-02 0.100D-02
Coeff-Com: -0.863D-02-0.114D-01 0.244D-01 0.484D-01-0.167D-01-0.174D+00
Coeff-Com: -0.131D+00 0.374D+00 0.891D+00
Coeff: 0.484D-05-0.213D-03-0.152D-03 0.393D-03 0.288D-02 0.100D-02
Coeff: -0.863D-02-0.114D-01 0.244D-01 0.484D-01-0.167D-01-0.174D+00
Coeff: -0.131D+00 0.374D+00 0.891D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.08D-08 MaxDP=5.77D-07 DE=-4.09D-12 OVMax= 8.96D-07

Cycle 19 Pass 1 IDiag 1:
RMSU= 1.50D-09 CP: 7.82D-01 1.06D+00 1.18D+00 2.13D+00 2.96D+00
CP: 2.58D+00 3.00D+00 2.25D+00 1.04D+00 2.48D+00
CP: 1.95D+00 2.44D+00 1.94D+00 2.50D+00 1.60D+00
E= -723.413890517091 Delta-E= -0.000000000005 Rises=F Damp=F
DIIS: error= 1.40D-08 at cycle 16 NSaved= 16.
NSaved=16 IEnMin=16 EnMin= -723.413890517091 IErMin=16 ErrMin= 1.40D-08
ErrMax= 1.40D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-14 BMatP= 5.33D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.346D-05-0.134D-03-0.986D-04 0.155D-03 0.151D-02 0.772D-03
Coeff-Com: -0.383D-02-0.619D-02 0.823D-02 0.203D-01 0.888D-02-0.504D-01
Coeff-Com: -0.107D+00-0.608D-01 0.475D+00 0.714D+00
Coeff: 0.346D-05-0.134D-03-0.986D-04 0.155D-03 0.151D-02 0.772D-03
Coeff: -0.383D-02-0.619D-02 0.823D-02 0.203D-01 0.888D-02-0.504D-01
Coeff: -0.107D+00-0.608D-01 0.475D+00 0.714D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.90D-09 MaxDP=2.70D-07 DE=-5.46D-12 OVMax= 3.88D-07

SCF Done: E(RwB97XD) = -723.413890517 A.U. after 19 cycles
NFock= 19 Conv=0.49D-08 -V/T= 2.0047
KE= 7.200600616239D+02 PE=-3.701525962443D+03 EE= 1.247824092669D+03
Leave Link 502 at Sat Sep 26 06:45:42 2026, MaxMem= 805306368 cpu: 8093.8 elap: 1349.4

Supporting Information file

(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23222 LenP2D= 51945.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 06:45:43 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 06:45:43 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 06:56:39 2026, MaxMem= 805306368 cpu: 3935.9 elap: 656.1
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.55024040D+00 3.94224005D-03 6.74863048D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000105471	-0.000671207	-0.000198676
2	6	0.000074868	0.000713915	0.000231202
3	6	-0.000123594	0.000687102	0.000231410
4	6	0.000182064	-0.000993204	-0.000271617
5	6	0.000090587	-0.000745562	-0.000201535
6	6	-0.000300162	0.000869520	-0.000012125
7	6	0.000194185	0.001010552	0.000251472
8	6	0.000339580	-0.000129320	-0.000204204
9	6	-0.000291256	-0.000876382	-0.000305190
10	6	-0.000344597	-0.000200878	0.000845818
11	6	0.000428732	0.000221615	-0.000131752
12	6	0.000293965	0.001195032	-0.000640841
13	6	-0.000443075	0.000238487	0.000628557
14	6	0.000515675	-0.000292384	-0.000481770

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    15        6       -0.000314460   0.000634614   0.000189718
    16        6       -0.000015022  -0.000982838  -0.000215499
    17        7        0.000495785  -0.001328128   0.000303108
    18        7       -0.000282637   0.000881370   0.000004114
    19        1        0.000078627   0.000219009  -0.000318153
    20        1       -0.000104530   0.000148666   0.000005723
    21        1        0.000106703  -0.000270275   0.000234838
    22        1       -0.000141663  -0.000202423   0.000017836
    23        1       -0.000078480   0.000020175   0.000125853
    24        1       -0.000103072  -0.000207712  -0.000058408
    25        1       -0.000062078   0.000060505   0.000032928
    26        1       -0.000090673  -0.000000248  -0.000062809
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.001328128 RMS     0.000448318
 Leave Link  716 at Sat Sep 26 06:56:39 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000894925 RMS     0.000314764
 Search for a local minimum.
 Step number  22 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .31476D-03 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points   18   19   20   21   22
 DE= -6.83D-05 DEPred=-9.99D-05 R= 6.83D-01
 TightC=F SS=  1.41D+00  RLast= 9.24D-02 DXNew= 1.3552D+00 2.7707D-01
 Trust test= 6.83D-01 RLast= 9.24D-02 DXMaxT set to 8.06D-01
 ITU=  1  1  1  1  1  1  1  1 -1  1  1  1  1  1  1  1  1  1  0  0
 ITU=  1  0
    Eigenvalues ---    0.00301   0.00501   0.01039   0.01313   0.01702
    Eigenvalues ---    0.01842   0.02672   0.02796   0.02926   0.03055
    Eigenvalues ---    0.03327   0.03655   0.03792   0.04333   0.04366
    Eigenvalues ---    0.04461   0.05025   0.05420   0.05500   0.08079
    Eigenvalues ---    0.09953   0.10084   0.11062   0.11211   0.11582
    Eigenvalues ---    0.11796   0.13872   0.15077   0.15394   0.15892
    Eigenvalues ---    0.15993   0.16001   0.16008   0.16213   0.16492
    Eigenvalues ---    0.21442   0.22434   0.24888   0.24994   0.24996
    Eigenvalues ---    0.25000   0.25000   0.25003   0.25437   0.28744
    Eigenvalues ---    0.30197   0.34756   0.37245   0.38666   0.41224
    Eigenvalues ---    0.45819   0.46139   0.47032   0.47644   0.47689
    Eigenvalues ---    0.47691   0.47814   0.48482   0.49957   0.52081
    Eigenvalues ---    0.54811   0.55382   0.55638   0.55660   0.57345
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    Eigenvalues ---    0.92344   0.93711   0.95031   0.95362   0.97724
    Eigenvalues ---    0.98947   1.37309
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    22   21   20
 RFO step:  Lambda=-5.77388330D-05.
 NNeg= 0 NGDIIS= 3 SimSw=  2.50D-01 Rises=F DC= -6.83D-05 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.7263306281D-02 NUsed= 3 OKEnD=T EnDIS=F
 InvSVX:  RCond= 1.14D-02 Info=          0 Equed=N FErr=  3.64D-15 BErr=  5.03D-17
 DidBck=T Rises=F RFO-DIIS coefs:    0.62288    0.02905    0.34807
 Iteration  1 RMS(Cart)=  0.01501863 RMS(Int)=  0.00021376
 Iteration  2 RMS(Cart)=  0.00022508 RMS(Int)=  0.00000427
 Iteration  3 RMS(Cart)=  0.00000004 RMS(Int)=  0.00000427
  ITry=  1 IFail=0 DXMaxC=  6.84D-02 DCOld=  1.00D+10 DXMaxT=  8.06D-01 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)    (Quad)   (Total)
    R1        2.32245   0.00019  -0.00067   0.00092   0.00024   2.32270
    R2        2.53670  -0.00038   0.00087  -0.00163  -0.00076   2.53594
    R3        2.53279  -0.00023   0.00090  -0.00132  -0.00042   2.53237
    R4        2.32240   0.00020  -0.00068   0.00092   0.00025   2.32265
    R5        2.31964   0.00016  -0.00069   0.00083   0.00014   2.31978
    R6        2.53290  -0.00022   0.00091  -0.00133  -0.00042   2.53248
    R7        2.53378  -0.00008   0.00078  -0.00092  -0.00013   2.53365
    R8        2.31955   0.00019  -0.00070   0.00085   0.00015   2.31970
    R9        2.31884   0.00022  -0.00037   0.00054   0.00017   2.31901
   R10        2.53387  -0.00004   0.00082  -0.00093  -0.00012   2.53376
   R11        2.62777  -0.00015   0.00068  -0.00105  -0.00037   2.62740
   R12        2.31874   0.00032  -0.00043   0.00059   0.00016   2.31891
   R13        2.69035   0.00065  -0.00247   0.00327   0.00080   2.69115
   R14        2.69344  -0.00021   0.00196  -0.00183   0.00013   2.69357
   R15        2.62798  -0.00021   0.00083  -0.00119  -0.00037   2.62761
   R16        2.69264   0.00067   0.00185  -0.00134   0.00051   2.69315
   R17        2.81664  -0.00089   0.00267  -0.00349  -0.00082   2.81582
   R18        2.05022   0.00018   0.00081  -0.00047   0.00034   2.05056
   R19        2.81601  -0.00043   0.00264  -0.00335  -0.00071   2.81529
   R20        2.05028   0.00009   0.00070  -0.00048   0.00022   2.05050
   R21        1.94313   0.00037   0.00118  -0.00046   0.00072   1.94385
   R22        1.91681   0.00016   0.00038  -0.00013   0.00024   1.91706
   R23        1.93030   0.00002  -0.00022  -0.00016  -0.00038   1.92992
   R24        1.94320   0.00032   0.00116  -0.00045   0.00071   1.94391
   R25        1.91678   0.00021   0.00041  -0.00015   0.00026   1.91705
   R26        1.93036  -0.00003  -0.00022  -0.00019  -0.00041   1.92996
    A1        2.55411   0.00027   0.00027   0.00102   0.00129   2.55540
    A2        2.62177  -0.00034  -0.00109  -0.00099  -0.00208   2.61969
    A3        2.55630   0.00029   0.00018   0.00104   0.00122   2.55752
    A4        2.70320   0.00058   0.00154   0.00154   0.00308   2.70629
    A5        2.61971  -0.00034  -0.00098  -0.00096  -0.00194   2.61777
    A6        2.85649  -0.00076  -0.00044  -0.00318  -0.00363   2.85286
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A7	2.70448	0.00063	0.00152	0.00157	0.00310	2.70758
A8	2.85544	-0.00072	-0.00038	-0.00312	-0.00350	2.85194
A9	2.08400	0.00025	0.00105	-0.00026	0.00079	2.08479
A10	2.10775	-0.00007	-0.00161	0.00131	-0.00030	2.10745
A11	2.09105	-0.00019	0.00047	-0.00106	-0.00059	2.09046
A12	2.08422	-0.00005	0.00083	-0.00025	0.00058	2.08480
A13	2.09108	-0.00018	0.00056	-0.00118	-0.00062	2.09046
A14	2.10724	0.00024	-0.00143	0.00158	0.00015	2.10739
A15	2.05664	-0.00004	-0.00396	0.00293	-0.00103	2.05560
A16	1.92496	0.00065	-0.00669	0.00758	0.00089	1.92585
A17	2.05803	-0.00032	-0.00410	0.00223	-0.00187	2.05615
A18	1.92769	-0.00031	-0.00752	0.00633	-0.00120	1.92649
A19	2.01405	0.00019	0.00011	-0.00023	-0.00012	2.01393
A20	1.92481	0.00005	-0.00047	0.00003	-0.00044	1.92437
A21	1.88664	-0.00006	0.00345	-0.00153	0.00193	1.88857
A22	1.89816	-0.00011	0.00003	-0.00024	-0.00021	1.89795
A23	1.84588	0.00002	-0.00177	0.00169	-0.00009	1.84579
A24	1.88929	-0.00010	-0.00149	0.00037	-0.00113	1.88817
A25	2.01383	0.00026	0.00007	0.00005	0.00012	2.01395
A26	1.92495	0.00009	-0.00051	-0.00008	-0.00059	1.92437
A27	1.88669	-0.00009	0.00361	-0.00159	0.00202	1.88871
A28	1.89814	-0.00015	0.00007	-0.00037	-0.00031	1.89783
A29	1.84590	-0.00005	-0.00179	0.00158	-0.00021	1.84570
A30	1.88933	-0.00009	-0.00160	0.00051	-0.00109	1.88823
A31	2.90295	0.00003	-0.00041	0.00128	0.00087	2.90383
A32	3.12608	0.00011	-0.00074	0.00074	-0.00001	3.12608
A33	2.90259	0.00011	-0.00013	0.00160	0.00147	2.90406
A34	3.12756	-0.00004	-0.00123	0.00008	-0.00115	3.12641
A35	3.98159	0.00061	-0.01065	0.01051	-0.00014	3.98145
A36	3.98572	-0.00063	-0.01162	0.00856	-0.00307	3.98265
A37	3.14487	-0.00005	-0.00005	0.00052	0.00049	3.14536
A38	3.12640	0.00082	0.00412	0.00601	0.01013	3.13653
A39	3.14447	0.00024	0.00014	0.00065	0.00077	3.14524
A40	3.14931	-0.00047	-0.00178	-0.00685	-0.00865	3.14066
A41	4.01246	0.00080	0.00935	-0.00626	0.00309	4.01554
A42	4.01589	-0.00014	0.00679	-0.00577	0.00102	4.01691
D1	0.01503	0.00016	0.00243	-0.00165	0.00077	0.01581
D2	-0.01385	0.00011	-0.00199	0.00242	0.00043	-0.01342
D3	-0.01288	0.00025	-0.00072	0.00255	0.00182	-0.01106
D4	0.01665	-0.00009	0.00199	-0.00249	-0.00049	0.01616
D5	0.00051	0.00015	0.00123	-0.00040	0.00083	0.00134
D6	-0.00951	-0.00013	-0.00162	0.00052	-0.00110	-0.01061
D7	-0.00874	-0.00002	0.00055	0.00614	0.00668	-0.00206
D8	3.09017	0.00022	0.00030	0.01073	0.01103	3.10121
D9	0.00246	-0.00018	0.00085	-0.00163	-0.00077	0.00169
D10	0.00627	-0.00010	-0.00324	-0.00241	-0.00565	0.00062
D11	3.11396	-0.00007	-0.00581	-0.00260	-0.00841	3.10555
D12	0.00722	-0.00001	0.00039	-0.00133	-0.00095	0.00627

D13	-3.09625	-0.00032	0.00138	-0.00584	-0.00447	-3.10072
D14	-3.10470	0.00031	0.00347	-0.00093	0.00253	-3.10217
D15	0.07501	-0.00000	0.00445	-0.00544	-0.00099	0.07402
D16	2.51791	0.00001	-0.00510	0.00050	-0.00460	2.51332
D17	-0.65376	-0.00031	-0.00816	0.00006	-0.00811	-0.66187
D18	-0.66487	0.00035	-0.00503	0.00778	0.00275	-0.66212
D19	2.51535	0.00004	-0.00409	0.00325	-0.00083	2.51452
D20	-1.12181	-0.00007	-0.02082	-0.00378	-0.02460	-1.14641
D21	1.03728	-0.00004	-0.02109	-0.00424	-0.02533	1.01195
D22	3.09962	-0.00017	-0.02111	-0.00469	-0.02580	3.07382
D23	-1.12275	-0.00012	-0.02110	-0.00396	-0.02506	-1.14781
D24	1.03626	-0.00005	-0.02137	-0.00449	-0.02586	1.01040
D25	3.09875	-0.00016	-0.02145	-0.00487	-0.02632	3.07243

Item	Value	Threshold	Converged?
Maximum Force	0.000895	0.000450	NO
RMS Force	0.000315	0.000300	NO
Maximum Displacement	0.068444	0.001800	NO
RMS Displacement	0.015027	0.001200	NO

Predicted change in Energy=-2.886725D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 06:56:39 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.017720	0.668293	0.050292
2	6	0	3.338452	1.690324	0.119432
3	6	0	4.016862	-0.670159	-0.046710
4	6	0	2.139698	2.287601	0.164609
5	6	0	3.338465	-1.692687	-0.116613
6	6	0	0.912606	2.321879	0.168357
7	6	0	2.139014	-2.288586	-0.163224
8	6	0	-0.382856	1.977152	0.144775
9	6	0	0.911976	-2.322984	-0.168885
10	6	0	-1.460719	1.392288	0.099161
11	6	0	-0.383288	-1.977155	-0.147592
12	6	0	-2.671464	0.710339	0.052903
13	6	0	-1.460827	-1.391648	-0.104066
14	6	0	-2.671572	-0.709687	-0.054645
15	6	0	-3.907742	1.412722	0.152729
16	6	0	-3.907817	-1.411887	-0.153009
17	7	0	-3.728146	2.877852	-0.050854
18	7	0	-3.725579	-2.876393	0.050667

19	1	0	-3.449999	3.160429	-1.000007
20	1	0	-4.576123	3.374126	0.201700
21	1	0	-3.444249	-3.158178	0.999148
22	1	0	-4.573627	-3.373968	-0.199048
23	1	0	-2.977535	3.195855	0.564330
24	1	0	-4.744403	1.049920	-0.435349
25	1	0	-4.744017	-1.049629	0.435997
26	1	0	-2.976315	-3.193742	-0.566525

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229118	0.000000			
3	C	1.341963	2.461650	0.000000		
4	C	2.482376	1.340072	3.509521	0.000000	
5	C	2.462412	3.391236	1.229095	4.166392	0.000000
6	C	3.519946	2.507187	4.316822	1.227577	4.699228
7	C	3.509738	4.165366	2.481772	4.587915	1.340131
8	C	4.592070	3.732432	5.138330	2.541664	5.232999
9	C	4.317571	4.698676	3.519527	4.782888	2.507559
10	C	5.526287	4.808460	5.854815	3.710643	5.709273
11	C	5.138718	5.231926	4.591267	4.964984	3.732736
12	C	6.689316	6.089654	6.830036	5.064337	6.474760
13	C	5.855054	5.708028	5.525298	5.154885	4.808741
14	C	6.830554	6.473852	6.688556	5.672753	6.090212
15	C	7.961006	7.251586	8.196189	6.110408	7.888195
16	C	8.196500	7.887100	7.960024	7.096445	7.251811
17	N	8.055484	7.167708	8.519011	5.901391	8.416124
18	N	8.516072	8.411907	8.051232	7.815452	7.164486
19	H	7.942336	7.035441	8.446075	5.776060	8.391446
20	H	9.011026	8.092123	9.500386	6.803247	9.402905
21	H	8.439383	8.383729	7.934244	7.844325	7.028356
22	H	9.498067	9.399441	9.007235	8.789445	8.089172
23	H	7.455628	6.508168	8.015049	5.212559	8.015820
24	H	8.783864	8.127142	8.936972	7.020160	8.541442
25	H	8.936893	8.540133	8.782369	7.654822	8.126833
26	H	8.013257	8.012548	7.452731	7.533476	6.506307

		6	7	8	9	10
6	C	0.000000				
7	C	4.782302	0.000000			
8	C	1.340752	4.964999	0.000000		
9	C	4.657090	1.227533	4.501793	0.000000	
10	C	2.549823	5.155168	1.227165	4.416421	0.000000
11	C	4.501206	2.541503	3.965100	1.340805	3.546109
12	C	3.931405	5.672827	2.617437	4.700137	1.390358
13	C	4.415618	3.710372	3.545808	2.549860	2.791343
14	C	4.699623	5.064233	3.535123	3.931615	2.430662
15	C	4.905361	7.096673	3.569799	6.106441	2.447694

16	C	6.105797	6.110063	4.898939	4.905176	3.730318
17	N	4.679075	7.818458	3.469942	6.970894	2.714891
18	N	6.967686	5.897858	5.894027	4.675616	4.832554
19	H	4.593535	7.850417	3.481097	7.055878	2.879536
20	H	5.588781	8.791618	4.420211	7.919194	3.693770
21	H	7.050065	5.768893	6.039345	4.586780	5.044909
22	H	7.916844	6.799918	6.805531	5.585456	5.700554
23	H	4.006722	7.535748	2.897174	6.791427	2.402075
24	H	5.829587	7.655136	4.496597	6.591063	3.344472
25	H	6.590606	7.019274	5.316572	5.829029	4.105662
26	H	6.788654	5.210427	5.828389	4.004390	4.875637

		11	12	13	14	15
11	C	0.000000				
12	C	3.535332	0.000000			
13	C	1.227113	2.430767	0.000000		
14	C	2.617511	1.424093	1.390474	0.000000	
15	C	4.899310	1.425374	3.730660	2.464901	0.000000
16	C	3.569574	2.464713	2.447562	1.425153	2.841107
17	N	5.896485	2.413598	4.834480	3.739893	1.490070
18	N	3.466821	3.738424	2.712473	2.411770	4.294194
19	H	6.043683	2.778071	5.047863	4.059243	2.143085
20	H	6.807208	3.278052	5.701856	4.513375	2.072737
21	H	3.475530	4.056846	2.876051	2.775359	4.671656
22	H	4.417316	4.512568	3.691631	3.276745	4.845570
23	H	5.830693	2.555978	4.877738	3.966106	2.052867
24	H	5.316513	2.156567	4.105224	2.745501	1.085109
25	H	4.496314	2.745857	3.344844	2.156691	2.615869
26	H	2.894716	3.964653	2.399607	2.554490	4.754407

		16	17	18	19	20
16	C	0.000000				
17	N	4.294715	0.000000			
18	N	1.489789	5.755141	0.000000		
19	H	4.672588	1.028643	6.133766	0.000000	
20	H	4.845448	1.014463	6.309930	1.660699	0.000000
21	H	2.142870	6.133250	1.028672	6.627326	6.677429
22	H	2.072483	6.310471	1.014457	6.678504	6.759983
23	H	4.755132	1.021271	6.139675	1.634511	1.648868
24	H	2.615356	2.126487	4.085357	2.539403	2.415798
25	H	1.085076	4.085845	2.126678	4.632622	4.433136
26	H	2.052729	6.139659	1.021290	6.386531	6.803414

		21	22	23	24	25
21	H	0.000000				
22	H	1.660643	0.000000			
23	H	6.385970	6.803883	0.000000		
24	H	4.632091	4.433484	2.954017	0.000000	
25	H	2.540180	2.415546	4.600116	2.273181	0.000000
26	H	1.634490	1.648917	6.488896	4.599131	2.954156

		26

Supporting Information file

26 H 0.000000
Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=2 Diff= 1.78D-03
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.524624	-0.671891	-0.025364
2	6	0	3.844881	-1.695419	-0.058123
3	6	0	4.524387	0.669172	0.023764
4	6	0	2.645851	-2.293362	-0.082242
5	6	0	3.846465	1.693865	0.056922
6	6	0	1.418743	-2.327173	-0.085076
7	6	0	2.647291	2.291615	0.081910
8	6	0	0.123441	-1.981211	-0.074155
9	6	0	1.420268	2.326773	0.086025
10	6	0	-0.954151	-1.394582	-0.049738
11	6	0	0.124843	1.981016	0.076769
12	6	0	-2.164578	-0.710844	-0.028179
13	6	0	-0.952968	1.394837	0.053911
14	6	0	-2.164029	0.712118	0.028573
15	6	0	-3.401171	-1.415760	-0.103167
16	6	0	-3.399959	1.417967	0.101474
17	7	0	-3.222329	-2.872767	0.152670
18	7	0	-3.216968	2.874176	-0.154341
19	1	0	-2.944543	-3.121390	1.111382
20	1	0	-4.070484	-3.377346	-0.082212
21	1	0	-2.935276	3.121767	-1.112210
22	1	0	-4.064836	3.380755	0.077224
23	1	0	-2.471723	-3.212897	-0.450570
24	1	0	-4.237797	-1.031787	0.471362
25	1	0	-4.236193	1.035295	-0.474429
26	1	0	-2.467698	3.213016	0.451312

Rotational constants (GHZ): 0.6025038 0.2708228 0.1875193
Leave Link 202 at Sat Sep 26 06:56:39 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.

606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.2115250298 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0153885009 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.1961365289 Hartrees.
Leave Link 301 at Sat Sep 26 06:56:39 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23221 LenP2D= 51946.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.88D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 06:56:40 2026, MaxMem= 805306368 cpu: 5.7 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 06:56:40 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000033 -0.000041 -0.000441 Ang= 0.05 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Generating alternative initial guess.
ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 4639 and IRadAn= 5 diagonalized for initial guess.

Supporting Information file

HarFok: IExCor= 4639 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Harris En= -691.982203540844
Leave Link 401 at Sat Sep 26 06:56:48 2026, MaxMem= 805306368 cpu: 45.0 elap: 7.5
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.
Integral accuracy reduced to 1.0D-05 until final iterations.

Cycle 1 Pass 0 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.413292559054
DIIS: error= 1.14D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413292559054 IErMin= 1 ErrMin= 1.14D-03
ErrMax= 1.14D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.51D-04 BMatP= 8.51D-04
IDIUse=3 WtCom= 9.89D-01 WtEn= 1.14D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.704 Goal= None Shift= 0.000
GapD= 0.704 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
RMSDP=8.48D-03 MaxDP=3.16D-01 OVMax= 5.29D-03

Cycle 2 Pass 0 IDiag 1:
RMSU= 7.14D-03 CP: 1.42D+00
E= -723.413971835849 Delta-E= -0.000679276795 Rises=F Damp=F
DIIS: error= 7.16D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413971835849 IErMin= 2 ErrMin= 7.16D-04
ErrMax= 7.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-04 BMatP= 8.51D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.16D-03
Coeff-Com: 0.103D+00 0.897D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.103D+00 0.897D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=5.68D-03 MaxDP=1.95D-01 DE=-6.79D-04 OVMax= 1.47D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 3.81D-03 CP: 1.14D+00 5.86D-01
E= -723.414008632498 Delta-E= -0.000036796648 Rises=F Damp=F
DIIS: error= 4.46D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.414008632498 IErMin= 2 ErrMin= 7.16D-04
ErrMax= 4.46D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.20D-04 BMatP= 1.16D-04
IDIUse=3 WtCom= 1.30D-01 WtEn= 8.70D-01
Coeff-Com: 0.513D-01 0.754D+00 0.194D+00
Coeff-En: 0.000D+00 0.000D+00 0.100D+01
Coeff: 0.668D-02 0.982D-01 0.895D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=7.58D+02 MaxDP=2.97D+04 DE=-3.68D-05 OVMax= 9.96D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.413815387726 Delta-E= 0.000193244771 Rises=F Damp=F
DIIS: error= 1.24D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413815387726 IErMin= 1 ErrMin= 1.24D-03
ErrMax= 1.24D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-04 BMatP= 1.73D-04
IDIUse=3 WtCom= 9.88D-01 WtEn= 1.24D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.180 Goal= None Shift= 0.000
GapD= 0.180 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=5.75D-03 MaxDP=1.58D-01 DE= 1.93D-04 OVMax= 1.62D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.27D-03 CP: 7.17D-01
E= -723.413927090870 Delta-E= -0.000111703144 Rises=F Damp=F
DIIS: error= 6.53D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413927090870 IErMin= 2 ErrMin= 6.53D-05
ErrMax= 6.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-06 BMatP= 1.73D-04
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.198D-01 0.102D+01
Coeff: -0.198D-01 0.102D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=3.26D-04 MaxDP=1.38D-02 DE=-1.12D-04 OVMax= 8.44D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.54D-04 CP: 7.22D-01 1.05D+00
E= -723.413924786054 Delta-E= 0.000002304816 Rises=F Damp=F
DIIS: error= 1.10D-04 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413927090870 IErMin= 2 ErrMin= 6.53D-05
ErrMax= 1.10D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.94D-06 BMatP= 1.61D-06
IDIUse=3 WtCom= 4.88D-01 WtEn= 5.12D-01
Coeff-Com: -0.208D-01 0.638D+00 0.382D+00
Coeff-En: 0.000D+00 0.673D+00 0.327D+00
Coeff: -0.101D-01 0.656D+00 0.354D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.45D-05 MaxDP=6.50D-04 DE= 2.30D-06 OVMax= 5.86D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 6.65D-06 CP: 7.23D-01 1.05D+00 1.04D+00
E= -723.413929242555 Delta-E= -0.000004456501 Rises=F Damp=F
DIIS: error= 5.17D-06 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413929242555 IErMin= 4 ErrMin= 5.17D-06
ErrMax= 5.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.58D-08 BMatP= 1.61D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.453D-02 0.105D+00 0.514D-01 0.848D+00
Coeff: -0.453D-02 0.105D+00 0.514D-01 0.848D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=2.24D-05 MaxDP=1.20D-03 DE=-4.46D-06 OVMax= 1.19D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 4.23D-06 CP: 7.24D-01 1.05D+00 1.11D+00 1.53D+00
E= -723.413929285013 Delta-E= -0.000000042458 Rises=F Damp=F
DIIS: error= 4.64D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413929285013 IErMin= 5 ErrMin= 4.64D-06
ErrMax= 4.64D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-08 BMatP= 2.58D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.196D-02-0.779D-01-0.537D-01 0.449D+00 0.681D+00
Coeff: 0.196D-02-0.779D-01-0.537D-01 0.449D+00 0.681D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.60D-06 MaxDP=5.11D-04 DE=-4.25D-08 OVMax= 1.26D-04

Cycle 9 Pass 1 IDiag 1:
RMSU= 1.16D-06 CP: 7.24D-01 1.05D+00 1.13D+00 1.86D+00 1.55D+00
E= -723.413929312668 Delta-E= -0.000000027654 Rises=F Damp=F
DIIS: error= 2.10D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413929312668 IErMin= 6 ErrMin= 2.10D-06
ErrMax= 2.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.14D-09 BMatP= 1.57D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.140D-02-0.475D-01-0.306D-01 0.112D+00 0.320D+00 0.645D+00
Coeff: 0.140D-02-0.475D-01-0.306D-01 0.112D+00 0.320D+00 0.645D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.30D-06 MaxDP=9.21D-05 DE=-2.77D-08 OVMax= 5.25D-05

```
Cycle  10  Pass 1  IDiag  1:
RMSU=  6.01D-07    CP:  7.24D-01  1.05D+00  1.13D+00  1.92D+00  1.72D+00
               CP:  1.41D+00
E= -723.413929318867     Delta-E=       -0.000000006199 Rises=F Damp=F
DIIS: error= 1.40D-06 at cycle   7 NSaved=   7.
NSaved= 7 IEnMin= 7 EnMin= -723.413929318867     IErMin= 7 ErrMin= 1.40D-06
ErrMax= 1.40D-06  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.84D-10 BMatP= 2.14D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.133D-03 0.842D-02 0.646D-02-0.114D+00-0.103D+00 0.229D+00
Coeff-Com:  0.973D+00
Coeff:     -0.133D-03 0.842D-02 0.646D-02-0.114D+00-0.103D+00 0.229D+00
Coeff:      0.973D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=1.25D-06 MaxDP=7.36D-05 DE=-6.20D-09 OVMax= 6.92D-05

Cycle  11  Pass 1  IDiag  1:
RMSU=  2.10D-07    CP:  7.24D-01  1.05D+00  1.13D+00  1.96D+00  1.83D+00
               CP:  1.89D+00  2.22D+00
E= -723.413929322606     Delta-E=       -0.000000003740 Rises=F Damp=F
DIIS: error= 9.51D-07 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -723.413929322606     IErMin= 8 ErrMin= 9.51D-07
ErrMax= 9.51D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-10 BMatP= 4.84D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.403D-03 0.155D-01 0.103D-01-0.794D-01-0.119D+00-0.584D-01
Coeff-Com:  0.438D+00 0.793D+00
Coeff:     -0.403D-03 0.155D-01 0.103D-01-0.794D-01-0.119D+00-0.584D-01
Coeff:      0.438D+00 0.793D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=7.12D-07 MaxDP=4.03D-05 DE=-3.74D-09 OVMax= 4.19D-05

Cycle  12  Pass 1  IDiag  1:
RMSU=  1.11D-07    CP:  7.24D-01  1.05D+00  1.13D+00  1.96D+00  1.86D+00
               CP:  2.10D+00  2.77D+00  1.67D+00
E= -723.413929323844     Delta-E=       -0.000000001237 Rises=F Damp=F
DIIS: error= 5.20D-07 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.413929323844     IErMin= 9 ErrMin= 5.20D-07
ErrMax= 5.20D-07  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.62D-11 BMatP= 1.58D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.874D-04 0.232D-02 0.132D-02 0.874D-02-0.201D-02-0.951D-01
Coeff-Com: -0.174D+00 0.261D+00 0.997D+00
Coeff:     -0.874D-04 0.232D-02 0.132D-02 0.874D-02-0.201D-02-0.951D-01
Coeff:     -0.174D+00 0.261D+00 0.997D+00
Gap=     0.180 Goal=   None    Shift=    0.000
RMSDP=3.92D-07 MaxDP=1.85D-05 DE=-1.24D-09 OVMax= 3.16D-05

Cycle  13  Pass 1  IDiag  1:
RMSU=  9.64D-08    CP:  7.24D-01  1.05D+00  1.13D+00  1.95D+00  1.85D+00
               CP:  2.19D+00  3.00D+00  2.01D+00  2.20D+00
```

E= -723.413929324323 Delta-E= -0.000000000479 Rises=F Damp=F
DIIS: error= 3.76D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413929324323 IErMin=10 ErrMin= 3.76D-07
ErrMax= 3.76D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-11 BMatP= 4.62D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.986D-04-0.443D-02-0.313D-02 0.352D-01 0.451D-01-0.372D-01
Coeff-Com: -0.279D+00-0.140D+00 0.606D+00 0.778D+00
Coeff: 0.986D-04-0.443D-02-0.313D-02 0.352D-01 0.451D-01-0.372D-01
Coeff: -0.279D+00-0.140D+00 0.606D+00 0.778D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.70D-07 MaxDP=8.38D-06 DE=-4.79D-10 OVMax= 1.98D-05

Cycle 14 Pass 1 IDiag 1:
RMSU= 3.96D-08 CP: 7.24D-01 1.05D+00 1.13D+00 1.95D+00 1.84D+00
CP: 2.22D+00 3.00D+00 2.11D+00 3.00D+00 1.95D+00
E= -723.413929324471 Delta-E= -0.000000000148 Rises=F Damp=F
DIIS: error= 1.18D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413929324471 IErMin=11 ErrMin= 1.18D-07
ErrMax= 1.18D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.00D-12 BMatP= 2.03D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.491D-04-0.193D-02-0.134D-02 0.107D-01 0.163D-01 0.498D-02
Coeff-Com: -0.669D-01-0.931D-01 0.482D-01 0.293D+00 0.790D+00
Coeff: 0.491D-04-0.193D-02-0.134D-02 0.107D-01 0.163D-01 0.498D-02
Coeff: -0.669D-01-0.931D-01 0.482D-01 0.293D+00 0.790D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=8.17D-08 MaxDP=6.95D-06 DE=-1.48D-10 OVMax= 5.49D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 6.15D-08 CP: 7.24D-01 1.05D+00 1.13D+00 1.95D+00 1.84D+00
CP: 2.20D+00 3.00D+00 2.05D+00 3.00D+00 2.19D+00
CP: 1.04D+00
E= -723.413929324489 Delta-E= -0.000000000018 Rises=F Damp=F
DIIS: error= 8.59D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413929324489 IErMin=12 ErrMin= 8.59D-08
ErrMax= 8.59D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-12 BMatP= 3.00D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.181D-04 0.943D-03 0.673D-03-0.974D-02-0.110D-01 0.183D-01
Coeff-Com: 0.839D-01 0.748D-02-0.237D+00-0.176D+00 0.376D+00 0.947D+00
Coeff: -0.181D-04 0.943D-03 0.673D-03-0.974D-02-0.110D-01 0.183D-01
Coeff: 0.839D-01 0.748D-02-0.237D+00-0.176D+00 0.376D+00 0.947D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=7.36D-08 MaxDP=6.35D-06 DE=-1.84D-11 OVMax= 4.76D-06

Cycle 16 Pass 1 IDiag 1:
RMSU= 9.71D-09 CP: 7.24D-01 1.05D+00 1.13D+00 1.95D+00 1.83D+00
CP: 2.19D+00 3.00D+00 1.99D+00 3.00D+00 2.40D+00
CP: 1.19D+00 1.87D+00
E= -723.413929324480 Delta-E= 0.000000000009 Rises=F Damp=F

DIIS: error= 3.09D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=12 EnMin= -723.413929324489 IErMin=13 ErrMin= 3.09D-08
ErrMax= 3.09D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-13 BMatP= 1.01D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.131D-04 0.604D-03 0.435D-03-0.512D-02-0.636D-02 0.680D-02
Coeff-Com: 0.410D-01 0.118D-01-0.984D-01-0.993D-01 0.370D-01 0.382D+00
Coeff-Com: 0.729D+00
Coeff: -0.131D-04 0.604D-03 0.435D-03-0.512D-02-0.636D-02 0.680D-02
Coeff: 0.410D-01 0.118D-01-0.984D-01-0.993D-01 0.370D-01 0.382D+00
Coeff: 0.729D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.45D-08 MaxDP=9.63D-07 DE= 8.64D-12 OVMax= 1.18D-06

Cycle 17 Pass 1 IDiag 1:
RMSU= 4.07D-09 CP: 7.24D-01 1.05D+00 1.13D+00 1.95D+00 1.83D+00
CP: 2.18D+00 3.00D+00 1.98D+00 3.00D+00 2.46D+00
CP: 1.29D+00 2.03D+00 1.42D+00
E= -723.413929324503 Delta-E= -0.000000000022 Rises=F Damp=F
DIIS: error= 1.56D-08 at cycle 14 NSaved= 14.
NSaved=14 IEnMin=14 EnMin= -723.413929324503 IErMin=14 ErrMin= 1.56D-08
ErrMax= 1.56D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.49D-14 BMatP= 1.61D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.394D-06-0.542D-04-0.336D-04 0.106D-02 0.851D-03-0.285D-02
Coeff-Com: -0.103D-01 0.119D-02 0.401D-01 0.207D-01-0.124D+00-0.143D+00
Coeff-Com: 0.337D+00 0.879D+00
Coeff: 0.394D-06-0.542D-04-0.336D-04 0.106D-02 0.851D-03-0.285D-02
Coeff: -0.103D-01 0.119D-02 0.401D-01 0.207D-01-0.124D+00-0.143D+00
Coeff: 0.337D+00 0.879D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=1.05D-08 MaxDP=8.47D-07 DE=-2.21D-11 OVMax= 6.69D-07

Cycle 18 Pass 1 IDiag 1:
RMSU= 1.94D-09 CP: 7.24D-01 1.05D+00 1.13D+00 1.95D+00 1.83D+00
CP: 2.18D+00 3.00D+00 1.97D+00 3.00D+00 2.49D+00
CP: 1.36D+00 2.09D+00 1.75D+00 1.97D+00
E= -723.413929324498 Delta-E= 0.000000000005 Rises=F Damp=F
DIIS: error= 9.63D-09 at cycle 15 NSaved= 15.
NSaved=15 IEnMin=14 EnMin= -723.413929324503 IErMin=15 ErrMin= 9.63D-09
ErrMax= 9.63D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-14 BMatP= 5.49D-14
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.361D-05-0.184D-03-0.128D-03 0.184D-02 0.201D-02-0.297D-02
Coeff-Com: -0.154D-01-0.356D-02 0.453D-01 0.365D-01-0.723D-01-0.161D+00
Coeff-Com: -0.275D-01 0.365D+00 0.833D+00
Coeff: 0.361D-05-0.184D-03-0.128D-03 0.184D-02 0.201D-02-0.297D-02
Coeff: -0.154D-01-0.356D-02 0.453D-01 0.365D-01-0.723D-01-0.161D+00
Coeff: -0.275D-01 0.365D+00 0.833D+00
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.56D-09 MaxDP=3.53D-07 DE= 4.55D-12 OVMax= 3.77D-07

Supporting Information file

SCF Done: E(RwB97XD) = -723.413929324 A.U. after 18 cycles
NFock= 18 Conv=0.46D-08 -V/T= 2.0047
KE= 7.200583522920D+02 PE=-3.701465428570D+03 EE= 1.247797010425D+03
Leave Link 502 at Sat Sep 26 07:16:34 2026, MaxMem= 805306368 cpu: 7114.0 elap: 1186.1
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23221 LenP2D= 51946.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 07:16:34 2026, MaxMem= 805306368 cpu: 2.9 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 07:16:34 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 07:27:30 2026, MaxMem= 805306368 cpu: 3930.6 elap: 655.2
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.54717760D+00-1.55498257D-03-2.06281018D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000063459	-0.000538203	-0.000192871
2	6	0.000028678	0.000578779	0.000202815
3	6	-0.000056576	0.000544341	0.000198967
4	6	0.000148303	-0.000742960	-0.000229235
5	6	0.000023076	-0.000585469	-0.000198637
6	6	-0.000233679	0.000617681	0.000118764
7	6	0.000167030	0.000741289	0.000225151
8	6	0.000202973	-0.000131755	-0.000077692

```
     9        6        -0.000246560   -0.000615769   -0.000169655
    10        6        -0.000182925   -0.000087151    0.000184798
    11        6         0.000253553    0.000141917    0.000021412
    12        6         0.000208275    0.000705044   -0.000048092
    13        6        -0.000267117    0.000114533    0.000075036
    14        6         0.000275348   -0.000390286   -0.000168212
    15        6        -0.000220806    0.000490051    0.000114358
    16        6        -0.000092535   -0.000569716   -0.000092345
    17        7         0.000258942   -0.000852949    0.000147029
    18        7         0.000022464    0.000602215   -0.000121890
    19        1         0.000078548    0.000204868   -0.000197571
    20        1        -0.000065171    0.000028159    0.000010747
    21        1         0.000082930   -0.000194535    0.000183490
    22        1        -0.000070332   -0.000061541   -0.000018545
    23        1        -0.000051397   -0.000060579   -0.000004156
    24        1        -0.000073857   -0.000089736   -0.000014151
    25        1        -0.000065052    0.000084239    0.000033468
    26        1        -0.000060655    0.000067536    0.000017015
 ----------------------------------------------------------------------
 Cartesian Forces:  Max     0.000852949 RMS     0.000294740
 Leave Link  716 at Sat Sep 26 07:27:30 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000636199 RMS     0.000186307
 Search for a local minimum.
 Step number  23 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .18631D-03 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points   18   19   20   21   22
                                                     23
 DE= -3.88D-05 DEPred=-2.89D-05 R= 1.34D+00
 TightC=F SS=  1.41D+00  RLast= 6.77D-02 DXNew= 1.3552D+00 2.0312D-01
 Trust test= 1.34D+00 RLast= 6.77D-02 DXMaxT set to 8.06D-01
 ITU=  1  1  1  1  1  1  1  1  1 -1  1  1  1  1  1  1  1  1  1  0
 ITU=  0  1  0
    Eigenvalues ---    0.00297   0.00500   0.01048   0.01326   0.01708
    Eigenvalues ---    0.01844   0.02671   0.02797   0.02906   0.03058
    Eigenvalues ---    0.03340   0.03585   0.03786   0.04322   0.04358
    Eigenvalues ---    0.04461   0.05025   0.05328   0.05540   0.08085
    Eigenvalues ---    0.09953   0.10130   0.10937   0.11210   0.11295
    Eigenvalues ---    0.11789   0.12933   0.14172   0.15495   0.15743
```

```
    Eigenvalues ---    0.15898   0.16001   0.16001   0.16281   0.16488
    Eigenvalues ---    0.19057   0.22365   0.23065   0.24968   0.24999
    Eigenvalues ---    0.25000   0.25000   0.25002   0.25009   0.28808
    Eigenvalues ---    0.29871   0.33644   0.37247   0.38107   0.40442
    Eigenvalues ---    0.45816   0.45974   0.46739   0.47550   0.47688
    Eigenvalues ---    0.47691   0.47759   0.47960   0.48640   0.52127
    Eigenvalues ---    0.54811   0.55303   0.55637   0.55660   0.57132
    Eigenvalues ---    0.91939   0.93711   0.95030   0.95339   0.97719
    Eigenvalues ---    0.98834   1.37127
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    23   22   21   20
 RFO step:  Lambda=-2.35045058D-05.
 NNeg= 0 NGDIIS= 4 SimSw=  2.50D-01 Rises=F DC= -3.88D-05 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.3884182391D-02 NUsed= 4 OKEnD=T EnDIS=F
 InvSVX:  RCond= 1.56D-04 Info=           0 Equed=N FErr=  6.77D-15 BErr=  7.01D-17
 DidBck=F Rises=F RFO-DIIS coefs:    1.61045   -0.47711   -0.07947   -0.05387
 Iteration  1 RMS(Cart)=  0.00778494 RMS(Int)=  0.00005438
 Iteration  2 RMS(Cart)=  0.00005632 RMS(Int)=  0.00000432
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000432
  ITry=  1  IFail=0  DXMaxC=  3.57D-02  DCOld=  1.00D+10  DXMaxT=  8.06D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                        (Linear)    (Quad)   (Total)
   R1       2.32270   0.00018   0.00032   0.00026   0.00058   2.32327
   R2       2.53594  -0.00029  -0.00071  -0.00067  -0.00138   2.53457
   R3       2.53237  -0.00018  -0.00049  -0.00042  -0.00091   2.53146
   R4       2.32265   0.00019   0.00032   0.00027   0.00059   2.32324
   R5       2.31978   0.00013   0.00025   0.00015   0.00040   2.32019
   R6       2.53248  -0.00018  -0.00049  -0.00041  -0.00091   2.53157
   R7       2.53365  -0.00007  -0.00026  -0.00017  -0.00043   2.53322
   R8       2.31970   0.00015   0.00026   0.00017   0.00043   2.32013
   R9       2.31901   0.00010   0.00020   0.00008   0.00028   2.31929
  R10       2.53376  -0.00006  -0.00027  -0.00015  -0.00042   2.53333
  R11       2.62740  -0.00009  -0.00040  -0.00028  -0.00068   2.62671
  R12       2.31891   0.00015   0.00021   0.00011   0.00032   2.31922
  R13       2.69115   0.00041   0.00110   0.00085   0.00195   2.69309
  R14       2.69357  -0.00007  -0.00033   0.00030  -0.00003   2.69353
  R15       2.62761  -0.00014  -0.00043  -0.00038  -0.00080   2.62681
  R16       2.69315   0.00019  -0.00015   0.00032   0.00017   2.69332
  R17       2.81582  -0.00064  -0.00118  -0.00141  -0.00258   2.81324
  R18       2.05056   0.00009   0.00002   0.00019   0.00021   2.05077
  R19       2.81529  -0.00040  -0.00111  -0.00129  -0.00240   2.81290
  R20       2.05050   0.00010  -0.00001   0.00026   0.00025   2.05075
  R21       1.94385   0.00026   0.00023   0.00055   0.00078   1.94463
  R22       1.91706   0.00007   0.00008   0.00012   0.00020   1.91726
  R23       1.92992  -0.00006  -0.00020  -0.00033  -0.00053   1.92939
  R24       1.94391   0.00025   0.00023   0.00055   0.00078   1.94469
  R25       1.91705   0.00009   0.00008   0.00014   0.00022   1.91727
```

R26	1.92996	-0.00008	-0.00021	-0.00034	-0.00056	1.92940
A1	2.55540	0.00020	0.00082	0.00097	0.00179	2.55719
A2	2.61969	-0.00026	-0.00116	-0.00150	-0.00266	2.61703
A3	2.55752	0.00020	0.00078	0.00095	0.00172	2.55924
A4	2.70629	0.00045	0.00176	0.00233	0.00409	2.71037
A5	2.61777	-0.00026	-0.00110	-0.00140	-0.00251	2.61526
A6	2.85286	-0.00054	-0.00235	-0.00286	-0.00521	2.84765
A7	2.70758	0.00045	0.00174	0.00237	0.00411	2.71169
A8	2.85194	-0.00052	-0.00230	-0.00274	-0.00505	2.84689
A9	2.08479	0.00011	0.00028	0.00019	0.00046	2.08526
A10	2.10745	-0.00004	0.00019	0.00005	0.00024	2.10769
A11	2.09046	-0.00007	-0.00047	-0.00022	-0.00069	2.08977
A12	2.08480	0.00004	0.00021	0.00036	0.00056	2.08536
A13	2.09046	-0.00005	-0.00054	-0.00010	-0.00064	2.08982
A14	2.10739	0.00001	0.00039	-0.00023	0.00016	2.10755
A15	2.05560	0.00009	0.00022	-0.00028	-0.00005	2.05555
A16	1.92585	0.00026	0.00195	-0.00004	0.00191	1.92776
A17	2.05615	-0.00006	-0.00018	-0.00028	-0.00047	2.05569
A18	1.92649	0.00007	0.00121	0.00056	0.00177	1.92826
A19	2.01393	0.00023	-0.00015	0.00191	0.00177	2.01569
A20	1.92437	-0.00005	-0.00020	-0.00034	-0.00054	1.92383
A21	1.88857	-0.00011	0.00063	-0.00103	-0.00040	1.88817
A22	1.89795	-0.00006	-0.00017	-0.00017	-0.00034	1.89761
A23	1.84579	-0.00003	0.00033	-0.00053	-0.00020	1.84559
A24	1.88817	0.00000	-0.00044	0.00006	-0.00039	1.88778
A25	2.01395	0.00021	-0.00003	0.00176	0.00173	2.01569
A26	1.92437	-0.00000	-0.00028	-0.00023	-0.00052	1.92385
A27	1.88871	-0.00012	0.00067	-0.00109	-0.00041	1.88829
A28	1.89783	-0.00006	-0.00023	-0.00008	-0.00031	1.89752
A29	1.84570	-0.00003	0.00028	-0.00044	-0.00016	1.84554
A30	1.88823	-0.00001	-0.00042	-0.00003	-0.00044	1.88779
A31	2.90383	0.00003	0.00077	0.00040	0.00116	2.90499
A32	3.12608	0.00006	-0.00000	0.00054	0.00053	3.12660
A33	2.90406	0.00004	0.00095	0.00066	0.00159	2.90565
A34	3.12641	0.00001	-0.00032	-0.00026	-0.00058	3.12582
A35	3.98145	0.00035	0.00217	-0.00031	0.00186	3.98331
A36	3.98265	0.00001	0.00102	0.00028	0.00130	3.98395
A37	3.14536	0.00002	0.00041	0.00005	0.00048	3.14583
A38	3.13653	0.00020	0.00310	0.00089	0.00399	3.14052
A39	3.14524	0.00007	0.00040	0.00007	0.00046	3.14570
A40	3.14066	-0.00000	-0.00265	0.00088	-0.00178	3.13888
A41	4.01554	0.00055	-0.00044	0.00237	0.00194	4.01748
A42	4.01691	0.00010	-0.00117	0.00096	-0.00021	4.01670
D1	0.01581	0.00003	-0.00022	-0.00091	-0.00113	0.01468
D2	-0.01342	0.00008	0.00071	0.00158	0.00230	-0.01112
D3	-0.01106	0.00007	0.00090	0.00128	0.00218	-0.00889
D4	0.01616	-0.00001	-0.00056	-0.00094	-0.00149	0.01467
D5	0.00134	0.00000	0.00007	-0.00090	-0.00084	0.00049

D6	-0.01061	0.00001	0.00008	0.00125	0.00133	-0.00928
D7	-0.00206	-0.00005	0.00258	-0.00156	0.00100	-0.00106
D8	3.10121	0.00007	0.00474	-0.00011	0.00463	3.10584
D9	0.00169	-0.00005	-0.00044	-0.00092	-0.00136	0.00033
D10	0.00062	-0.00006	-0.00141	-0.00151	-0.00291	-0.00229
D11	3.10555	0.00002	-0.00155	-0.00007	-0.00164	3.10391
D12	0.00627	0.00002	-0.00066	0.00148	0.00082	0.00709
D13	-3.10072	-0.00005	-0.00233	0.00059	-0.00175	-3.10247
D14	-3.10217	0.00005	-0.00026	0.00057	0.00031	-3.10186
D15	0.07402	-0.00001	-0.00193	-0.00033	-0.00226	0.07176
D16	2.51332	0.00003	-0.00146	0.00059	-0.00088	2.51244
D17	-0.66187	-0.00000	-0.00187	0.00152	-0.00036	-0.66222
D18	-0.66212	0.00006	0.00182	-0.00157	0.00025	-0.66187
D19	2.51452	-0.00000	0.00013	-0.00249	-0.00236	2.51216
D20	-1.14641	-0.00003	-0.01301	-0.00021	-0.01321	-1.15962
D21	1.01195	0.00003	-0.01350	0.00073	-0.01277	0.99918
D22	3.07382	-0.00006	-0.01378	-0.00001	-0.01378	3.06004
D23	-1.14781	-0.00004	-0.01324	-0.00014	-0.01338	-1.16119
D24	1.01040	0.00003	-0.01379	0.00090	-0.01289	0.99750
D25	3.07243	-0.00005	-0.01406	0.00009	-0.01397	3.05846

Item	Value	Threshold	Converged?
Maximum Force	0.000636	0.000450	NO
RMS Force	0.000186	0.000300	YES
Maximum Displacement	0.035675	0.001800	NO
RMS Displacement	0.007788	0.001200	NO

Predicted change in Energy=-1.175885D-05
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 07:27:30 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.014808	0.669249	0.047030
2	6	0	3.337058	1.692718	0.115188
3	6	0	4.014142	-0.668692	-0.046912
4	6	0	2.138132	2.288569	0.160348
5	6	0	3.337485	-1.692871	-0.114980
6	6	0	0.910943	2.326468	0.166491
7	6	0	2.138076	-2.287909	-0.159842
8	6	0	-0.383553	1.978808	0.146000
9	6	0	0.910937	-2.326573	-0.165573
10	6	0	-1.460976	1.392629	0.102972
11	6	0	-0.383558	-1.978739	-0.144367

12	6	0	-2.671103	0.710481	0.054373
13	6	0	-1.461246	-1.393145	-0.100946
14	6	0	-2.671224	-0.710512	-0.054034
15	6	0	-3.907940	1.412161	0.151932
16	6	0	-3.908012	-1.411912	-0.152566
17	7	0	-3.724924	2.875701	-0.050038
18	7	0	-3.725472	-2.875429	0.048654
19	1	0	-3.431121	3.159086	-0.994669
20	1	0	-4.577020	3.372006	0.188646
21	1	0	-3.431453	-3.159346	0.993088
22	1	0	-4.577846	-3.371336	-0.189875
23	1	0	-2.984945	3.193853	0.577364
24	1	0	-4.743101	1.049392	-0.438498
25	1	0	-4.743744	-1.048903	0.436887
26	1	0	-2.985828	-3.193675	-0.579103

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229423	0.000000			
3	C	1.341235	2.461905	0.000000		
4	C	2.481321	1.339590	3.508242	0.000000	
5	C	2.462646	3.393404	1.229407	4.167267	0.000000
6	C	3.520601	2.508048	4.318144	1.227790	4.703448
7	C	3.508519	4.166364	2.480774	4.587665	1.339651
8	C	4.590242	3.731721	5.136749	2.540679	5.234067
9	C	4.319047	4.703147	3.520302	4.786624	2.508440
10	C	5.523643	4.807425	5.852215	3.709391	5.709032
11	C	5.137519	5.233541	4.589715	4.966053	3.732124
12	C	6.686042	6.088225	6.826776	5.062640	6.473632
13	C	5.853421	5.709027	5.523371	5.155464	4.808103
14	C	6.827663	6.473299	6.685500	5.671891	6.088786
15	C	7.958195	7.250522	8.193221	6.109267	7.887246
16	C	8.194031	7.886790	7.957641	7.095585	7.251040
17	N	8.048684	7.162286	8.512102	5.896136	8.411522
18	N	8.513323	8.411404	8.048629	7.814166	7.163140
19	H	7.919993	7.013577	8.425085	5.753993	8.374328
20	H	9.008023	8.090614	9.496883	6.802051	9.401306
21	H	8.426148	8.374125	7.919712	7.835401	7.014049
22	H	9.498219	9.401245	9.008162	8.789854	8.091682
23	H	7.459989	6.514195	8.018490	5.219134	8.020757
24	H	8.779591	8.124617	8.932774	7.017517	8.539353
25	H	8.933995	8.539282	8.779475	7.653457	8.125609
26	H	8.020171	8.021083	7.460452	7.540342	6.515528

		6	7	8	9	10
6	C	0.000000				
7	C	4.785898	0.000000			
8	C	1.340524	4.965583	0.000000		

9	C	4.664875	1.227761	4.506560	0.000000	
10	C	2.549919	5.154474	1.227313	4.419339	0.000000
11	C	4.506347	2.540563	3.968184	1.340581	3.547975
12	C	3.931289	5.671369	2.617237	4.701392	1.389998
13	C	4.419765	3.709338	3.548587	2.550043	2.793228
14	C	4.701467	5.062483	3.536367	3.931408	2.431574
15	C	4.904875	7.095211	3.569654	6.107415	2.447532
16	C	6.107340	6.109222	4.899789	4.905002	3.730782
17	N	4.673308	7.813430	3.465200	6.969090	2.710789
18	N	6.969214	5.896595	5.894193	4.673695	4.831895
19	H	4.571112	7.834707	3.461481	7.045093	2.864726
20	H	5.586714	8.789118	4.419048	7.919403	3.692560
21	H	7.045127	5.753981	6.033894	4.570816	5.039401
22	H	7.919518	6.802817	6.806537	5.587384	5.700526
23	H	4.012370	7.539133	2.903386	6.797423	2.406644
24	H	5.827962	7.652831	4.495677	6.590886	3.344151
25	H	6.591033	7.017882	5.316287	5.828449	4.104771
26	H	6.797993	5.220209	5.835425	4.013434	4.881044

		11	12	13	14	15
11	C	0.000000				
12	C	3.536137	0.000000			
13	C	1.227281	2.431691	0.000000		
14	C	2.617245	1.425123	1.390048	0.000000	
15	C	4.899720	1.425356	3.730951	2.465285	0.000000
16	C	3.569753	2.465222	2.447382	1.425242	2.840441
17	N	5.893998	2.410315	4.832171	3.737811	1.488704
18	N	3.465501	3.737710	2.710399	2.410155	4.292713
19	H	6.033896	2.770159	5.040035	4.054138	2.143315
20	H	6.806357	3.276319	5.700752	4.511974	2.071234
21	H	3.460824	4.053996	2.863231	2.769693	4.672607
22	H	4.419666	4.511824	3.692471	3.276224	4.842256
23	H	5.834708	2.557176	4.880810	3.967512	2.051180
24	H	5.316174	2.156608	4.104936	2.745497	1.085220
25	H	4.495962	2.745467	3.344033	2.156584	2.614689
26	H	2.904630	3.967717	2.407258	2.557493	4.753780

		16	17	18	19	20
16	C	0.000000				
17	N	4.292745	0.000000			
18	N	1.488520	5.751977	0.000000		
19	H	4.672321	1.029056	6.131112	0.000000	
20	H	4.842506	1.014572	6.306756	1.660920	0.000000
21	H	2.143166	6.131561	1.029083	6.623728	6.679671
22	H	2.071090	6.306545	1.014575	6.679004	6.753957
23	H	4.753727	1.020991	6.137108	1.634494	1.648497
24	H	2.614794	2.126733	4.083761	2.545865	2.411520
25	H	1.085209	4.083822	2.126923	4.634598	4.431010
26	H	2.051107	6.137060	1.020996	6.381893	6.799228

		21	22	23	24	25

```
  21  H    0.000000
  22  H    1.660891   0.000000
  23  H    6.382424   6.799095   0.000000
  24  H    4.635012   4.430797   2.953270   0.000000
  25  H    2.546653   2.411234   4.595006   2.273574   0.000000
  26  H    1.634486   1.648509   6.491374   4.594714   2.953397
            26
  26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=3 Diff= 9.69D-04
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.522512   -0.670149   -0.022893
    2          6           0        3.844827   -1.695429   -0.054897
    3          6           0        4.521760    0.670275    0.023717
    4          6           0        2.645939   -2.292577   -0.079065
    5          6           0        3.845038    1.696178    0.055505
    6          6           0        1.418752   -2.330744   -0.083956
    7          6           0        2.645591    2.292356    0.079224
    8          6           0        0.124235   -1.982656   -0.075858
    9          6           0        1.418450    2.331124    0.083494
   10          6           0       -0.953226   -1.395389   -0.053650
   11          6           0        0.123976    1.982679    0.074495
   12          6           0       -2.163396   -0.712024   -0.029274
   13          6           0       -0.953674    1.395850    0.051712
   14          6           0       -2.163608    0.711912    0.028857
   15          6           0       -3.400185   -1.416788   -0.102072
   16          6           0       -3.400445    1.416280    0.102453
   17          7           0       -3.217099   -2.872268    0.151497
   18          7           0       -3.217975    2.871785   -0.150338
   19          1           0       -2.923352   -3.122081    1.105573
   20          1           0       -4.069147   -3.376748   -0.069566
   21          1           0       -2.923900    3.122173   -1.104193
   22          1           0       -4.070396    3.375758    0.070456
   23          1           0       -2.477053   -3.212343   -0.464217
   24          1           0       -4.235412   -1.033435    0.475110
   25          1           0       -4.236111    1.032619   -0.473868
   26          1           0       -2.478398    3.212058    0.465837
---------------------------------------------------------------------
Rotational constants (GHZ):          0.6022165          0.2710366          0.1875868
```

Leave Link 202 at Sat Sep 26 07:27:30 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.3238101100 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0153915018 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.3084186081 Hartrees.
Leave Link 301 at Sat Sep 26 07:27:30 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51951.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.87D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 07:27:31 2026, MaxMem= 805306368 cpu: 5.7 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 07:27:31 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 -0.000000 0.000000

```
      Rot=    1.000000    0.000017   -0.000011   -0.000220 Ang=   0.03 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Generating alternative initial guess.
 ExpMin= 9.52D-02 ExpMax= 1.97D+04 ExpMxC= 6.73D+02 IAcc=3 IRadAn=          5 AccDes=
0.00D+00
 Harris functional with IExCor= 4639 and IRadAn=       5 diagonalized for initial guess.
 HarFok:  IExCor= 4639 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
      NFxFlg=          0 DoJE=T BraDBF=F KetDBF=T FulRan=T
      wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=          0
      NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Petite list used in FoFCou.
 Harris En= -691.982042050579
 Leave Link  401 at Sat Sep 26 07:27:39 2026, MaxMem=    805306368 cpu:                45.9 elap:
7.7
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.
 Integral accuracy reduced to 1.0D-05 until final iterations.

 Cycle   1  Pass 0  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=          0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=          0 FMFlag=      100000 FMFlg1=          0
      NFxFlg=          0 DoJE=T BraDBF=F KetDBF=F FulRan=T
      wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=          0 NGrid=          0
      NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.413732906385
 DIIS: error= 1.15D-03 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -723.413732906385     IErMin= 1 ErrMin= 1.15D-03
 ErrMax= 1.15D-03  0.00D+00 EMaxC= 1.00D-01 BMatC= 3.73D-04 BMatP= 3.73D-04
 IDIUse=3 WtCom= 9.88D-01 WtEn= 1.15D-02
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=     0.704 Goal=   None    Shift=    0.000
 GapD=    0.704 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.
 RMSDP=8.05D-03 MaxDP=2.99D-01              OVMax= 2.68D-03
```

Cycle 2 Pass 0 IDiag 1:
RMSU= 6.81D-03 CP: 1.40D+00
E= -723.414009321531 Delta-E= -0.000276415146 Rises=F Damp=F
DIIS: error= 7.11D-04 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.414009321531 IErMin= 2 ErrMin= 7.11D-04
ErrMax= 7.11D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-04 BMatP= 3.73D-04
IDIUse=3 WtCom= 9.93D-01 WtEn= 7.11D-03
Coeff-Com: 0.243D+00 0.757D+00
Coeff-En: 0.000D+00 0.100D+01
Coeff: 0.241D+00 0.759D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=6.04D-03 MaxDP=2.26D-01 DE=-2.76D-04 OVMax= 1.20D-03

Cycle 3 Pass 0 IDiag 1:
RMSU= 3.07D-03 CP: 1.04D+00 4.78D-01
E= -723.414030370424 Delta-E= -0.000021048892 Rises=F Damp=F
DIIS: error= 4.22D-03 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.414030370424 IErMin= 2 ErrMin= 7.11D-04
ErrMax= 4.22D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.02D-04 BMatP= 1.04D-04
IDIUse=3 WtCom= 1.33D-01 WtEn= 8.67D-01
Coeff-Com: 0.127D+00 0.672D+00 0.201D+00
Coeff-En: 0.000D+00 0.294D+00 0.706D+00
Coeff: 0.169D-01 0.344D+00 0.639D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=7.51D+02 MaxDP=2.98D+04 DE=-2.10D-05 OVMax= 9.97D-01

Problem detected with inexpensive integrals.
Switching to full accuracy and repeating last cycle.
Cycle 4 Pass 1 IDiag 1:
E= -723.413844741065 Delta-E= 0.000185629358 Rises=F Damp=F
DIIS: error= 1.21D-03 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413844741065 IErMin= 1 ErrMin= 1.21D-03
ErrMax= 1.21D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-04 BMatP= 1.52D-04
IDIUse=3 WtCom= 9.88D-01 WtEn= 1.21D-02
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.179 Goal= None Shift= 0.000
GapD= 0.179 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.
RMSDP=4.35D-03 MaxDP=1.07D-01 DE= 1.86D-04 OVMax= 1.38D-03

Cycle 5 Pass 1 IDiag 1:
RMSU= 3.74D-03 CP: 8.18D-01
E= -723.413941562140 Delta-E= -0.000096821075 Rises=F Damp=F
DIIS: error= 6.58D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413941562140 IErMin= 2 ErrMin= 6.58D-05
ErrMax= 6.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.96D-07 BMatP= 1.52D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.274D-01 0.103D+01
Coeff: -0.274D-01 0.103D+01
Gap= 0.180 Goal= None Shift= 0.000
RMSDP=4.16D-04 MaxDP=1.80D-02 DE=-9.68D-05 OVMax= 3.66D-04

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.09D-04 CP: 8.32D-01 1.06D+00
E= -723.413941180950 Delta-E= 0.000000381190 Rises=F Damp=F
DIIS: error= 7.41D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 2 EnMin= -723.413941562140 IErMin= 2 ErrMin= 6.58D-05
ErrMax= 7.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-06 BMatP= 6.96D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.201D-01 0.629D+00 0.391D+00
Coeff: -0.201D-01 0.629D+00 0.391D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.07D-05 MaxDP=9.84D-04 DE= 3.81D-07 OVMax= 3.47D-04

Cycle 7 Pass 1 IDiag 1:
RMSU= 5.24D-06 CP: 8.33D-01 1.06D+00 1.05D+00
E= -723.413942576941 Delta-E= -0.000001395991 Rises=F Damp=F
DIIS: error= 9.50D-06 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413942576941 IErMin= 4 ErrMin= 9.50D-06
ErrMax= 9.50D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-08 BMatP= 6.96D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.601D-04-0.220D-01 0.731D-01 0.949D+00
Coeff: 0.601D-04-0.220D-01 0.731D-01 0.949D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.15D-05 MaxDP=1.53D-03 DE=-1.40D-06 OVMax= 1.26D-04

Cycle 8 Pass 1 IDiag 1:
RMSU= 3.70D-06 CP: 8.35D-01 1.06D+00 1.12D+00 1.97D+00
E= -723.413942630109 Delta-E= -0.000000053168 Rises=F Damp=F
DIIS: error= 6.27D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413942630109 IErMin= 5 ErrMin= 6.27D-06
ErrMax= 6.27D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.82D-09 BMatP= 2.02D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.248D-02-0.886D-01-0.430D-02 0.509D+00 0.582D+00
Coeff: 0.248D-02-0.886D-01-0.430D-02 0.509D+00 0.582D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=6.66D-06 MaxDP=3.31D-04 DE=-5.32D-08 OVMax= 9.78D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 4.81D-07 CP: 8.35D-01 1.06D+00 1.14D+00 2.24D+00 1.25D+00
E= -723.413942649051 Delta-E= -0.000000018942 Rises=F Damp=F
DIIS: error= 3.66D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413942649051 IErMin= 6 ErrMin= 3.66D-06
ErrMax= 3.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-09 BMatP= 8.82D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.637D-03-0.186D-01-0.115D-01-0.640D-01 0.716D-01 0.102D+01
Coeff: 0.637D-03-0.186D-01-0.115D-01-0.640D-01 0.716D-01 0.102D+01
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=9.48D-07 MaxDP=6.18D-05 DE=-1.89D-08 OVMax= 8.06D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 4.60D-07 CP: 8.35D-01 1.06D+00 1.14D+00 2.34D+00 1.34D+00
CP: 1.79D+00
E= -723.413942658073 Delta-E= -0.000000009022 Rises=F Damp=F
DIIS: error= 3.17D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413942658073 IErMin= 7 ErrMin= 3.17D-06
ErrMax= 3.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.96D-10 BMatP= 1.21D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.723D-03 0.289D-01-0.456D-02-0.291D+00-0.267D+00 0.761D+00
Coeff-Com: 0.773D+00
Coeff: -0.723D-03 0.289D-01-0.456D-02-0.291D+00-0.267D+00 0.761D+00
Coeff: 0.773D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.03D-06 MaxDP=4.26D-05 DE=-9.02D-09 OVMax= 8.73D-05

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.94D-07 CP: 8.35D-01 1.06D+00 1.14D+00 2.37D+00 1.36D+00
CP: 2.51D+00 1.82D+00
E= -723.413942662985 Delta-E= -0.000000004913 Rises=F Damp=F
DIIS: error= 1.12D-06 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413942662985 IErMin= 8 ErrMin= 1.12D-06
ErrMax= 1.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.55D-11 BMatP= 9.96D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.215D-03 0.741D-02 0.250D-02-0.295D-01-0.737D-01-0.580D-01
Coeff-Com: 0.168D+00 0.984D+00
Coeff: -0.215D-03 0.741D-02 0.250D-02-0.295D-01-0.737D-01-0.580D-01
Coeff: 0.168D+00 0.984D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.19D-06 MaxDP=5.81D-05 DE=-4.91D-09 OVMax= 3.06D-05

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.24D-07 CP: 8.35D-01 1.06D+00 1.13D+00 2.32D+00 1.31D+00
CP: 2.59D+00 2.17D+00 1.71D+00
E= -723.413942663706 Delta-E= -0.000000000721 Rises=F Damp=F
DIIS: error= 5.62D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413942663706 IErMin= 9 ErrMin= 5.62D-07
ErrMax= 5.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.98D-11 BMatP= 9.55D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.993D-04-0.473D-02 0.336D-02 0.763D-01 0.340D-01-0.290D+00
Coeff-Com: -0.136D+00 0.608D+00 0.709D+00
Coeff: 0.993D-04-0.473D-02 0.336D-02 0.763D-01 0.340D-01-0.290D+00
Coeff: -0.136D+00 0.608D+00 0.709D+00

Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.86D-07 MaxDP=3.03D-05 DE=-7.21D-10 OVMax= 1.85D-05

Cycle 13 Pass 1 IDiag 1:
RMSU= 4.67D-08 CP: 8.35D-01 1.06D+00 1.13D+00 2.30D+00 1.28D+00
CP: 2.59D+00 2.35D+00 2.17D+00 1.60D+00
E= -723.413942663929 Delta-E= -0.000000000223 Rises=F Damp=F
DIIS: error= 3.01D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413942663929 IErMin=10 ErrMin= 3.01D-07
ErrMax= 3.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.38D-12 BMatP= 4.98D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.826D-04-0.343D-02 0.115D-02 0.394D-01 0.261D-01-0.117D+00
Coeff-Com: -0.832D-01 0.910D-01 0.302D+00 0.744D+00
Coeff: 0.826D-04-0.343D-02 0.115D-02 0.394D-01 0.261D-01-0.117D+00
Coeff: -0.832D-01 0.910D-01 0.302D+00 0.744D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=7.72D-08 MaxDP=4.12D-06 DE=-2.23D-10 OVMax= 4.64D-06

Cycle 14 Pass 1 IDiag 1:
RMSU= 2.12D-08 CP: 8.35D-01 1.06D+00 1.13D+00 2.30D+00 1.27D+00
CP: 2.55D+00 2.37D+00 2.28D+00 1.85D+00 1.45D+00
E= -723.413942663940 Delta-E= -0.000000000010 Rises=F Damp=F
DIIS: error= 1.04D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413942663940 IErMin=11 ErrMin= 1.04D-07
ErrMax= 1.04D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-12 BMatP= 6.38D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.300D-05 0.305D-03-0.604D-03-0.959D-02-0.281D-02 0.474D-01
Coeff-Com: 0.161D-01-0.152D+00-0.110D+00 0.235D+00 0.976D+00
Coeff: -0.300D-05 0.305D-03-0.604D-03-0.959D-02-0.281D-02 0.474D-01
Coeff: 0.161D-01-0.152D+00-0.110D+00 0.235D+00 0.976D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=6.42D-08 MaxDP=4.18D-06 DE=-1.05D-11 OVMax= 2.91D-06

Cycle 15 Pass 1 IDiag 1:
RMSU= 1.21D-08 CP: 8.35D-01 1.06D+00 1.13D+00 2.30D+00 1.27D+00
CP: 2.53D+00 2.37D+00 2.32D+00 1.97D+00 1.77D+00
CP: 1.84D+00
E= -723.413942663955 Delta-E= -0.000000000015 Rises=F Damp=F
DIIS: error= 5.79D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413942663955 IErMin=12 ErrMin= 5.79D-08
ErrMax= 5.79D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.56D-13 BMatP= 1.33D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.180D-04 0.833D-03-0.507D-03-0.124D-01-0.666D-02 0.453D-01
Coeff-Com: 0.249D-01-0.897D-01-0.111D+00-0.433D-01 0.443D+00 0.749D+00
Coeff: -0.180D-04 0.833D-03-0.507D-03-0.124D-01-0.666D-02 0.453D-01
Coeff: 0.249D-01-0.897D-01-0.111D+00-0.433D-01 0.443D+00 0.749D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.09D-08 MaxDP=1.33D-06 DE=-1.50D-11 OVMax= 1.00D-06

Supporting Information file

Cycle 16 Pass 1 IDiag 1:
RMSU= 3.59D-09 CP: 8.35D-01 1.06D+00 1.13D+00 2.30D+00 1.27D+00
CP: 2.52D+00 2.37D+00 2.32D+00 1.98D+00 1.88D+00
CP: 2.11D+00 1.44D+00
E= -723.413942663954 Delta-E= 0.000000000001 Rises=F Damp=F
DIIS: error= 1.98D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=12 EnMin= -723.413942663955 IErMin=13 ErrMin= 1.98D-08
ErrMax= 1.98D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.77D-14 BMatP= 3.56D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.682D-05 0.283D-03-0.934D-04-0.325D-02-0.212D-02 0.934D-02
Coeff-Com: 0.747D-02-0.847D-02-0.228D-01-0.615D-01-0.632D-02 0.294D+00
Coeff-Com: 0.793D+00
Coeff: -0.682D-05 0.283D-03-0.934D-04-0.325D-02-0.212D-02 0.934D-02
Coeff: 0.747D-02-0.847D-02-0.228D-01-0.615D-01-0.632D-02 0.294D+00
Coeff: 0.793D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.18D-09 MaxDP=2.50D-07 DE= 1.14D-12 OVMax= 4.17D-07

SCF Done: E(RwB97XD) = -723.413942664 A.U. after 16 cycles
NFock= 16 Conv=0.52D-08 -V/T= 2.0047
KE= 7.200605605142D+02 PE=-3.701690389587D+03 EE= 1.247907467800D+03
Leave Link 502 at Sat Sep 26 07:46:50 2026, MaxMem= 805306368 cpu: 6904.0 elap: 1151.2
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51951.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 07:46:50 2026, MaxMem= 805306368 cpu: 3.5 elap: 0.6
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 07:46:50 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 07:58:45 2026, MaxMem= 805306368 cpu: 4287.9 elap: 714.8
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.54254381D+00-1.15705223D-03 2.02739411D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000067272	-0.000183338	-0.000149487
2	6	0.000112652	0.000282737	0.000166720
3	6	-0.000056801	0.000178713	0.000148451
4	6	-0.000057625	-0.000395619	-0.000183019
5	6	0.000098100	-0.000276357	-0.000172800
6	6	-0.000000401	0.000317481	0.000157166
7	6	-0.000046894	0.000390732	0.000188368
8	6	0.000046595	-0.000101159	-0.000038448
9	6	-0.000018002	-0.000311447	-0.000131839
10	6	-0.000041038	0.000025270	-0.000046067
11	6	0.000056613	0.000078626	0.000050217
12	6	-0.000010436	-0.000209921	0.000019260
13	6	0.000003252	0.000012710	-0.000054046
14	6	-0.000027263	0.000186705	0.000049764
15	6	0.000096243	0.000013511	-0.000027860
16	6	0.000099834	0.000063183	0.000004129
17	7	-0.000216782	-0.000088013	0.000102517
18	7	-0.000232645	0.000036658	-0.000080705
19	1	0.000053797	0.000044097	-0.000086446
20	1	0.000005315	0.000049186	0.000004038
21	1	0.000056929	-0.000039588	0.000084045
22	1	0.000005252	-0.000050103	-0.000011892
23	1	0.000081942	0.000086338	0.000008788
24	1	-0.000004900	-0.000003460	-0.000003851
25	1	-0.000013824	-0.000027608	0.000004511
26	1	0.000077359	-0.000079333	-0.000001513

Cartesian Forces: Max 0.000395619 RMS 0.000129204
Leave Link 716 at Sat Sep 26 07:58:46 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000287446 RMS 0.000079184
Search for a local minimum.

Supporting Information file

```
 Step number  24 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .79184D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points   18   19   20   21   22
                                                     23   24
 DE= -1.33D-05 DEPred=-1.18D-05 R= 1.13D+00
 TightC=F SS=  1.41D+00  RLast= 3.63D-02 DXNew= 1.3552D+00 1.0876D-01
 Trust test= 1.13D+00 RLast= 3.63D-02 DXMaxT set to 8.06D-01
 ITU=  1  1  1  1  1  1  1  1  1 -1  1  1  1  1  1  1  1  1
 ITU=  0  0  1  0
    Eigenvalues ---    0.00283   0.00503   0.01051   0.01315   0.01709
    Eigenvalues ---    0.01840   0.02671   0.02794   0.02901   0.03063
    Eigenvalues ---    0.03307   0.03530   0.03783   0.04319   0.04340
    Eigenvalues ---    0.04461   0.05025   0.05380   0.05582   0.08066
    Eigenvalues ---    0.09847   0.09960   0.10372   0.11110   0.11205
    Eigenvalues ---    0.11790   0.11924   0.14030   0.15553   0.15651
    Eigenvalues ---    0.15896   0.16001   0.16003   0.16295   0.16464
    Eigenvalues ---    0.17732   0.22374   0.22794   0.24966   0.25000
    Eigenvalues ---    0.25000   0.25000   0.25005   0.25026   0.28910
    Eigenvalues ---    0.29985   0.35326   0.37245   0.38475   0.43192
    Eigenvalues ---    0.45813   0.46449   0.46732   0.47687   0.47690
    Eigenvalues ---    0.47696   0.47843   0.47973   0.48541   0.52039
    Eigenvalues ---    0.54815   0.55295   0.55637   0.55660   0.57408
    Eigenvalues ---    0.91781   0.93716   0.95029   0.95372   0.97720
    Eigenvalues ---    0.98775   1.37103
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    24   23   22   21   20
 RFO step:  Lambda=-3.01668865D-06.
 NNeg= 0 NGDIIS= 5 SimSw=  2.50D-01 Rises=F DC= -1.33D-05 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.8408216524D-03 NUsed= 5 OKEnD=T EnDIS=F
 InvSVX:  RCond= 3.56D-06 Info=           0 Equed=N FErr=  3.44D-14 BErr=  4.95D-17
 DidBck=F Rises=F RFO-DIIS coefs:    1.14474   -0.10847    0.01724   -0.03475   -0.01876
 Iteration  1 RMS(Cart)=  0.00119366 RMS(Int)=  0.00000150
 Iteration  2 RMS(Cart)=  0.00000185 RMS(Int)=  0.00000111
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000111
  ITry=  1  IFail=0  DXMaxC=  4.24D-03  DCOld=  1.00D+10  DXMaxT=  8.06D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                       (Linear)    (Quad)   (Total)
    R1       2.32327   0.00006   0.00016   0.00004   0.00020   2.32347
    R2       2.53457  -0.00008  -0.00032  -0.00011  -0.00043   2.53414
    R3       2.53146  -0.00004  -0.00024  -0.00002  -0.00025   2.53120
    R4       2.32324   0.00005   0.00016   0.00003   0.00019   2.32344
    R5       2.32019  -0.00000   0.00013  -0.00003   0.00010   2.32028
    R6       2.53157  -0.00005  -0.00024  -0.00004  -0.00028   2.53129
    R7       2.53322   0.00002  -0.00014   0.00008  -0.00006   2.53317
```

R8	2.32013	-0.00000	0.00013	-0.00004	0.00010	2.32023
R9	2.31929	0.00003	0.00009	-0.00001	0.00008	2.31937
R10	2.53333	-0.00000	-0.00014	0.00004	-0.00010	2.53323
R11	2.62671	0.00001	-0.00018	0.00007	-0.00011	2.62660
R12	2.31922	0.00003	0.00009	-0.00001	0.00008	2.31931
R13	2.69309	-0.00008	0.00055	-0.00032	0.00023	2.69332
R14	2.69353	0.00004	-0.00015	0.00005	-0.00010	2.69343
R15	2.62681	0.00003	-0.00021	0.00012	-0.00009	2.62672
R16	2.69332	0.00005	-0.00013	0.00014	0.00001	2.69332
R17	2.81324	0.00008	-0.00066	0.00033	-0.00034	2.81290
R18	2.05077	0.00001	-0.00003	0.00008	0.00005	2.05082
R19	2.81290	0.00012	-0.00063	0.00035	-0.00028	2.81262
R20	2.05075	0.00000	-0.00001	0.00005	0.00004	2.05079
R21	1.94463	0.00011	0.00006	0.00026	0.00032	1.94495
R22	1.91726	0.00002	0.00002	0.00001	0.00003	1.91729
R23	1.92939	0.00009	-0.00008	0.00017	0.00009	1.92948
R24	1.94469	0.00011	0.00006	0.00025	0.00031	1.94500
R25	1.91727	0.00002	0.00001	0.00002	0.00004	1.91730
R26	1.92940	0.00008	-0.00008	0.00014	0.00006	1.92946
A1	2.55719	0.00008	0.00033	0.00033	0.00066	2.55785
A2	2.61703	-0.00018	-0.00043	-0.00076	-0.00119	2.61585
A3	2.55924	0.00007	0.00031	0.00027	0.00058	2.55983
A4	2.71037	0.00029	0.00067	0.00122	0.00189	2.71226
A5	2.61526	-0.00018	-0.00041	-0.00080	-0.00121	2.61405
A6	2.84765	-0.00023	-0.00095	-0.00093	-0.00188	2.84577
A7	2.71169	0.00028	0.00066	0.00109	0.00176	2.71344
A8	2.84689	-0.00023	-0.00094	-0.00102	-0.00196	2.84493
A9	2.08526	0.00002	0.00002	0.00012	0.00014	2.08540
A10	2.10769	-0.00003	0.00016	-0.00024	-0.00008	2.10761
A11	2.08977	0.00001	-0.00016	0.00011	-0.00005	2.08972
A12	2.08536	0.00001	0.00005	0.00002	0.00007	2.08543
A13	2.08982	-0.00000	-0.00018	0.00008	-0.00010	2.08972
A14	2.10755	-0.00001	0.00014	-0.00011	0.00003	2.10758
A15	2.05555	-0.00003	0.00028	-0.00018	0.00010	2.05565
A16	1.92776	-0.00007	0.00083	-0.00014	0.00069	1.92845
A17	2.05569	0.00001	0.00023	0.00003	0.00026	2.05595
A18	1.92826	-0.00012	0.00096	-0.00080	0.00016	1.92842
A19	2.01569	-0.00001	0.00022	-0.00005	0.00017	2.01586
A20	1.92383	0.00006	-0.00007	0.00017	0.00010	1.92392
A21	1.88817	0.00008	-0.00018	0.00053	0.00035	1.88852
A22	1.89761	-0.00002	-0.00007	-0.00007	-0.00014	1.89747
A23	1.84559	-0.00007	0.00011	-0.00046	-0.00035	1.84524
A24	1.88778	-0.00004	-0.00001	-0.00015	-0.00016	1.88762
A25	2.01569	-0.00002	0.00021	-0.00002	0.00019	2.01587
A26	1.92385	0.00006	-0.00007	0.00017	0.00010	1.92395
A27	1.88829	0.00007	-0.00018	0.00048	0.00030	1.88859
A28	1.89752	-0.00001	-0.00007	-0.00001	-0.00009	1.89744
A29	1.84554	-0.00007	0.00012	-0.00050	-0.00037	1.84517

A30	1.88779	-0.00003	-0.00002	-0.00015	-0.00016	1.88763
A31	2.90499	0.00003	0.00030	0.00051	0.00081	2.90580
A32	3.12660	-0.00001	0.00007	-0.00062	-0.00056	3.12605
A33	2.90565	0.00003	0.00030	0.00009	0.00040	2.90605
A34	3.12582	0.00003	0.00003	0.00048	0.00051	3.12633
A35	3.98331	-0.00010	0.00111	-0.00032	0.00079	3.98410
A36	3.98395	-0.00011	0.00119	-0.00077	0.00042	3.98437
A37	3.14583	-0.00000	0.00014	-0.00027	-0.00014	3.14569
A38	3.14052	-0.00005	-0.00036	-0.00037	-0.00074	3.13979
A39	3.14570	-0.00002	0.00006	-0.00007	0.00000	3.14570
A40	3.13888	0.00003	0.00057	0.00019	0.00076	3.13964
A41	4.01748	-0.00016	-0.00050	-0.00021	-0.00071	4.01677
A42	4.01670	-0.00017	-0.00069	-0.00005	-0.00074	4.01596
D1	0.01468	-0.00004	-0.00040	-0.00068	-0.00108	0.01360
D2	-0.01112	0.00002	0.00052	0.00047	0.00099	-0.01013
D3	-0.00889	0.00001	0.00028	0.00048	0.00076	-0.00813
D4	0.01467	-0.00002	-0.00032	-0.00061	-0.00093	0.01374
D5	0.00049	-0.00004	-0.00027	-0.00064	-0.00090	-0.00041
D6	-0.00928	0.00003	0.00046	0.00072	0.00118	-0.00810
D7	-0.00106	0.00001	-0.00027	-0.00027	-0.00054	-0.00159
D8	3.10584	-0.00002	0.00019	-0.00103	-0.00084	3.10499
D9	0.00033	-0.00001	-0.00020	-0.00052	-0.00072	-0.00039
D10	-0.00229	0.00001	0.00023	0.00029	0.00051	-0.00178
D11	3.10391	0.00000	0.00096	0.00020	0.00116	3.10507
D12	0.00709	-0.00000	0.00005	0.00016	0.00022	0.00731
D13	-3.10247	0.00003	-0.00022	0.00039	0.00017	-3.10230
D14	-3.10186	-0.00001	-0.00061	0.00050	-0.00011	-3.10197
D15	0.07176	0.00002	-0.00088	0.00073	-0.00016	0.07161
D16	2.51244	0.00001	0.00023	-0.00055	-0.00033	2.51211
D17	-0.66222	0.00002	0.00090	-0.00089	0.00001	-0.66222
D18	-0.66187	0.00001	0.00013	0.00118	0.00130	-0.66057
D19	2.51216	0.00004	-0.00015	0.00140	0.00125	2.51342
D20	-1.15962	-0.00000	-0.00222	0.00003	-0.00219	-1.16181
D21	0.99918	0.00000	-0.00221	0.00004	-0.00217	0.99701
D22	3.06004	0.00004	-0.00237	0.00027	-0.00210	3.05794
D23	-1.16119	-0.00001	-0.00224	0.00005	-0.00219	-1.16338
D24	0.99750	0.00001	-0.00223	0.00015	-0.00209	0.99542
D25	3.05846	0.00004	-0.00240	0.00035	-0.00205	3.05641

Item	Value	Threshold	Converged?
Maximum Force	0.000287	0.000450	YES
RMS Force	0.000079	0.000300	YES
Maximum Displacement	0.004239	0.001800	NO
RMS Displacement	0.001194	0.001200	YES

Predicted change in Energy=-1.505092D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Supporting Information file

Leave Link 103 at Sat Sep 26 07:58:46 2026, MaxMem= 805306368 cpu: 0.4 elap: 0.1
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.014271	0.668922	0.047345
2	6	0	3.337082	1.692893	0.115438
3	6	0	4.013672	-0.668819	-0.046191
4	6	0	2.137925	2.288020	0.160010
5	6	0	3.337606	-1.693498	-0.114469
6	6	0	0.910734	2.327537	0.165923
7	6	0	2.137981	-2.287767	-0.159329
8	6	0	-0.383532	1.979177	0.144811
9	6	0	0.910840	-2.327833	-0.165686
10	6	0	-1.461127	1.393244	0.101533
11	6	0	-0.383328	-1.978953	-0.145004
12	6	0	-2.670978	0.710680	0.053601
13	6	0	-1.460825	-1.392877	-0.102095
14	6	0	-2.670840	-0.710434	-0.054788
15	6	0	-3.907924	1.412021	0.151416
16	6	0	-3.907589	-1.411978	-0.152830
17	7	0	-3.725066	2.875591	-0.049167
18	7	0	-3.725280	-2.875280	0.049084
19	1	0	-3.429651	3.159959	-0.993182
20	1	0	-4.577711	3.371536	0.188369
21	1	0	-3.429872	-3.158893	0.993355
22	1	0	-4.578136	-3.371148	-0.187882
23	1	0	-2.986248	3.193877	0.579608
24	1	0	-4.743205	1.049095	-0.438797
25	1	0	-4.743659	-1.048513	0.435904
26	1	0	-2.986628	-3.194482	-0.579403

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229527	0.000000			
3	C	1.341007	2.462028	0.000000		
4	C	2.480896	1.339455	3.507683	0.000000	
5	C	2.462740	3.394187	1.229509	4.167380	0.000000
6	C	3.520937	2.508483	4.318722	1.227841	4.705002
7	C	3.507875	4.166413	2.480324	4.586917	1.339503
8	C	4.589873	3.731728	5.136513	2.540346	5.234753
9	C	4.319398	4.704457	3.520535	4.787265	2.508824
10	C	5.523365	4.807577	5.852123	3.709072	5.709858
11	C	5.136839	5.233712	4.589098	4.965562	3.731993

12	C	6.685382	6.088132	6.826237	5.062101	6.473902
13	C	5.852351	5.708696	5.522454	5.154483	4.807855
14	C	6.826694	6.473028	6.684646	5.671074	6.088629
15	C	7.957650	7.250538	8.192717	6.108988	7.887500
16	C	8.193051	7.886537	7.956760	7.094793	7.250764
17	N	8.048356	7.162389	8.511810	5.896072	8.412026
18	N	8.512463	8.411277	8.047914	7.813395	7.162941
19	H	7.918328	7.012132	8.423739	5.752219	8.374004
20	H	9.008116	8.091175	9.496912	6.802542	9.402049
21	H	8.423916	8.372708	7.917542	7.833497	7.012376
22	H	9.497734	9.401446	9.007875	8.789350	8.091902
23	H	7.460963	6.515590	8.019409	5.220516	8.022426
24	H	8.779194	8.124820	8.932427	7.017368	8.539702
25	H	8.933191	8.539110	8.778806	7.652762	8.125624
26	H	8.020679	8.022378	7.461065	7.540928	6.516522

		6	7	8	9	10
6	C	0.000000				
7	C	4.786748	0.000000			
8	C	1.340494	4.965616	0.000000		
9	C	4.667165	1.227812	4.508008	0.000000	
10	C	2.550054	5.154753	1.227355	4.420865	0.000000
11	C	4.507452	2.540191	3.968726	1.340528	3.548823
12	C	3.931348	5.671165	2.617214	4.702134	1.389939
13	C	4.420136	3.708842	3.548559	2.550094	2.793553
14	C	4.701665	5.061983	3.536329	3.931502	2.431729
15	C	4.904879	7.094925	3.569740	6.107990	2.447377
16	C	6.107521	6.108680	4.899745	4.904714	3.730838
17	N	4.673037	7.813305	3.465117	6.969994	2.710255
18	N	6.969618	5.896308	5.894251	4.673268	4.832126
19	H	4.568960	7.834000	3.459496	7.045599	2.862650
20	H	5.586901	8.789148	4.419468	7.920376	3.692462
21	H	7.044602	5.752263	6.033239	4.569007	5.039172
22	H	7.920093	6.802996	6.806714	5.587294	5.700784
23	H	4.013496	7.540039	2.904940	6.799415	2.407661
24	H	5.828133	7.652678	4.495820	6.591393	3.344014
25	H	6.591112	7.017623	5.316235	5.828545	4.104753
26	H	6.799826	5.221132	5.836723	4.014038	4.882423

		11	12	13	14	15
11	C	0.000000				
12	C	3.536511	0.000000			
13	C	1.227325	2.431803	0.000000		
14	C	2.617248	1.425242	1.390001	0.000000	
15	C	4.899933	1.425301	3.730954	2.465302	0.000000
16	C	3.569585	2.465259	2.447365	1.425246	2.840342
17	N	5.894319	2.410083	4.832123	3.737780	1.488525
18	N	3.465504	3.737738	2.710744	2.410226	4.292410
19	H	6.033896	2.769531	5.039705	4.054173	2.143393
20	H	6.806741	3.276270	5.700788	4.511958	2.071154

21	H	3.459704	4.053721	2.862861	2.769419	4.672328
22	H	4.420006	4.511861	3.693040	3.276414	4.841799
23	H	5.835960	2.557801	4.881593	3.968071	2.051303
24	H	5.316382	2.156642	4.104950	2.745561	1.085248
25	H	4.496183	2.745346	3.344403	2.156770	2.614119
26	H	2.905750	3.968705	2.408667	2.558405	4.754235

		16	17	18	19	20
16	C	0.000000				
17	N	4.292704	0.000000			
18	N	1.488374	5.751710	0.000000		
19	H	4.673032	1.029223	6.131706	0.000000	
20	H	4.842261	1.014587	6.306247	1.660985	0.000000
21	H	2.143284	6.130986	1.029247	6.623761	6.679224
22	H	2.071040	6.306244	1.014594	6.680036	6.753173
23	H	4.753866	1.021037	6.136961	1.634449	1.648449
24	H	2.614749	2.127089	4.083493	2.547256	2.411319
25	H	1.085232	4.083064	2.126923	4.634667	4.430084
26	H	2.051207	6.137770	1.021026	6.383290	6.799530

		21	22	23	24	25
21	H	0.000000				
22	H	1.660988	0.000000			
23	H	6.381667	6.798728	0.000000		
24	H	4.634982	4.430435	2.953665	0.000000	
25	H	2.547644	2.410631	4.594238	2.272677	0.000000
26	H	1.634412	1.648453	6.492645	4.594918	2.953504

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=2 Diff= 1.91D-04
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.521895	-0.670380	-0.023171
2	6	0	3.844654	-1.696079	-0.055172
3	6	0	4.521364	0.669828	0.023098
4	6	0	2.645467	-2.292341	-0.078867
5	6	0	3.845352	1.696316	0.055086
6	6	0	1.418274	-2.331974	-0.083539
7	6	0	2.645757	2.291865	0.078793
8	6	0	0.124026	-1.983015	-0.074900
9	6	0	1.418617	2.332197	0.083575

```
    10        6        0       -0.953539   -1.395861   -0.052464
    11        6        0        0.124431    1.982877    0.075053
    12        6        0       -2.163355   -0.711963   -0.028804
    13        6        0       -0.953096    1.395711    0.052715
    14        6        0       -2.163145    0.712091    0.029366
    15        6        0       -3.400330   -1.416251   -0.101966
    16        6        0       -3.399865    1.416727    0.102432
    17        7        0       -3.217586   -2.871840    0.150165
    18        7        0       -3.217443    2.871981   -0.150974
    19        1        0       -2.922306   -3.122733    1.103666
    20        1        0       -4.070230   -3.375812   -0.069830
    21        1        0       -2.921899    3.122077   -1.104628
    22        1        0       -4.070299    3.375950    0.068236
    23        1        0       -2.478708   -3.212159   -0.466891
    24        1        0       -4.235664   -1.032675    0.474965
    25        1        0       -4.235883    1.032757   -0.473216
    26        1        0       -2.478851    3.213123    0.465952
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6021231           0.2710664           0.1875909
 Leave Link  202 at Sat Sep 26 07:58:46 2026, MaxMem=    805306368 cpu:                 0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1010.3224204540 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.222036 cShort=   0.000000 cLong=
0.777964
  DFx   wShort=   0.000000 wLong=   0.200000 cFull=   0.000000 cShort=   0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0153911331 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1010.3070293208 Hartrees.
 Leave Link  301 at Sat Sep 26 07:58:46 2026, MaxMem=    805306368 cpu:                 0.4 elap:
0.1
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
```

Supporting Information file

One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51951.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.86D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 07:58:48 2026, MaxMem= 805306368 cpu: 11.3 elap: 1.9
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 07:58:48 2026, MaxMem= 805306368 cpu: 1.2 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= 0.000000 -0.000000 -0.000000
Rot= 1.000000 0.000004 -0.000000 0.000055 Ang= 0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Sat Sep 26 07:58:49 2026, MaxMem= 805306368 cpu: 5.9 elap: 1.0
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.413937077451
DIIS: error= 1.33D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413937077451 IErMin= 1 ErrMin= 1.33D-04
ErrMax= 1.33D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-05 BMatP= 1.51D-05
IDIUse=3 WtCom= 9.99D-01 WtEn= 1.33D-03

Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap=   0.704 Goal=   None   Shift=   0.000
RMSDP=6.74D-05 MaxDP=2.73D-03   OVMax= 5.87D-04

Cycle   2 Pass 1 IDiag 1:
RMSU= 6.00D-05   CP: 1.00D+00
E= -723.413944430592   Delta-E=   -0.000007353141 Rises=F Damp=F
DIIS: error= 1.35D-05 at cycle   2 NSaved=   2.
NSaved= 2 IEnMin= 2 EnMin= -723.413944430592   IErMin= 2 ErrMin= 1.35D-05
ErrMax= 1.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-07 BMatP= 1.51D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.383D-01 0.104D+01
Coeff: -0.383D-01 0.104D+01
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=7.55D-06 MaxDP=2.89D-04 DE=-7.35D-06 OVMax= 1.77D-04

Cycle   3 Pass 1 IDiag 1:
RMSU= 4.43D-06   CP: 1.00D+00 1.09D+00
E= -723.413944739273   Delta-E=   -0.000000308681 Rises=F Damp=F
DIIS: error= 1.04D-05 at cycle   3 NSaved=   3.
NSaved= 3 IEnMin= 3 EnMin= -723.413944739273   IErMin= 3 ErrMin= 1.04D-05
ErrMax= 1.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.51D-08 BMatP= 1.30D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.151D-01 0.253D+00 0.762D+00
Coeff: -0.151D-01 0.253D+00 0.762D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=1.62D-06 MaxDP=5.42D-05 DE=-3.09D-07 OVMax= 1.64D-04

Cycle   4 Pass 1 IDiag 1:
RMSU= 1.43D-06   CP: 1.00D+00 1.09D+00 1.17D+00
E= -723.413944774110   Delta-E=   -0.000000034838 Rises=F Damp=F
DIIS: error= 9.64D-06 at cycle   4 NSaved=   4.
NSaved= 4 IEnMin= 4 EnMin= -723.413944774110   IErMin= 4 ErrMin= 9.64D-06
ErrMax= 9.64D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.93D-08 BMatP= 3.51D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.895D-03-0.128D+00 0.503D+00 0.624D+00
Coeff: 0.895D-03-0.128D+00 0.503D+00 0.624D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=1.15D-06 MaxDP=5.49D-05 DE=-3.48D-08 OVMax= 6.14D-05

Cycle   5 Pass 1 IDiag 1:
RMSU= 7.65D-07   CP: 1.00D+00 1.09D+00 1.35D+00 1.09D+00
E= -723.413944814302   Delta-E=   -0.000000040192 Rises=F Damp=F
DIIS: error= 2.57D-06 at cycle   5 NSaved=   5.
NSaved= 5 IEnMin= 5 EnMin= -723.413944814302   IErMin= 5 ErrMin= 2.57D-06
ErrMax= 2.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.75D-09 BMatP= 2.93D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.259D-02-0.102D+00 0.166D+00 0.304D+00 0.630D+00
Coeff: 0.259D-02-0.102D+00 0.166D+00 0.304D+00 0.630D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=6.06D-07 MaxDP=2.90D-05 DE=-4.02D-08 OVMax= 4.58D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 3.02D-07 CP: 1.00D+00 1.08D+00 1.42D+00 1.24D+00 1.33D+00
E= -723.413944820313 Delta-E= -0.000000006011 Rises=F Damp=F
DIIS: error= 1.83D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413944820313 IErMin= 6 ErrMin= 1.83D-06
ErrMax= 1.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-10 BMatP= 2.75D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.655D-03-0.550D-02-0.441D-01-0.464D-01 0.150D+00 0.946D+00
Coeff: 0.655D-03-0.550D-02-0.441D-01-0.464D-01 0.150D+00 0.946D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.91D-07 MaxDP=2.66D-05 DE=-6.01D-09 OVMax= 4.03D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.41D-07 CP: 1.00D+00 1.08D+00 1.46D+00 1.37D+00 1.73D+00
CP: 1.62D+00
E= -723.413944822891 Delta-E= -0.000000002578 Rises=F Damp=F
DIIS: error= 1.33D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413944822891 IErMin= 7 ErrMin= 1.33D-06
ErrMax= 1.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-10 BMatP= 4.17D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.495D-03 0.304D-01-0.746D-01-0.135D+00-0.159D+00 0.519D+00
Coeff-Com: 0.819D+00
Coeff: -0.495D-03 0.304D-01-0.746D-01-0.135D+00-0.159D+00 0.519D+00
Coeff: 0.819D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.19D-07 MaxDP=1.60D-05 DE=-2.58D-09 OVMax= 3.60D-05

Cycle 8 Pass 1 IDiag 1:
RMSU= 9.71D-08 CP: 1.00D+00 1.08D+00 1.47D+00 1.46D+00 1.99D+00
CP: 2.04D+00 1.64D+00
E= -723.413944823998 Delta-E= -0.000000001107 Rises=F Damp=F
DIIS: error= 6.34D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413944823998 IErMin= 8 ErrMin= 6.34D-07
ErrMax= 6.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-11 BMatP= 2.23D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.405D-03 0.159D-01-0.209D-01-0.546D-01-0.123D+00 0.773D-02
Coeff-Com: 0.406D+00 0.770D+00
Coeff: -0.405D-03 0.159D-01-0.209D-01-0.546D-01-0.123D+00 0.773D-02
Coeff: 0.406D+00 0.770D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.11D-07 MaxDP=1.16D-05 DE=-1.11D-09 OVMax= 1.48D-05

Supporting Information file

Cycle 9 Pass 1 IDiag 1:
RMSU= 4.27D-08 CP: 1.00D+00 1.08D+00 1.47D+00 1.48D+00 2.10D+00
CP: 2.20D+00 2.19D+00 1.64D+00
E= -723.413944824245 Delta-E= -0.000000000247 Rises=F Damp=F
DIIS: error= 2.72D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413944824245 IErMin= 9 ErrMin= 2.72D-07
ErrMax= 2.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.89D-12 BMatP= 5.26D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.576D-05-0.241D-02 0.128D-01 0.134D-01-0.109D-01-0.124D+00
Coeff-Com: -0.484D-01 0.292D+00 0.868D+00
Coeff: -0.576D-05-0.241D-02 0.128D-01 0.134D-01-0.109D-01-0.124D+00
Coeff: -0.484D-01 0.292D+00 0.868D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.05D-07 MaxDP=6.66D-06 DE=-2.47D-10 OVMax= 1.00D-05

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.33D-08 CP: 1.00D+00 1.08D+00 1.47D+00 1.48D+00 2.12D+00
CP: 2.29D+00 2.53D+00 2.09D+00 1.57D+00
E= -723.413944824315 Delta-E= -0.000000000070 Rises=F Damp=F
DIIS: error= 2.37D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413944824315 IErMin=10 ErrMin= 2.37D-07
ErrMax= 2.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.64D-12 BMatP= 9.89D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.929D-04-0.490D-02 0.119D-01 0.192D-01 0.208D-01-0.641D-01
Coeff-Com: -0.116D+00-0.400D-01 0.445D+00 0.728D+00
Coeff: 0.929D-04-0.490D-02 0.119D-01 0.192D-01 0.208D-01-0.641D-01
Coeff: -0.116D+00-0.400D-01 0.445D+00 0.728D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.91D-08 MaxDP=3.20D-06 DE=-7.05D-11 OVMax= 3.65D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 8.56D-09 CP: 1.00D+00 1.08D+00 1.47D+00 1.48D+00 2.12D+00
CP: 2.30D+00 2.69D+00 2.32D+00 1.96D+00 1.36D+00
E= -723.413944824329 Delta-E= -0.000000000013 Rises=F Damp=F
DIIS: error= 6.93D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413944824329 IErMin=11 ErrMin= 6.93D-08
ErrMax= 6.93D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.62D-13 BMatP= 3.64D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.564D-04-0.200D-02 0.241D-02 0.605D-02 0.144D-01 0.487D-02
Coeff-Com: -0.488D-01-0.123D+00-0.384D-01 0.373D+00 0.811D+00
Coeff: 0.564D-04-0.200D-02 0.241D-02 0.605D-02 0.144D-01 0.487D-02
Coeff: -0.488D-01-0.123D+00-0.384D-01 0.373D+00 0.811D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.10D-08 MaxDP=1.98D-06 DE=-1.34D-11 OVMax= 2.74D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 5.27D-09 CP: 1.00D+00 1.08D+00 1.47D+00 1.48D+00 2.13D+00
CP: 2.32D+00 2.78D+00 2.47D+00 2.19D+00 1.68D+00

CP: 1.50D+00
E= -723.413944824335 Delta-E= -0.000000000007 Rises=F Damp=F
DIIS: error= 6.37D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413944824335 IErMin=12 ErrMin= 6.37D-08
ErrMax= 6.37D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.93D-13 BMatP= 9.62D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.226D-07 0.415D-03-0.186D-02-0.230D-02 0.485D-03 0.192D-01
Coeff-Com: 0.115D-01-0.373D-01-0.125D+00-0.452D-01 0.301D+00 0.880D+00
Coeff: -0.226D-07 0.415D-03-0.186D-02-0.230D-02 0.485D-03 0.192D-01
Coeff: 0.115D-01-0.373D-01-0.125D+00-0.452D-01 0.301D+00 0.880D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.08D-08 MaxDP=4.46D-07 DE=-6.59D-12 OVMax= 1.01D-06

Cycle 13 Pass 1 IDiag 1:
RMSU= 2.94D-09 CP: 1.00D+00 1.08D+00 1.47D+00 1.48D+00 2.13D+00
CP: 2.32D+00 2.80D+00 2.49D+00 2.26D+00 1.86D+00
CP: 1.97D+00 1.49D+00
E= -723.413944824327 Delta-E= 0.000000000008 Rises=F Damp=F
DIIS: error= 1.46D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=12 EnMin= -723.413944824335 IErMin=13 ErrMin= 1.46D-08
ErrMax= 1.46D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.97D-14 BMatP= 1.93D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.154D-04 0.716D-03-0.145D-02-0.263D-02-0.375D-02 0.621D-02
Coeff-Com: 0.183D-01 0.195D-01-0.405D-01-0.126D+00-0.106D+00 0.380D+00
Coeff-Com: 0.855D+00
Coeff: -0.154D-04 0.716D-03-0.145D-02-0.263D-02-0.375D-02 0.621D-02
Coeff: 0.183D-01 0.195D-01-0.405D-01-0.126D+00-0.106D+00 0.380D+00
Coeff: 0.855D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.64D-09 MaxDP=2.65D-07 DE= 8.19D-12 OVMax= 5.05D-07

SCF Done: E(RwB97XD) = -723.413944824 A.U. after 13 cycles
NFock= 13 Conv=0.56D-08 -V/T= 2.0047
KE= 7.200597200467D+02 PE=-3.701688488590D+03 EE= 1.247907794398D+03
Leave Link 502 at Sat Sep 26 08:15:21 2026, MaxMem= 805306368 cpu: 5951.4 elap: 992.3
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51951.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 08:15:22 2026, MaxMem= 805306368 cpu: 3.1 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.

Supporting Information file

Leave Link 702 at Sat Sep 26 08:15:22 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 08:26:17 2026, MaxMem= 805306368 cpu: 3927.0 elap: 654.6
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.54307285D+00-9.47348407D-04-1.20646896D-03
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000069150	-0.000060594	-0.000128721
2	6	0.000123662	0.000157062	0.000149755
3	6	-0.000052943	0.000058823	0.000130395
4	6	-0.000099909	-0.000254138	-0.000168908
5	6	0.000119454	-0.000146886	-0.000149551
6	6	0.000041372	0.000197275	0.000132456
7	6	-0.000102312	0.000240049	0.000164461
8	6	-0.000012596	-0.000060832	-0.000035029
9	6	0.000057772	-0.000193842	-0.000128013
10	6	0.000044427	0.000015158	-0.000004793
11	6	-0.000019673	0.000072466	0.000043061
12	6	-0.000043612	-0.000226909	-0.000012849
13	6	0.000010110	-0.000054295	-0.000017140
14	6	-0.000064952	0.000204586	0.000030043
15	6	0.000121898	-0.000055027	-0.000001821
16	6	0.000110644	0.000122587	0.000017413
17	7	-0.000204118	0.000030845	0.000008597
18	7	-0.000155362	-0.000073740	-0.000015497
19	1	0.000020457	-0.000000473	-0.000011071
20	1	0.000004230	0.000035700	0.000003388
21	1	0.000012246	0.000010456	0.000007547
22	1	0.000009611	-0.000032989	-0.000008675
23	1	0.000052941	0.000038029	-0.000006246
24	1	0.000010230	0.000064022	-0.000002927
25	1	0.000022889	-0.000042990	0.000004491

Supporting Information file

```
    26        1          0.000062686   -0.000044345   -0.000000367
 ----------------------------------------------------------------------
 Cartesian Forces:  Max     0.000254138 RMS     0.000097366
 Leave Link  716 at Sat Sep 26 08:26:17 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000200646 RMS     0.000061213
 Search for a local minimum.
 Step number  25 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .61213D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points   18   19   20   21   22
                                     23   24   25
 DE= -2.16D-06 DEPred=-1.51D-06 R= 1.44D+00
 TightC=F SS=  1.41D+00  RLast= 7.99D-03 DXNew= 1.3552D+00 2.3984D-02
 Trust test= 1.44D+00 RLast= 7.99D-03 DXMaxT set to 8.06D-01
 ITU=  1  1  1  1  1  1  1  1  1  1 -1  1  1  1  1  1  1  1
 ITU=  1  0  0  1  0
    Eigenvalues ---    0.00326   0.00508   0.01044   0.01310   0.01744
    Eigenvalues ---    0.01891   0.02497   0.02674   0.02887   0.03014
    Eigenvalues ---    0.03071   0.03483   0.03791   0.04223   0.04333
    Eigenvalues ---    0.04461   0.05024   0.05485   0.05540   0.07211
    Eigenvalues ---    0.08156   0.09984   0.10228   0.11088   0.11204
    Eigenvalues ---    0.11569   0.11790   0.13997   0.15397   0.15524
    Eigenvalues ---    0.15897   0.15985   0.16005   0.16005   0.16588
    Eigenvalues ---    0.16917   0.22397   0.22581   0.24921   0.24998
    Eigenvalues ---    0.25000   0.25000   0.25001   0.25060   0.28623
    Eigenvalues ---    0.30049   0.34249   0.37245   0.38668   0.40700
    Eigenvalues ---    0.45853   0.46093   0.47034   0.47629   0.47691
    Eigenvalues ---    0.47693   0.47829   0.48426   0.49865   0.52063
    Eigenvalues ---    0.54857   0.55142   0.55635   0.55661   0.56663
    Eigenvalues ---    0.92163   0.93718   0.95029   0.95423   0.97721
    Eigenvalues ---    0.98908   1.37082
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    25   24   23   22   21   20
 RFO step:  Lambda=-3.53683113D-06.
 NNeg= 0 NGDIIS= 6 SimSw=  2.50D-01 Rises=F DC= -2.16D-06 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.1047337815D-02 NUsed= 6 OKEnD=F EnDIS=F
 InvSVX:  RCond= 1.12D-06 Info=           0 Equed=N FErr=  7.00D-14 BErr=  1.08D-16
 DidBck=F Rises=F RFO-DIIS coefs:    1.83827   -0.40561   -0.71090    0.21746    0.05839
              RFO-DIIS coefs:    0.00240
```

Supporting Information file

Iteration 1 RMS(Cart)= 0.00098962 RMS(Int)= 0.00000193
Iteration 2 RMS(Cart)= 0.00000236 RMS(Int)= 0.00000169
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000169
ITry= 1 IFail=0 DXMaxC= 3.55D-03 DCOld= 1.00D+10 DXMaxT= 8.06D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.32347	0.00000	0.00029	-0.00008	0.00021	2.32368
R2	2.53414	-0.00002	-0.00065	0.00015	-0.00050	2.53364
R3	2.53120	-0.00000	-0.00041	0.00014	-0.00027	2.53093
R4	2.32344	0.00001	0.00029	-0.00007	0.00022	2.32365
R5	2.32028	-0.00004	0.00016	-0.00011	0.00005	2.32034
R6	2.53129	0.00001	-0.00043	0.00017	-0.00026	2.53103
R7	2.53317	0.00002	-0.00014	0.00011	-0.00003	2.53314
R8	2.32023	-0.00003	0.00017	-0.00011	0.00007	2.32029
R9	2.31937	-0.00001	0.00011	-0.00006	0.00005	2.31941
R10	2.53323	0.00003	-0.00017	0.00017	-0.00000	2.53323
R11	2.62660	0.00003	-0.00022	0.00019	-0.00004	2.62657
R12	2.31931	-0.00001	0.00013	-0.00005	0.00007	2.31938
R13	2.69332	-0.00010	0.00061	-0.00058	0.00003	2.69335
R14	2.69343	0.00005	-0.00004	0.00002	-0.00003	2.69340
R15	2.62672	0.00003	-0.00026	0.00022	-0.00004	2.62668
R16	2.69332	-0.00003	0.00008	-0.00017	-0.00009	2.69324
R17	2.81290	0.00009	-0.00095	0.00070	-0.00025	2.81265
R18	2.05082	-0.00003	0.00009	-0.00010	-0.00001	2.05081
R19	2.81262	0.00013	-0.00085	0.00071	-0.00014	2.81248
R20	2.05079	-0.00003	0.00012	-0.00015	-0.00003	2.05076
R21	1.94495	0.00002	0.00044	-0.00014	0.00030	1.94525
R22	1.91729	0.00001	0.00005	-0.00002	0.00004	1.91733
R23	1.92948	0.00005	-0.00005	0.00021	0.00016	1.92964
R24	1.94500	0.00001	0.00043	-0.00016	0.00027	1.94526
R25	1.91730	0.00001	0.00006	-0.00003	0.00003	1.91734
R26	1.92946	0.00006	-0.00008	0.00026	0.00018	1.92963
A1	2.55785	0.00005	0.00091	0.00001	0.00092	2.55877
A2	2.61585	-0.00014	-0.00153	-0.00040	-0.00192	2.61392
A3	2.55983	0.00004	0.00085	0.00000	0.00085	2.56068
A4	2.71226	0.00020	0.00241	0.00040	0.00281	2.71507
A5	2.61405	-0.00013	-0.00152	-0.00029	-0.00181	2.61224
A6	2.84577	-0.00014	-0.00267	-0.00009	-0.00275	2.84302
A7	2.71344	0.00019	0.00233	0.00047	0.00280	2.71625
A8	2.84493	-0.00013	-0.00268	0.00004	-0.00265	2.84228
A9	2.08540	-0.00000	0.00014	-0.00004	0.00011	2.08551
A10	2.10761	-0.00002	0.00001	-0.00015	-0.00013	2.10748
A11	2.08972	0.00002	-0.00014	0.00017	0.00003	2.08975
A12	2.08543	0.00002	0.00016	0.00002	0.00018	2.08561
A13	2.08972	0.00003	-0.00012	0.00016	0.00003	2.08976
A14	2.10758	-0.00006	-0.00002	-0.00020	-0.00022	2.10736
A15	2.05565	0.00002	0.00013	0.00005	0.00018	2.05583

A16	1.92845	-0.00016	0.00083	-0.00092	-0.00010	1.92835
A17	2.05595	0.00002	0.00026	0.00006	0.00032	2.05626
A18	1.92842	-0.00009	0.00058	-0.00057	0.00001	1.92842
A19	2.01586	-0.00003	0.00098	-0.00087	0.00012	2.01598
A20	1.92392	0.00005	-0.00003	0.00036	0.00033	1.92426
A21	1.88852	0.00003	-0.00038	0.00064	0.00026	1.88878
A22	1.89747	-0.00001	-0.00018	0.00003	-0.00015	1.89732
A23	1.84524	-0.00004	-0.00045	-0.00006	-0.00051	1.84473
A24	1.88762	-0.00001	-0.00001	-0.00008	-0.00009	1.88753
A25	2.01587	-0.00004	0.00095	-0.00091	0.00004	2.01592
A26	1.92395	0.00005	0.00002	0.00032	0.00034	1.92429
A27	1.88859	0.00004	-0.00047	0.00074	0.00027	1.88886
A28	1.89744	-0.00000	-0.00010	0.00001	-0.00009	1.89735
A29	1.84517	-0.00003	-0.00044	-0.00006	-0.00050	1.84467
A30	1.88763	-0.00001	-0.00004	-0.00007	-0.00011	1.88752
A31	2.90580	0.00001	0.00080	-0.00031	0.00050	2.90630
A32	3.12605	0.00002	-0.00015	0.00062	0.00047	3.12652
A33	2.90605	0.00001	0.00059	0.00024	0.00084	2.90688
A34	3.12633	-0.00001	0.00033	-0.00068	-0.00034	3.12599
A35	3.98410	-0.00015	0.00096	-0.00087	0.00009	3.98419
A36	3.98437	-0.00007	0.00083	-0.00051	0.00032	3.98469
A37	3.14569	-0.00001	-0.00013	-0.00000	-0.00014	3.14556
A38	3.13979	-0.00002	0.00022	-0.00028	-0.00006	3.13972
A39	3.14570	-0.00001	0.00003	-0.00008	-0.00005	3.14566
A40	3.13964	0.00000	0.00044	-0.00029	0.00015	3.13979
A41	4.01677	-0.00017	0.00012	-0.00082	-0.00069	4.01607
A42	4.01596	-0.00014	-0.00037	-0.00064	-0.00101	4.01495
D1	0.01360	-0.00003	-0.00135	-0.00045	-0.00180	0.01180
D2	-0.01013	0.00002	0.00158	0.00023	0.00182	-0.00832
D3	-0.00813	0.00002	0.00132	0.00051	0.00183	-0.00630
D4	0.01374	-0.00003	-0.00131	-0.00057	-0.00188	0.01187
D5	-0.00041	-0.00002	-0.00115	-0.00047	-0.00162	-0.00203
D6	-0.00810	0.00002	0.00147	0.00033	0.00180	-0.00630
D7	-0.00159	0.00001	-0.00078	0.00090	0.00013	-0.00146
D8	3.10499	-0.00001	-0.00026	0.00047	0.00021	3.10520
D9	-0.00039	-0.00002	-0.00110	-0.00049	-0.00159	-0.00199
D10	-0.00178	0.00001	-0.00048	0.00096	0.00049	-0.00129
D11	3.10507	-0.00001	0.00048	-0.00023	0.00024	3.10531
D12	0.00731	-0.00001	0.00082	-0.00076	0.00005	0.00736
D13	-3.10230	0.00002	0.00016	0.00021	0.00037	-3.10193
D14	-3.10197	-0.00000	0.00034	-0.00045	-0.00011	-3.10208
D15	0.07161	0.00002	-0.00031	0.00052	0.00021	0.07182
D16	2.51211	0.00002	0.00016	0.00057	0.00073	2.51284
D17	-0.66222	0.00002	0.00064	0.00026	0.00090	-0.66132
D18	-0.66057	-0.00001	0.00089	-0.00062	0.00027	-0.66030
D19	2.51342	0.00001	0.00023	0.00036	0.00059	2.51401
D20	-1.16181	-0.00000	0.00009	0.00012	0.00021	-1.16160
D21	0.99701	0.00001	0.00057	-0.00021	0.00036	0.99738

D22 3.05794 0.00004 0.00031 0.00029 0.00060 3.05854
D23 -1.16338 0.00001 0.00014 0.00033 0.00046 -1.16292
D24 0.99542 0.00001 0.00074 -0.00008 0.00066 0.99607
D25 3.05641 0.00005 0.00043 0.00045 0.00088 3.05729

Item	Value	Threshold	Converged?
Maximum Force	0.000201	0.000450	YES
RMS Force	0.000061	0.000300	YES
Maximum Displacement	0.003546	0.001800	NO
RMS Displacement	0.000990	0.001200	YES

Predicted change in Energy=-1.713692D-06
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 08:26:17 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.013692	0.669015	0.047048
2	6	0	3.337369	1.693672	0.115430
3	6	0	4.013115	-0.668496	-0.045979
4	6	0	2.137730	2.287531	0.159596
5	6	0	3.337872	-1.693837	-0.114546
6	6	0	0.910585	2.329223	0.165904
7	6	0	2.137806	-2.286933	-0.158956
8	6	0	-0.383329	1.979623	0.144715
9	6	0	0.910708	-2.329257	-0.165623
10	6	0	-1.460672	1.393163	0.101603
11	6	0	-0.383181	-1.979361	-0.144771
12	6	0	-2.670509	0.710594	0.053990
13	6	0	-1.460737	-1.393315	-0.101865
14	6	0	-2.670534	-0.710542	-0.054338
15	6	0	-3.907339	1.412103	0.151880
16	6	0	-3.907294	-1.411959	-0.152505
17	7	0	-3.725020	2.875524	-0.049283
18	7	0	-3.725756	-2.875383	0.048685
19	1	0	-3.430649	3.159855	-0.993809
20	1	0	-4.577327	3.371672	0.189115
21	1	0	-3.431582	-3.159785	0.993256
22	1	0	-4.578293	-3.371124	-0.189758
23	1	0	-2.985289	3.194338	0.578291
24	1	0	-4.743069	1.048902	-0.437516
25	1	0	-4.743664	-1.048493	0.435773
26	1	0	-2.986122	-3.194653	-0.578764

Supporting Information file

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229638	0.000000			
3	C	1.340742	2.462219	0.000000		
4	C	2.480221	1.339310	3.506769	0.000000	
5	C	2.462907	3.395306	1.229625	4.167348	0.000000
6	C	3.521319	2.509134	4.319364	1.227869	4.706950
7	C	3.506995	4.166468	2.479695	4.585543	1.339364
8	C	4.589229	3.731784	5.135914	2.539836	5.235347
9	C	4.320113	4.706551	3.520990	4.788119	2.509481
10	C	5.522320	4.807462	5.851030	3.708336	5.709844
11	C	5.136456	5.234631	4.588632	4.965280	3.732114
12	C	6.684334	6.088088	6.825153	5.061329	6.473820
13	C	5.851902	5.709512	5.521915	5.154217	4.808028
14	C	6.825857	6.473326	6.683786	5.670416	6.088632
15	C	7.956500	7.250268	8.191558	6.108133	7.887390
16	C	8.192209	7.886816	7.955938	7.094078	7.250747
17	N	8.047709	7.162488	8.511099	5.895863	8.412357
18	N	8.512450	8.412398	8.047946	7.813351	7.163626
19	H	7.918704	7.013285	8.424029	5.753098	8.375220
20	H	9.007227	8.090953	9.495995	6.802075	9.402232
21	H	8.425385	8.375280	7.918967	7.834889	7.014395
22	H	9.497421	9.402287	9.007617	8.789050	8.092257
23	H	7.459571	6.514770	8.018033	5.219475	8.022259
24	H	8.778381	8.124958	8.931602	7.016847	8.539821
25	H	8.932649	8.539624	8.778249	7.652380	8.125919
26	H	8.019786	8.022728	7.460205	7.540118	6.516200

		6	7	8	9	10
6	C	0.000000				
7	C	4.787536	0.000000			
8	C	1.340478	4.965062	0.000000		
9	C	4.670261	1.227846	4.509688	0.000000	
10	C	2.550137	5.153644	1.227380	4.421680	0.000000
11	C	4.509351	2.539720	3.969554	1.340526	3.549029
12	C	3.931504	5.670133	2.617224	4.702556	1.389919
13	C	4.421782	3.708278	3.549411	2.550256	2.793897
14	C	4.702455	5.061233	3.536654	3.931655	2.431802
15	C	4.904456	7.093889	3.569422	6.108367	2.447257
16	C	6.108173	6.108097	4.899949	4.904564	3.730850
17	N	4.672642	7.812536	3.465137	6.970885	2.710615
18	N	6.971177	5.896673	5.895093	4.673433	4.832586
19	H	4.569595	7.834039	3.460541	7.047241	2.863902
20	H	5.586092	8.788287	4.419207	7.921171	3.692655
21	H	7.047562	5.753915	6.035345	4.570367	5.040721
22	H	7.921378	6.803118	6.807356	5.587057	5.701131
23	H	4.012022	7.538830	2.904086	6.800168	2.407471
24	H	5.828133	7.651917	4.495839	6.591743	3.344143

25	H	6.591838	7.017269	5.316646	5.828718	4.105045
26	H	6.800887	5.220617	5.837045	4.013089	4.882413

		11	12	13	14	15
11	C	0.000000				
12	C	3.536557	0.000000			
13	C	1.227363	2.431927	0.000000		
14	C	2.617262	1.425259	1.389980	0.000000	
15	C	4.899971	1.425287	3.731033	2.465326	0.000000
16	C	3.569506	2.465260	2.447151	1.425201	2.840418
17	N	5.894651	2.410307	4.832465	3.737892	1.488391
18	N	3.465990	3.738021	2.710996	2.410527	4.292569
19	H	6.034854	2.770302	5.040582	4.054671	2.143472
20	H	6.807048	3.276515	5.701132	4.512162	2.071276
21	H	3.461395	4.054786	2.864251	2.770458	4.672945
22	H	4.420180	4.512148	3.693049	3.276673	4.842123
23	H	5.836175	2.557921	4.881949	3.968297	2.051430
24	H	5.316455	2.156741	4.104971	2.745519	1.085241
25	H	4.496372	2.745563	3.344483	2.156917	2.614300
26	H	2.905269	3.968746	2.408122	2.558403	4.754437

		16	17	18	19	20
16	C	0.000000				
17	N	4.292596	0.000000			
18	N	1.488302	5.751741	0.000000		
19	H	4.672950	1.029382	6.131718	0.000000	
20	H	4.842394	1.014606	6.306393	1.661038	0.000000
21	H	2.143355	6.131717	1.029387	6.624672	6.679769
22	H	2.071222	6.306221	1.014611	6.679616	6.753433
23	H	4.754169	1.021124	6.137612	1.634329	1.648481
24	H	2.614496	2.126898	4.083054	2.547161	2.411514
25	H	1.085216	4.082992	2.126852	4.634426	4.430166
26	H	2.051402	6.137863	1.021118	6.383544	6.799868

		21	22	23	24	25
21	H	0.000000				
22	H	1.661064	0.000000			
23	H	6.383280	6.799475	0.000000		
24	H	4.634669	4.430031	2.953735	0.000000	
25	H	2.547529	2.411069	4.594977	2.271938	0.000000
26	H	1.634288	1.648477	6.492918	4.595059	2.953682

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=3 Diff= 1.68D-04
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Supporting Information file

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.521359	-0.669914	-0.022926
2	6	0	3.845100	-1.696385	-0.055202
3	6	0	4.520698	0.670046	0.022873
4	6	0	2.645499	-2.291503	-0.078525
5	6	0	3.845391	1.697127	0.055164
6	6	0	1.418357	-2.333464	-0.083490
7	6	0	2.645287	2.291350	0.078500
8	6	0	0.124421	-1.983411	-0.074783
9	6	0	1.418186	2.333810	0.083539
10	6	0	-0.952959	-1.395859	-0.052496
11	6	0	0.124319	1.983320	0.074901
12	6	0	-2.162839	-0.712107	-0.029115
13	6	0	-0.953201	1.396061	0.052575
14	6	0	-2.162954	0.711966	0.029027
15	6	0	-3.399619	-1.416704	-0.102336
16	6	0	-3.399764	1.416335	0.102264
17	7	0	-3.217241	-2.872110	0.150332
18	7	0	-3.218285	2.871764	-0.150392
19	1	0	-2.922958	-3.122936	1.104330
20	1	0	-4.069495	-3.376408	-0.070512
21	1	0	-2.924023	3.122695	-1.104374
22	1	0	-4.070875	3.375556	0.070328
23	1	0	-2.477424	-3.212815	-0.465528
24	1	0	-4.235434	-1.032993	0.473795
25	1	0	-4.236050	1.032299	-0.472920
26	1	0	-2.478738	3.213008	0.465485

Rotational constants (GHZ): 0.6019771 0.2710943 0.1875894
Leave Link 202 at Sat Sep 26 08:26:17 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0
(Enter /home/user/gauss16/g16/l301.exe)
Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.3062630450 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964

DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0153894613 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.2908735837 Hartrees.
Leave Link 301 at Sat Sep 26 08:26:17 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51950.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.85D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 08:26:18 2026, MaxMem= 805306368 cpu: 5.8 elap: 1.0
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 08:26:18 2026, MaxMem= 805306368 cpu: 0.7 elap: 0.1
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 0.000000 0.000000
Rot= 1.000000 0.000003 -0.000001 -0.000052 Ang= 0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.
Leave Link 401 at Sat Sep 26 08:26:18 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l502.exe)
Integral symmetry usage will be decided dynamically.
Closed shell SCF:
Using DIIS extrapolation, IDIIS= 1040.
NGot= 805306368 LenX= 804326778 LenY= 803841666
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Fock matrices will be formed incrementally for 20 cycles.

Supporting Information file

Cycle 1 Pass 1 IDiag 1:
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
E= -723.413936715894
DIIS: error= 1.81D-04 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -723.413936715894 IErMin= 1 ErrMin= 1.81D-04
ErrMax= 1.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-05 BMatP= 2.02D-05
IDIUse=3 WtCom= 9.98D-01 WtEn= 1.81D-03
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.704 Goal= None Shift= 0.000
RMSDP=8.43D-05 MaxDP=3.21D-03 OVMax= 6.66D-04

Cycle 2 Pass 1 IDiag 1:
RMSU= 7.63D-05 CP: 1.00D+00
E= -723.413946325264 Delta-E= -0.000009609370 Rises=F Damp=F
DIIS: error= 1.67D-05 at cycle 2 NSaved= 2.
NSaved= 2 IEnMin= 2 EnMin= -723.413946325264 IErMin= 2 ErrMin= 1.67D-05
ErrMax= 1.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D-07 BMatP= 2.02D-05
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.383D-01 0.104D+01
Coeff: -0.383D-01 0.104D+01
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.03D-05 MaxDP=4.80D-04 DE=-9.61D-06 OVMax= 2.01D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 5.56D-06 CP: 1.00D+00 1.09D+00
E= -723.413946724570 Delta-E= -0.000000399306 Rises=F Damp=F
DIIS: error= 1.12D-05 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.413946724570 IErMin= 3 ErrMin= 1.12D-05
ErrMax= 1.12D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-08 BMatP= 1.66D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.140D-01 0.240D+00 0.774D+00
Coeff: -0.140D-01 0.240D+00 0.774D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.67D-06 MaxDP=1.67D-04 DE=-3.99D-07 OVMax= 1.70D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 1.75D-06 CP: 1.00D+00 1.10D+00 1.30D+00
E= -723.413946773530 Delta-E= -0.000000048960 Rises=F Damp=F
DIIS: error= 1.59D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -723.413946773530 IErMin= 3 ErrMin= 1.12D-05
ErrMax= 1.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.47D-08 BMatP= 4.21D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.227D-02-0.161D+00 0.501D+00 0.659D+00
Coeff: 0.227D-02-0.161D+00 0.501D+00 0.659D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.54D-06 MaxDP=9.63D-05 DE=-4.90D-08 OVMax= 9.24D-05

Cycle 5 Pass 1 IDiag 1:
RMSU= 7.21D-07 CP: 1.00D+00 1.11D+00 1.49D+00 1.12D+00
E= -723.413946824572 Delta-E= -0.000000051042 Rises=F Damp=F
DIIS: error= 4.66D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413946824572 IErMin= 5 ErrMin= 4.66D-06
ErrMax= 4.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.36D-09 BMatP= 3.47D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.266D-02-0.108D+00 0.192D+00 0.324D+00 0.590D+00
Coeff: 0.266D-02-0.108D+00 0.192D+00 0.324D+00 0.590D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.51D-07 MaxDP=2.55D-05 DE=-5.10D-08 OVMax= 4.51D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 2.55D-07 CP: 1.00D+00 1.11D+00 1.53D+00 1.21D+00 1.27D+00
E= -723.413946831731 Delta-E= -0.000000007159 Rises=F Damp=F
DIIS: error= 2.52D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413946831731 IErMin= 6 ErrMin= 2.52D-06
ErrMax= 2.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.91D-10 BMatP= 3.36D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.374D-04 0.213D-01-0.101D+00-0.150D+00 0.124D+00 0.111D+01
Coeff: 0.374D-04 0.213D-01-0.101D+00-0.150D+00 0.124D+00 0.111D+01
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.60D-07 MaxDP=2.39D-05 DE=-7.16D-09 OVMax= 5.36D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.90D-07 CP: 1.00D+00 1.11D+00 1.57D+00 1.34D+00 1.63D+00
CP: 1.53D+00
E= -723.413946835635 Delta-E= -0.000000003904 Rises=F Damp=F
DIIS: error= 1.05D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413946835635 IErMin= 7 ErrMin= 1.05D-06
ErrMax= 1.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-10 BMatP= 5.91D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.546D-03 0.311D-01-0.763D-01-0.132D+00-0.867D-01 0.445D+00
Coeff-Com: 0.820D+00
Coeff: -0.546D-03 0.311D-01-0.763D-01-0.132D+00-0.867D-01 0.445D+00
Coeff: 0.820D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.94D-07 MaxDP=5.97D-06 DE=-3.90D-09 OVMax= 2.06D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.88D-08 CP: 1.00D+00 1.11D+00 1.57D+00 1.36D+00 1.73D+00
CP: 1.92D+00 1.42D+00
E= -723.413946836485 Delta-E= -0.000000000850 Rises=F Damp=F
DIIS: error= 5.44D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413946836485 IErMin= 8 ErrMin= 5.44D-07
ErrMax= 5.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.16D-11 BMatP= 1.65D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.266D-03 0.890D-02-0.778D-02-0.263D-01-0.847D-01-0.738D-01
Coeff-Com: 0.416D+00 0.768D+00
Coeff: -0.266D-03 0.890D-02-0.778D-02-0.263D-01-0.847D-01-0.738D-01
Coeff: 0.416D+00 0.768D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.46D-07 MaxDP=8.24D-06 DE=-8.50D-10 OVMax= 1.48D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 4.55D-08 CP: 1.00D+00 1.11D+00 1.57D+00 1.35D+00 1.73D+00
CP: 2.02D+00 1.85D+00 1.58D+00
E= -723.413946836718 Delta-E= -0.000000000232 Rises=F Damp=F
DIIS: error= 2.94D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413946836718 IErMin= 9 ErrMin= 2.94D-07
ErrMax= 2.94D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-11 BMatP= 5.16D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.686D-05-0.224D-02 0.124D-01 0.140D-01-0.264D-01-0.121D+00
Coeff-Com: 0.313D-01 0.373D+00 0.718D+00
Coeff: -0.686D-05-0.224D-02 0.124D-01 0.140D-01-0.264D-01-0.121D+00
Coeff: 0.313D-01 0.373D+00 0.718D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=9.71D-08 MaxDP=5.39D-06 DE=-2.32D-10 OVMax= 4.70D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 1.73D-08 CP: 1.00D+00 1.11D+00 1.56D+00 1.34D+00 1.70D+00
CP: 2.07D+00 2.03D+00 2.02D+00 1.45D+00
E= -723.413946836758 Delta-E= -0.000000000040 Rises=F Damp=F
DIIS: error= 1.28D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413946836758 IErMin=10 ErrMin= 1.28D-07
ErrMax= 1.28D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.28D-12 BMatP= 1.18D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.829D-04-0.412D-02 0.943D-02 0.158D-01 0.831D-02-0.418D-01
Coeff-Com: -0.112D+00-0.292D-01 0.358D+00 0.795D+00
Coeff: 0.829D-04-0.412D-02 0.943D-02 0.158D-01 0.831D-02-0.418D-01
Coeff: -0.112D+00-0.292D-01 0.358D+00 0.795D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=7.15D-08 MaxDP=3.77D-06 DE=-4.02D-11 OVMax= 3.86D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 9.10D-09 CP: 1.00D+00 1.11D+00 1.56D+00 1.33D+00 1.67D+00
CP: 2.08D+00 2.16D+00 2.33D+00 1.87D+00 1.54D+00
E= -723.413946836777 Delta-E= -0.000000000018 Rises=F Damp=F

DIIS: error= 1.05D-07 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413946836777 IErMin=11 ErrMin= 1.05D-07
ErrMax= 1.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.68D-13 BMatP= 3.28D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.421D-04-0.138D-02 0.142D-02 0.404D-02 0.105D-01 0.121D-01
Coeff-Com: -0.590D-01-0.110D+00-0.383D-01 0.354D+00 0.827D+00
Coeff: 0.421D-04-0.138D-02 0.142D-02 0.404D-02 0.105D-01 0.121D-01
Coeff: -0.590D-01-0.110D+00-0.383D-01 0.354D+00 0.827D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.08D-08 MaxDP=2.07D-06 DE=-1.84D-11 OVMax= 1.98D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 5.00D-09 CP: 1.00D+00 1.11D+00 1.55D+00 1.33D+00 1.65D+00
CP: 2.09D+00 2.22D+00 2.49D+00 2.12D+00 1.98D+00
CP: 1.27D+00
E= -723.413946836780 Delta-E= -0.000000000004 Rises=F Damp=F
DIIS: error= 4.21D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413946836780 IErMin=12 ErrMin= 4.21D-08
ErrMax= 4.21D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-13 BMatP= 8.68D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.760D-05 0.730D-03-0.243D-02-0.348D-02 0.209D-02 0.205D-01
Coeff-Com: 0.132D-01-0.400D-01-0.150D+00-0.116D+00 0.427D+00 0.848D+00
Coeff: -0.760D-05 0.730D-03-0.243D-02-0.348D-02 0.209D-02 0.205D-01
Coeff: 0.132D-01-0.400D-01-0.150D+00-0.116D+00 0.427D+00 0.848D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.87D-08 MaxDP=8.69D-07 DE=-3.64D-12 OVMax= 1.12D-06

Cycle 13 Pass 1 IDiag 1:
RMSU= 3.10D-09 CP: 1.00D+00 1.11D+00 1.55D+00 1.33D+00 1.64D+00
CP: 2.08D+00 2.24D+00 2.55D+00 2.24D+00 2.26D+00
CP: 1.69D+00 1.49D+00
E= -723.413946836784 Delta-E= -0.000000000004 Rises=F Damp=F
DIIS: error= 2.23D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=13 EnMin= -723.413946836784 IErMin=13 ErrMin= 2.23D-08
ErrMax= 2.23D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.71D-14 BMatP= 2.96D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.132D-04 0.625D-03-0.133D-02-0.242D-02-0.176D-02 0.447D-02
Coeff-Com: 0.207D-01 0.129D-01-0.553D-01-0.143D+00-0.344D-01 0.362D+00
Coeff-Com: 0.837D+00
Coeff: -0.132D-04 0.625D-03-0.133D-02-0.242D-02-0.176D-02 0.447D-02
Coeff: 0.207D-01 0.129D-01-0.553D-01-0.143D+00-0.344D-01 0.362D+00
Coeff: 0.837D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.38D-09 MaxDP=1.80D-07 DE=-3.64D-12 OVMax= 6.21D-07

SCF Done: E(RwB97XD) = -723.413946837 A.U. after 13 cycles
NFock= 13 Conv=0.44D-08 -V/T= 2.0047
KE= 7.200588079746D+02 PE=-3.701657396579D+03 EE= 1.247893768184D+03

Supporting Information file

Leave Link 502 at Sat Sep 26 08:40:45 2026, MaxMem= 805306368 cpu: 5199.9 elap: 866.9
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23226 LenP2D= 51950.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 08:40:46 2026, MaxMem= 805306368 cpu: 3.5 elap: 0.6
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 08:40:46 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 08:52:13 2026, MaxMem= 805306368 cpu: 4122.8 elap: 687.2
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.54203847D+00-6.20825037D-04 2.86918554D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000048111	0.000069733	-0.000101381
2	6	0.000108239	-0.000010702	0.000118704
3	6	-0.000041498	-0.000075706	0.000101986
4	6	-0.000118348	-0.000035988	-0.000136644
5	6	0.000104303	0.000019186	-0.000118697
6	6	0.000093070	0.000031130	0.000107593
7	6	-0.000125506	0.000031748	0.000135140
8	6	-0.000060824	-0.000028191	-0.000029927
9	6	0.000098519	-0.000026129	-0.000109257
10	6	0.000041159	0.000043228	0.000006033
11	6	-0.000094715	0.000032714	0.000036754
12	6	-0.000041605	-0.000151108	-0.000015384

```
    13        6        0.000088242  -0.000055379  -0.000004287
    14        6       -0.000086474   0.000101172   0.000005568
    15        6        0.000079847  -0.000096497  -0.000003109
    16        6        0.000057015   0.000135833   0.000009290
    17        7       -0.000063076   0.000147589  -0.000068222
    18        7       -0.000017356  -0.000149422   0.000070678
    19        1       -0.000027392  -0.000049179   0.000068662
    20        1        0.000005364   0.000006416   0.000003256
    21        1       -0.000036818   0.000048488  -0.000067912
    22        1        0.000007383  -0.000003025  -0.000001762
    23        1        0.000011774  -0.000013387  -0.000009210
    24        1        0.000018885   0.000055971  -0.000000094
    25        1        0.000026905  -0.000043589  -0.000000081
    26        1        0.000021018   0.000015095   0.000002304
 ----------------------------------------------------------------
 Cartesian Forces:  Max     0.000151108 RMS     0.000070888
 Leave Link  716 at Sat Sep 26 08:52:13 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000101538 RMS     0.000036957
 Search for a local minimum.
 Step number  26 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .36957D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points   18   19   20   21   22
                                     23   24   25   26
 DE= -2.01D-06 DEPred=-1.71D-06 R= 1.17D+00
 TightC=F SS=  1.41D+00  RLast= 8.36D-03 DXNew= 1.3552D+00 2.5085D-02
 Trust test= 1.17D+00 RLast= 8.36D-03 DXMaxT set to 8.06D-01
 ITU=  1  1  1  1  1  1  1  1  1  1  1  1 -1  1  1  1  1  1  1  1
 ITU=  1  1  0  0  1  0
    Eigenvalues ---    0.00287   0.00507   0.01034   0.01292   0.01744
    Eigenvalues ---    0.01893   0.02234   0.02673   0.02922   0.02969
    Eigenvalues ---    0.03071   0.03498   0.03792   0.04197   0.04333
    Eigenvalues ---    0.04461   0.05020   0.05382   0.05608   0.07723
    Eigenvalues ---    0.08153   0.09984   0.10227   0.11044   0.11203
    Eigenvalues ---    0.11453   0.11788   0.13850   0.14912   0.15525
    Eigenvalues ---    0.15896   0.15946   0.16004   0.16006   0.16545
    Eigenvalues ---    0.16931   0.21692   0.22430   0.24808   0.24998
    Eigenvalues ---    0.25000   0.25001   0.25001   0.25020   0.28473
    Eigenvalues ---    0.29780   0.32229   0.37244   0.37927   0.39622
```

```
    Eigenvalues ---    0.45858   0.45945   0.46941   0.47597   0.47691
    Eigenvalues ---    0.47699   0.47825   0.48388   0.49275   0.52054
    Eigenvalues ---    0.54857   0.55161   0.55635   0.55661   0.57553
    Eigenvalues ---    0.92422   0.93732   0.95032   0.95390   0.97751
    Eigenvalues ---    0.99062   1.37097
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    26   25   24   23   22   21   20
 RFO step:  Lambda=-1.40227635D-06.
 NNeg= 0 NGDIIS= 7 SimSw=  2.50D-01 Rises=F DC= -2.01D-06 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.1647224521D-02 NUsed= 7 OKEnD=F EnDIS=F
 InvSVX:  RCond= 2.87D-07 Info=          0 Equed=N FErr=  3.38D-13 BErr=  1.09D-16
 DidBck=F Rises=F RFO-DIIS coefs:    1.50992   -0.23385   -0.25137   -0.24160    0.14794
              RFO-DIIS coefs:    0.07426   -0.00530
 Iteration  1 RMS(Cart)=  0.00333299 RMS(Int)=  0.00001170
 Iteration  2 RMS(Cart)=  0.00001189 RMS(Int)=  0.00000197
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000197
  ITry=  1  IFail=0  DXMaxC=  1.35D-02  DCOld=  1.00D+10  DXMaxT=  8.06D-01  DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)    (Quad)   (Total)
   R1        2.32368  -0.00004   0.00007  -0.00007  -0.00001   2.32367
   R2        2.53364   0.00004  -0.00015   0.00013  -0.00002   2.53362
   R3        2.53093   0.00005  -0.00006   0.00013   0.00006   2.53099
   R4        2.32365  -0.00005   0.00007  -0.00008  -0.00001   2.32364
   R5        2.32034  -0.00005  -0.00002  -0.00005  -0.00007   2.32027
   R6        2.53103   0.00005  -0.00006   0.00011   0.00005   2.53108
   R7        2.53314   0.00004   0.00004   0.00009   0.00012   2.53326
   R8        2.32029  -0.00006  -0.00001  -0.00007  -0.00008   2.32021
   R9        2.31941  -0.00003  -0.00002  -0.00001  -0.00003   2.31938
  R10        2.53323   0.00003   0.00004   0.00006   0.00010   2.53333
  R11        2.62657   0.00003   0.00008   0.00003   0.00011   2.62667
  R12        2.31938  -0.00007  -0.00000  -0.00006  -0.00007   2.31931
  R13        2.69335  -0.00008  -0.00024  -0.00003  -0.00027   2.69308
  R14        2.69340   0.00000   0.00001  -0.00001  -0.00001   2.69339
  R15        2.62668   0.00004   0.00008   0.00005   0.00013   2.62681
  R16        2.69324  -0.00005  -0.00000  -0.00008  -0.00008   2.69316
  R17        2.81265   0.00008   0.00011   0.00012   0.00023   2.81288
  R18        2.05081  -0.00003  -0.00002  -0.00007  -0.00009   2.05072
  R19        2.81248   0.00009   0.00017   0.00012   0.00029   2.81277
  R20        2.05076  -0.00004  -0.00002  -0.00009  -0.00011   2.05065
  R21        1.94525  -0.00008   0.00012  -0.00031  -0.00019   1.94506
  R22        1.91733  -0.00000  -0.00002   0.00001  -0.00001   1.91731
  R23        1.92964  -0.00000   0.00018  -0.00002   0.00016   1.92980
  R24        1.94526  -0.00009   0.00009  -0.00031  -0.00021   1.94505
  R25        1.91734  -0.00000  -0.00002   0.00000  -0.00002   1.91732
  R26        1.92963   0.00001   0.00018   0.00000   0.00018   1.92982
   A1        2.55877   0.00001   0.00033  -0.00003   0.00030   2.55907
   A2        2.61392  -0.00005  -0.00084   0.00006  -0.00078   2.61314
```

A3	2.56068	0.00000	0.00031	-0.00006	0.00025	2.56093
A4	2.71507	0.00006	0.00124	-0.00010	0.00115	2.71622
A5	2.61224	-0.00005	-0.00081	0.00002	-0.00079	2.61144
A6	2.84302	-0.00001	-0.00106	0.00030	-0.00075	2.84227
A7	2.71625	0.00006	0.00123	-0.00016	0.00107	2.71731
A8	2.84228	-0.00001	-0.00103	0.00022	-0.00080	2.84148
A9	2.08551	-0.00000	-0.00005	0.00004	-0.00000	2.08551
A10	2.10748	-0.00002	-0.00011	-0.00004	-0.00015	2.10732
A11	2.08975	0.00003	0.00014	-0.00001	0.00014	2.08988
A12	2.08561	0.00000	0.00000	-0.00005	-0.00005	2.08556
A13	2.08976	0.00003	0.00018	-0.00000	0.00018	2.08994
A14	2.10736	-0.00004	-0.00019	0.00005	-0.00014	2.10722
A15	2.05583	0.00003	0.00016	0.00002	0.00018	2.05601
A16	1.92835	-0.00010	-0.00027	-0.00029	-0.00056	1.92779
A17	2.05626	0.00004	0.00037	-0.00011	0.00025	2.05651
A18	1.92842	-0.00005	-0.00031	-0.00012	-0.00042	1.92800
A19	2.01598	-0.00004	0.00023	-0.00042	-0.00018	2.01580
A20	1.92426	0.00003	0.00029	0.00014	0.00043	1.92469
A21	1.88878	-0.00001	-0.00024	-0.00015	-0.00038	1.88840
A22	1.89732	0.00001	-0.00004	0.00005	0.00000	1.89732
A23	1.84473	0.00001	-0.00042	0.00035	-0.00007	1.84467
A24	1.88753	0.00001	0.00015	0.00005	0.00021	1.88773
A25	2.01592	-0.00004	0.00018	-0.00038	-0.00020	2.01572
A26	1.92429	0.00002	0.00032	0.00012	0.00044	1.92473
A27	1.88886	-0.00001	-0.00028	-0.00015	-0.00043	1.88843
A28	1.89735	0.00001	0.00002	-0.00003	-0.00001	1.89733
A29	1.84467	0.00001	-0.00042	0.00039	-0.00003	1.84463
A30	1.88752	0.00001	0.00015	0.00009	0.00023	1.88775
A31	2.90630	-0.00000	0.00015	0.00008	0.00024	2.90653
A32	3.12652	-0.00001	0.00023	-0.00048	-0.00025	3.12627
A33	2.90688	-0.00001	0.00023	-0.00032	-0.00009	2.90680
A34	3.12599	0.00001	0.00003	0.00049	0.00052	3.12651
A35	3.98419	-0.00007	-0.00011	-0.00027	-0.00038	3.98381
A36	3.98469	-0.00001	0.00006	-0.00023	-0.00017	3.98452
A37	3.14556	-0.00001	-0.00031	0.00029	-0.00002	3.14554
A38	3.13972	-0.00001	0.00004	-0.00006	-0.00002	3.13970
A39	3.14566	-0.00001	-0.00013	-0.00003	-0.00017	3.14549
A40	3.13979	-0.00001	-0.00020	0.00022	0.00002	3.13982
A41	4.01607	-0.00010	-0.00044	0.00014	-0.00030	4.01577
A42	4.01495	-0.00004	-0.00031	0.00010	-0.00021	4.01474
D1	0.01180	-0.00002	-0.00113	-0.00030	-0.00144	0.01036
D2	-0.00832	0.00001	0.00105	0.00040	0.00145	-0.00686
D3	-0.00630	0.00002	0.00114	0.00033	0.00146	-0.00484
D4	0.01187	-0.00002	-0.00122	-0.00028	-0.00150	0.01036
D5	-0.00203	-0.00002	-0.00105	-0.00038	-0.00143	-0.00346
D6	-0.00630	0.00002	0.00105	0.00037	0.00142	-0.00487
D7	-0.00146	0.00001	-0.00011	0.00073	0.00062	-0.00084
D8	3.10520	-0.00000	-0.00047	0.00051	0.00004	3.10524

D9	-0.00199	-0.00002	-0.00106	-0.00036	-0.00141	-0.00340
D10	-0.00129	0.00001	0.00006	0.00038	0.00045	-0.00084
D11	3.10531	-0.00000	-0.00036	0.00053	0.00017	3.10548
D12	0.00736	-0.00000	0.00033	-0.00054	-0.00021	0.00716
D13	-3.10193	-0.00000	0.00053	-0.00050	0.00003	-3.10189
D14	-3.10208	0.00001	0.00058	-0.00024	0.00034	-3.10174
D15	0.07182	0.00001	0.00079	-0.00021	0.00058	0.07240
D16	2.51284	0.00001	0.00078	0.00002	0.00080	2.51364
D17	-0.66132	-0.00000	0.00053	-0.00028	0.00025	-0.66107
D18	-0.66030	-0.00000	0.00062	-0.00037	0.00025	-0.66005
D19	2.51401	-0.00000	0.00082	-0.00033	0.00049	2.51450
D20	-1.16160	0.00001	0.00604	0.00009	0.00613	-1.15547
D21	0.99738	0.00001	0.00639	-0.00005	0.00634	1.00372
D22	3.05854	0.00003	0.00660	0.00001	0.00661	3.06515
D23	-1.16292	0.00002	0.00626	0.00021	0.00646	-1.15646
D24	0.99607	0.00001	0.00669	-0.00003	0.00666	1.00273
D25	3.05729	0.00003	0.00688	0.00006	0.00694	3.06423

Item	Value	Threshold	Converged?
Maximum Force	0.000102	0.000450	YES
RMS Force	0.000037	0.000300	YES
Maximum Displacement	0.013499	0.001800	NO
RMS Displacement	0.003333	0.001200	NO

Predicted change in Energy=-6.759734D-07
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 08:52:13 2026, MaxMem= 805306368 cpu: 0.1 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.013705	0.668631	0.047017
2	6	0	3.337720	1.693479	0.115811
3	6	0	4.013093	-0.668876	-0.045912
4	6	0	2.137780	2.286817	0.159770
5	6	0	3.338082	-1.694331	-0.114923
6	6	0	0.910701	2.329342	0.166292
7	6	0	2.137648	-2.286761	-0.159141
8	6	0	-0.383254	1.979659	0.144929
9	6	0	0.910615	-2.329675	-0.165994
10	6	0	-1.460686	1.393407	0.101666
11	6	0	-0.383218	-1.979378	-0.144911
12	6	0	-2.670525	0.710737	0.053878
13	6	0	-1.460509	-1.392920	-0.101966
14	6	0	-2.670446	-0.710260	-0.054400

15	6	0	-3.907287	1.412290	0.152237
16	6	0	-3.906984	-1.411951	-0.152797
17	7	0	-3.725763	2.875847	-0.049553
18	7	0	-3.725594	-2.875474	0.048932
19	1	0	-3.437792	3.160267	-0.995913
20	1	0	-4.575959	3.372615	0.194987
21	1	0	-3.437809	-3.159889	0.995344
22	1	0	-4.575759	-3.372216	-0.195775
23	1	0	-2.981203	3.193676	0.572928
24	1	0	-4.743405	1.049117	-0.436536
25	1	0	-4.743740	-1.048742	0.434986
26	1	0	-2.980898	-3.193332	-0.573384

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229635	0.000000			
3	C	1.340732	2.462317	0.000000		
4	C	2.479987	1.339343	3.506455	0.000000	
5	C	2.462982	3.395659	1.229618	4.167220	0.000000
6	C	3.521479	2.509440	4.319627	1.227832	4.707569
7	C	3.506626	4.166303	2.479449	4.584683	1.339391
8	C	4.589294	3.732076	5.136051	2.539719	5.235844
9	C	4.320229	4.707019	3.521086	4.787907	2.509754
10	C	5.522431	4.807801	5.851244	3.708169	5.710448
11	C	5.136314	5.234811	4.588548	4.964744	3.732322
12	C	6.684366	6.088401	6.825251	5.061130	6.474273
13	C	5.851427	5.709316	5.521567	5.153314	4.808065
14	C	6.825650	6.473407	6.683673	5.669866	6.088881
15	C	7.956520	7.250553	8.191638	6.108002	7.887828
16	C	8.191828	7.886798	7.955577	7.093500	7.250665
17	N	8.048633	7.163668	8.512049	5.896771	8.413603
18	N	8.512193	8.412504	8.047693	7.812854	7.163621
19	H	7.925955	7.021038	8.430928	5.760688	8.381870
20	H	9.006429	8.090247	9.495447	6.801065	9.402236
21	H	8.431011	8.380726	7.924980	7.839131	7.020916
22	H	9.495593	9.401144	9.005493	8.787643	8.090162
23	H	7.455278	6.510633	8.013891	5.215082	8.018673
24	H	8.778700	8.125570	8.931985	7.016993	8.540514
25	H	8.932678	8.540003	8.778251	7.652255	8.126194
26	H	8.013996	8.017534	7.454329	7.534614	6.510507

		6	7	8	9	10
6	C	0.000000				
7	C	4.787454	0.000000			
8	C	1.340543	4.964850	0.000000		
9	C	4.670852	1.227803	4.510114	0.000000	
10	C	2.550222	5.153607	1.227365	4.422222	0.000000
11	C	4.509562	2.539578	3.969632	1.340581	3.549284

12	C	3.931628	5.670000	2.617263	4.702873	1.389975
13	C	4.421519	3.707958	3.549045	2.550262	2.793757
14	C	4.702394	5.061037	3.536474	3.931788	2.431726
15	C	4.904507	7.093742	3.569422	6.108662	2.447196
16	C	6.108124	6.107611	4.899830	4.904248	3.730838
17	N	4.673549	7.813074	3.466028	6.971874	2.711286
18	N	6.971307	5.896396	5.895148	4.673171	4.832797
19	H	4.577178	7.839378	3.467789	7.052438	2.869743
20	H	5.585042	8.787859	4.418327	7.921422	3.692005
21	H	7.051846	5.760288	6.038913	4.576762	5.043825
22	H	7.920865	6.800691	6.807037	5.584629	5.701168
23	H	4.007412	7.534836	2.899373	6.797034	2.403129
24	H	5.828491	7.652054	4.496102	6.592221	3.344315
25	H	6.592144	7.017064	5.316878	5.828696	4.105318
26	H	6.796440	5.214689	5.832972	4.006962	4.879028

		11	12	13	14	15
11	C	0.000000				
12	C	3.536666	0.000000			
13	C	1.227327	2.431830	0.000000		
14	C	2.617301	1.425117	1.390049	0.000000	
15	C	4.900078	1.425283	3.731024	2.465298	0.000000
16	C	3.569167	2.465228	2.447077	1.425158	2.840666
17	N	5.895330	2.410794	4.832856	3.738166	1.488513
18	N	3.465839	3.738195	2.711337	2.410843	4.292855
19	H	6.039088	2.773258	5.043838	4.056631	2.143385
20	H	6.807234	3.276612	5.701275	4.512543	2.071672
21	H	3.467609	4.056701	2.869841	2.773353	4.672907
22	H	4.418143	4.512510	3.692046	3.276616	4.843497
23	H	5.833122	2.555567	4.879022	3.966211	2.051329
24	H	5.316771	2.156812	4.105227	2.745650	1.085192
25	H	4.496277	2.745766	3.344605	2.156992	2.614628
26	H	2.899174	3.966301	2.403186	2.555655	4.753575

		16	17	18	19	20
16	C	0.000000				
17	N	4.292868	0.000000			
18	N	1.488454	5.752165	0.000000		
19	H	4.672919	1.029281	6.132267	0.000000	
20	H	4.843610	1.014599	6.307382	1.660951	0.000000
21	H	2.143277	6.132278	1.029275	6.626423	6.679039
22	H	2.071653	6.307311	1.014601	6.678962	6.756141
23	H	4.753478	1.021209	6.137041	1.634274	1.648668
24	H	2.614759	2.126569	4.083385	2.544501	2.413608
25	H	1.085159	4.083315	2.126642	4.633436	4.431044
26	H	2.051304	6.137114	1.021216	6.384004	6.800462

		21	22	23	24	25
21	H	0.000000				
22	H	1.660957	0.000000			
23	H	6.383942	6.800328	0.000000		

```
  24  H    4.633637   4.431056   2.953559   0.000000
  25  H    2.544876   2.413422   4.596051   2.271687   0.000000
  26  H    1.634256   1.648688   6.489061   4.596034   2.953589
            26
  26  H    0.000000
 Stoichiometry    C16H8N2
 Framework group  C1[X(C16H8N2)]
 Deg. of freedom    72
 Full point group                 C1      NOp   1
 RotChk:  IX=0 Diff= 2.52D-04
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        4.521236   -0.670350   -0.022857
     2          6           0        3.845136   -1.696910   -0.055506
     3          6           0        4.520774    0.669604    0.022797
     4          6           0        2.645130   -2.291291   -0.078628
     5          6           0        3.845877    1.696934    0.055488
     6          6           0        1.418047   -2.333878   -0.083785
     7          6           0        2.645510    2.290694    0.078629
     8          6           0        0.124131   -1.983510   -0.074926
     9          6           0        1.418480    2.333965    0.083822
    10          6           0       -0.953236   -1.395971   -0.052509
    11          6           0        0.124608    1.983292    0.074971
    12          6           0       -2.162998   -0.711900   -0.028988
    13          6           0       -0.952748    1.395807    0.052634
    14          6           0       -2.162762    0.712034    0.029059
    15          6           0       -3.399833   -1.416345   -0.102660
    16          6           0       -3.399226    1.416904    0.102483
    17          7           0       -3.218507   -2.871888    0.150690
    18          7           0       -3.217640    2.872372   -0.150765
    19          1           0       -2.930673   -3.122756    1.106534
    20          1           0       -4.068735   -3.376881   -0.076257
    21          1           0       -2.929717    3.123166   -1.106595
    22          1           0       -4.067772    3.377541    0.076157
    23          1           0       -2.473916   -3.211579   -0.460097
    24          1           0       -4.235973   -1.032517    0.472830
    25          1           0       -4.235961    1.033268   -0.472207
    26          1           0       -2.472974    3.211915    0.460026
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6019459           0.2710843           0.1875825
 Leave Link  202 at Sat Sep 26 08:52:13 2026, MaxMem=    805306368 cpu:                0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
```

Supporting Information file

Standard basis: def2TZVP (5D, 7F)
Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.
There are 696 symmetry adapted cartesian basis functions of A symmetry.
There are 606 symmetry adapted basis functions of A symmetry.
606 basis functions, 982 primitive gaussians, 696 cartesian basis functions
59 alpha electrons 59 beta electrons
nuclear repulsion energy 1010.2932342357 Hartrees.
IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX= 1.000000
ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000
IRadAn= 5 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=121
HFx wShort= 0.000000 wLong= 0.200000 cFull= 0.222036 cShort= 0.000000 cLong= 0.777964
DFx wShort= 0.000000 wLong= 0.200000 cFull= 0.000000 cShort= 0.000000 cLong= 1.000000
NAtoms= 26 NActive= 26 NUniq= 26 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
R6Disp: Grimme-D2 Dispersion energy= -0.0153864232 Hartrees.
Nuclear repulsion after empirical dispersion term = 1010.2778478125 Hartrees.
Leave Link 301 at Sat Sep 26 08:52:14 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l302.exe)
NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1
NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23224 LenP2D= 51949.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 606 RedAO= T EigKep= 1.85D-06 NBF= 606
NBsUse= 606 1.00D-06 EigRej= -1.00D+00 NBFU= 606
Precomputing XC quadrature grid using
IXCGrd= 4 IRadAn= 5 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.
Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32
NSgBfM= 683 683 683 683 683 MxSgAt= 26 MxSgA2= 26.
Leave Link 302 at Sat Sep 26 08:52:14 2026, MaxMem= 805306368 cpu: 5.6 elap: 0.9
(Enter /home/user/gauss16/g16/l303.exe)
DipDrv: MaxL=1.
Leave Link 303 at Sat Sep 26 08:52:15 2026, MaxMem= 805306368 cpu: 0.8 elap: 0.2
(Enter /home/user/gauss16/g16/l401.exe)
Initial guess from the checkpoint file: "cdca-n2-b-4h2.chk"
B after Tr= -0.000000 -0.000000 -0.000000
Rot= 1.000000 -0.000004 0.000002 0.000072 Ang= -0.01 deg.
Guess basis will be translated and rotated to current coordinates.
JPrj=2 DoOrth=T DoCkMO=T.

Supporting Information file

```
 Leave Link  401 at Sat Sep 26 08:52:15 2026, MaxMem=    805306368 cpu:                2.9 elap:
0.5
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.413922271616
 DIIS: error= 2.31D-04 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -723.413922271616     IErMin= 1 ErrMin= 2.31D-04
 ErrMax= 2.31D-04  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.07D-05 BMatP= 2.07D-05
 IDIUse=3 WtCom= 9.98D-01 WtEn= 2.31D-03
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=     0.704 Goal=   None    Shift=    0.000
 RMSDP=4.05D-05 MaxDP=1.65D-03             OVMax= 1.20D-03

 Cycle   2  Pass 1  IDiag  1:
 RMSU=  3.98D-05    CP:  1.00D+00
 E= -723.413946382104     Delta-E=       -0.000024110488 Rises=F Damp=F
 DIIS: error= 3.50D-05 at cycle   2 NSaved=   2.
 NSaved= 2 IEnMin= 2 EnMin= -723.413946382104     IErMin= 2 ErrMin= 3.50D-05
 ErrMax= 3.50D-05  0.00D+00 EMaxC= 1.00D-01 BMatC= 5.63D-07 BMatP= 2.07D-05
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: -0.134D+00 0.113D+01
 Coeff:     -0.134D+00 0.113D+01
 Gap=     0.179 Goal=   None    Shift=    0.000
 RMSDP=1.07D-05 MaxDP=5.62D-04 DE=-2.41D-05 OVMax= 3.38D-04

 Cycle   3  Pass 1  IDiag  1:
 RMSU=  6.76D-06    CP:  1.00D+00  1.18D+00
 E= -723.413947563111     Delta-E=       -0.000001181007 Rises=F Damp=F
 DIIS: error= 1.95D-05 at cycle   3 NSaved=   3.
```

NSaved= 3 IEnMin= 3 EnMin= -723.413947563111 IErMin= 3 ErrMin= 1.95D-05
ErrMax= 1.95D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-07 BMatP= 5.63D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.581D-01 0.406D+00 0.652D+00
Coeff: -0.581D-01 0.406D+00 0.652D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.67D-06 MaxDP=1.79D-04 DE=-1.18D-06 OVMax= 1.95D-04

Cycle 4 Pass 1 IDiag 1:
RMSU= 2.70D-06 CP: 1.00D+00 1.19D+00 1.27D+00
E= -723.413947658922 Delta-E= -0.000000095811 Rises=F Damp=F
DIIS: error= 2.17D-05 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413947658922 IErMin= 3 ErrMin= 1.95D-05
ErrMax= 2.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.04D-08 BMatP= 1.36D-07
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.684D-02-0.120D+00 0.450D+00 0.663D+00
Coeff: 0.684D-02-0.120D+00 0.450D+00 0.663D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.47D-06 MaxDP=1.73D-04 DE=-9.58D-08 OVMax= 1.27D-04

Cycle 5 Pass 1 IDiag 1:
RMSU= 1.45D-06 CP: 1.00D+00 1.21D+00 1.59D+00 1.20D+00
E= -723.413947763106 Delta-E= -0.000000104184 Rises=F Damp=F
DIIS: error= 3.12D-06 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413947763106 IErMin= 5 ErrMin= 3.12D-06
ErrMax= 3.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-09 BMatP= 8.04D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.662D-02-0.796D-01 0.169D+00 0.301D+00 0.603D+00
Coeff: 0.662D-02-0.796D-01 0.169D+00 0.301D+00 0.603D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=9.98D-07 MaxDP=4.68D-05 DE=-1.04D-07 OVMax= 4.35D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 4.57D-07 CP: 1.00D+00 1.21D+00 1.66D+00 1.34D+00 1.22D+00
E= -723.413947768677 Delta-E= -0.000000005572 Rises=F Damp=F
DIIS: error= 1.67D-06 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413947768677 IErMin= 6 ErrMin= 1.67D-06
ErrMax= 1.67D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.74D-10 BMatP= 3.43D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.116D-02-0.734D-02-0.184D-01-0.149D-01 0.213D+00 0.826D+00
Coeff: 0.116D-02-0.734D-02-0.184D-01-0.149D-01 0.213D+00 0.826D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=9.23D-07 MaxDP=4.63D-05 DE=-5.57D-09 OVMax= 2.73D-05

Cycle 7 Pass 1 IDiag 1:
RMSU= 1.50D-07 CP: 1.00D+00 1.22D+00 1.73D+00 1.46D+00 1.50D+00
CP: 1.26D+00
E= -723.413947770417 Delta-E= -0.000000001739 Rises=F Damp=F

DIIS: error= 1.17D-06 at cycle 7 NSaved= 7.
NSaved= 7 IEnMin= 7 EnMin= -723.413947770417 IErMin= 7 ErrMin= 1.17D-06
ErrMax= 1.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-10 BMatP= 4.74D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.103D-02 0.151D-01-0.454D-01-0.759D-01-0.498D-01 0.323D+00
Coeff-Com: 0.834D+00
Coeff: -0.103D-02 0.151D-01-0.454D-01-0.759D-01-0.498D-01 0.323D+00
Coeff: 0.834D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=5.84D-07 MaxDP=2.77D-05 DE=-1.74D-09 OVMax= 1.79D-05

Cycle 8 Pass 1 IDiag 1:
RMSU= 5.56D-08 CP: 1.00D+00 1.22D+00 1.77D+00 1.54D+00 1.68D+00
CP: 1.55D+00 1.29D+00
E= -723.413947771051 Delta-E= -0.000000000635 Rises=F Damp=F
DIIS: error= 4.44D-07 at cycle 8 NSaved= 8.
NSaved= 8 IEnMin= 8 EnMin= -723.413947771051 IErMin= 8 ErrMin= 4.44D-07
ErrMax= 4.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.87D-11 BMatP= 1.26D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.833D-03 0.973D-02-0.181D-01-0.355D-01-0.838D-01-0.511D-01
Coeff-Com: 0.440D+00 0.739D+00
Coeff: -0.833D-03 0.973D-02-0.181D-01-0.355D-01-0.838D-01-0.511D-01
Coeff: 0.440D+00 0.739D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=2.57D-07 MaxDP=1.21D-05 DE=-6.35D-10 OVMax= 1.04D-05

Cycle 9 Pass 1 IDiag 1:
RMSU= 2.79D-08 CP: 1.00D+00 1.22D+00 1.79D+00 1.57D+00 1.76D+00
CP: 1.66D+00 1.51D+00 1.51D+00
E= -723.413947771277 Delta-E= -0.000000000226 Rises=F Damp=F
DIIS: error= 4.14D-07 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 9 EnMin= -723.413947771277 IErMin= 9 ErrMin= 4.14D-07
ErrMax= 4.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-11 BMatP= 4.87D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.134D-04-0.121D-02 0.822D-02 0.111D-01-0.167D-01-0.132D+00
Coeff-Com: -0.998D-01 0.275D+00 0.956D+00
Coeff: 0.134D-04-0.121D-02 0.822D-02 0.111D-01-0.167D-01-0.132D+00
Coeff: -0.998D-01 0.275D+00 0.956D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.03D-07 MaxDP=3.96D-06 DE=-2.26D-10 OVMax= 8.84D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 2.28D-08 CP: 1.00D+00 1.22D+00 1.80D+00 1.58D+00 1.79D+00
CP: 1.71D+00 1.63D+00 2.00D+00 1.72D+00
E= -723.413947771365 Delta-E= -0.000000000087 Rises=F Damp=F
DIIS: error= 1.39D-07 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413947771365 IErMin=10 ErrMin= 1.39D-07
ErrMax= 1.39D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.88D-12 BMatP= 1.07D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.219D-03-0.311D-02 0.890D-02 0.150D-01 0.129D-01-0.570D-01
Coeff-Com: -0.156D+00-0.509D-01 0.500D+00 0.730D+00
Coeff: 0.219D-03-0.311D-02 0.890D-02 0.150D-01 0.129D-01-0.570D-01
Coeff: -0.156D+00-0.509D-01 0.500D+00 0.730D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=2.58D-08 MaxDP=1.54D-06 DE=-8.71D-11 OVMax= 3.63D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 1.00D-08   CP: 1.00D+00 1.22D+00 1.80D+00 1.58D+00 1.79D+00
                CP: 1.71D+00 1.64D+00 2.23D+00 2.14D+00 1.58D+00
E= -723.413947771389   Delta-E=   -0.000000000024 Rises=F Damp=F
DIIS: error= 7.67D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413947771389   IErMin=11 ErrMin= 7.67D-08
ErrMax= 7.67D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.83D-13 BMatP= 3.88D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.665D-04-0.639D-03 0.297D-03 0.155D-02 0.971D-02 0.200D-01
Coeff-Com: -0.166D-01-0.108D+00-0.136D+00 0.253D+00 0.977D+00
Coeff: 0.665D-04-0.639D-03 0.297D-03 0.155D-02 0.971D-02 0.200D-01
Coeff: -0.166D-01-0.108D+00-0.136D+00 0.253D+00 0.977D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=3.02D-08 MaxDP=1.58D-06 DE=-2.43D-11 OVMax= 2.29D-06

Cycle 12 Pass 1 IDiag 1:
RMSU= 4.54D-09   CP: 1.00D+00 1.22D+00 1.79D+00 1.57D+00 1.79D+00
                CP: 1.70D+00 1.61D+00 2.36D+00 2.55D+00 2.18D+00
                CP: 1.41D+00
E= -723.413947771390   Delta-E=   -0.000000000002 Rises=F Damp=F
DIIS: error= 3.00D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413947771390   IErMin=12 ErrMin= 3.00D-08
ErrMax= 3.00D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.75D-13 BMatP= 7.83D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.166D-04 0.406D-03-0.202D-02-0.281D-02 0.243D-02 0.248D-01
Coeff-Com: 0.305D-01-0.475D-01-0.200D+00-0.408D-01 0.530D+00 0.706D+00
Coeff: -0.166D-04 0.406D-03-0.202D-02-0.281D-02 0.243D-02 0.248D-01
Coeff: 0.305D-01-0.475D-01-0.200D+00-0.408D-01 0.530D+00 0.706D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=1.43D-08 MaxDP=6.94D-07 DE=-1.59D-12 OVMax= 8.59D-07

Cycle 13 Pass 1 IDiag 1:
RMSU= 1.93D-09   CP: 1.00D+00 1.22D+00 1.79D+00 1.57D+00 1.78D+00
                CP: 1.69D+00 1.59D+00 2.39D+00 2.69D+00 2.44D+00
                CP: 1.71D+00 1.27D+00
E= -723.413947771390   Delta-E=   0.000000000000 Rises=F Damp=F
DIIS: error= 1.23D-08 at cycle 13 NSaved= 13.
NSaved=13 IEnMin=12 EnMin= -723.413947771390   IErMin=13 ErrMin= 1.23D-08
ErrMax= 1.23D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.67D-14 BMatP= 2.75D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

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Coeff-Com: -0.202D-04 0.291D-03-0.885D-03-0.140D-02-0.969D-03 0.545D-02
Coeff-Com: 0.159D-01 0.295D-02-0.511D-01-0.645D-01 0.173D-01 0.262D+00
Coeff-Com: 0.815D+00
Coeff: -0.202D-04 0.291D-03-0.885D-03-0.140D-02-0.969D-03 0.545D-02
Coeff: 0.159D-01 0.295D-02-0.511D-01-0.645D-01 0.173D-01 0.262D+00
Coeff: 0.815D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.89D-09 MaxDP=1.52D-07 DE= 2.27D-13 OVMax= 3.26D-07

SCF Done: E(RwB97XD) = -723.413947771 A.U. after 13 cycles
NFock= 13 Conv=0.39D-08 -V/T= 2.0047
KE= 7.200588944968D+02 PE=-3.701631334125D+03 EE= 1.247880644044D+03
Leave Link 502 at Sat Sep 26 09:09:32 2026, MaxMem= 805306368 cpu: 6221.6 elap: 1037.2
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23224 LenP2D= 51949.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 09:09:33 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 09:09:33 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 09:21:38 2026, MaxMem= 805306368 cpu: 4350.1 elap: 725.1
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.53962769D+00-6.32062678D-05 3.06568222D-04
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z

1	6	-0.000027911	0.000063890	-0.000089294
2	6	0.000054716	-0.000044296	0.000103344
3	6	-0.000017989	-0.000064537	0.000088776
4	6	-0.000065637	0.000028461	-0.000120279
5	6	0.000053915	0.000050408	-0.000102539
6	6	0.000051580	-0.000019719	0.000096453
7	6	-0.000069229	-0.000036929	0.000120093
8	6	-0.000047666	-0.000004061	-0.000031644
9	6	0.000067207	0.000019627	-0.000095890
10	6	0.000049427	0.000006614	0.000002407
11	6	-0.000047477	0.000012441	0.000029483
12	6	-0.000013237	-0.000001489	0.000004537
13	6	0.000023968	-0.000024915	-0.000004390
14	6	-0.000013400	0.000003724	0.000003552
15	6	-0.000006398	-0.000035121	-0.000004729
16	6	-0.000009215	0.000034450	-0.000004824
17	7	0.000038252	0.000072611	-0.000048505
18	7	0.000049515	-0.000070037	0.000044585
19	1	-0.000023836	-0.000026495	0.000042645
20	1	-0.000000153	-0.000004845	0.000000088
21	1	-0.000027501	0.000024916	-0.000040777
22	1	-0.000000653	0.000004973	0.000000448
23	1	-0.000011062	-0.000015746	0.000004470
24	1	-0.000002435	0.000002546	0.000004721
25	1	0.000003576	0.000004688	-0.000000052
26	1	-0.000008356	0.000018840	-0.000002678

Cartesian Forces: Max 0.000120279 RMS 0.000045600
Leave Link 716 at Sat Sep 26 09:21:38 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000052636 RMS 0.000016495
Search for a local minimum.
Step number 27 out of a maximum of 103
All quantities printed in internal units (Hartrees-Bohrs-Radians)
RMS Force = .16495D-04 SwitMx=.10000D-02 MixMth= 2
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 19 20 21 22
23 24 25 26 27
DE= -9.35D-07 DEPred=-6.76D-07 R= 1.38D+00
Trust test= 1.38D+00 RLast= 1.67D-02 DXMaxT set to 8.06D-01
ITU= 0 1 1 1 1 1 1 1 1 1 1 1 1 -1 1 1 1 1 1 1

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```
 ITU=  1  1  1  0  0  1  0
    Eigenvalues ---    0.00242   0.00508   0.01003   0.01287   0.01744
    Eigenvalues ---    0.01896   0.01993   0.02674   0.02920   0.03021
    Eigenvalues ---    0.03074   0.03491   0.03788   0.04171   0.04337
    Eigenvalues ---    0.04461   0.05018   0.05446   0.05551   0.08115
    Eigenvalues ---    0.08560   0.10005   0.10270   0.10941   0.11203
    Eigenvalues ---    0.11322   0.11788   0.13494   0.15227   0.15639
    Eigenvalues ---    0.15897   0.15992   0.16006   0.16101   0.16720
    Eigenvalues ---    0.16877   0.21613   0.22444   0.24587   0.24992
    Eigenvalues ---    0.25000   0.25000   0.25005   0.25031   0.28340
    Eigenvalues ---    0.29768   0.31648   0.37242   0.37617   0.39496
    Eigenvalues ---    0.45857   0.45972   0.46855   0.47503   0.47691
    Eigenvalues ---    0.47698   0.47810   0.48163   0.48816   0.52065
    Eigenvalues ---    0.54880   0.55164   0.55635   0.55663   0.57445
    Eigenvalues ---    0.92173   0.93736   0.95032   0.95263   0.97782
    Eigenvalues ---    0.98881   1.37095
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    27   26   25   24   23   22   21   20
 RFO step:  Lambda=-2.11947240D-07.
 NNeg= 0 NGDIIS= 8 SimSw=  2.50D-01 Rises=F DC= -9.35D-07 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.6283467096D-03 NUsed= 8 OKEnD=F EnDIS=F
 InvSVX:  RCond= 1.11D-07 Info=           0 Equed=N FErr=  5.18D-13 BErr=  9.94D-17
 DidBck=F Rises=F RFO-DIIS coefs:    1.08843    0.15836   -0.29408    0.00965    0.01932
              RFO-DIIS coefs:    0.01271    0.00976   -0.00415
 Iteration  1 RMS(Cart)=  0.00109916 RMS(Int)=  0.00000128
 Iteration  2 RMS(Cart)=  0.00000127 RMS(Int)=  0.00000036
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000036
  ITry=  1  IFail=0  DXMaxC=  4.56D-03  DCOld=  1.00D+10  DXMaxT=  8.06D-01  DXLimC=
3.00D+00 Rises=F
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                          (Linear)    (Quad)   (Total)
    R1        2.32367  -0.00004   0.00001  -0.00005  -0.00003   2.32364
    R2        2.53362   0.00003  -0.00003   0.00007   0.00004   2.53365
    R3        2.53099   0.00003  -0.00001   0.00006   0.00005   2.53104
    R4        2.32364  -0.00003   0.00002  -0.00004  -0.00003   2.32361
    R5        2.32027  -0.00004  -0.00002  -0.00003  -0.00004   2.32022
    R6        2.53108   0.00004  -0.00000   0.00007   0.00006   2.53115
    R7        2.53326   0.00001   0.00002   0.00002   0.00004   2.53330
    R8        2.32021  -0.00004  -0.00001  -0.00003  -0.00004   2.32017
    R9        2.31938  -0.00003  -0.00001  -0.00002  -0.00003   2.31935
   R10        2.53333   0.00003   0.00003   0.00004   0.00007   2.53340
   R11        2.62667   0.00001   0.00004  -0.00000   0.00004   2.62671
   R12        2.31931  -0.00002  -0.00001  -0.00002  -0.00002   2.31929
   R13        2.69308  -0.00001  -0.00012   0.00006  -0.00005   2.69303
   R14        2.69339   0.00000  -0.00001   0.00003   0.00002   2.69341
   R15        2.62681   0.00001   0.00004   0.00001   0.00005   2.62686
   R16        2.69316  -0.00002  -0.00004   0.00004  -0.00001   2.69315
   R17        2.81288   0.00003   0.00009   0.00002   0.00011   2.81300
```

R18	2.05072	-0.00000	-0.00003	0.00003	-0.00000	2.05071
R19	2.81277	0.00002	0.00011	0.00001	0.00012	2.81290
R20	2.05065	-0.00000	-0.00004	0.00003	-0.00001	2.05065
R21	1.94506	-0.00005	-0.00001	-0.00011	-0.00012	1.94494
R22	1.91731	-0.00000	-0.00001	0.00001	-0.00000	1.91731
R23	1.92980	-0.00001	0.00008	-0.00004	0.00004	1.92984
R24	1.94505	-0.00005	-0.00002	-0.00010	-0.00012	1.94493
R25	1.91732	-0.00000	-0.00001	0.00001	-0.00000	1.91731
R26	1.92982	-0.00001	0.00009	-0.00005	0.00004	1.92986
A1	2.55907	0.00000	0.00012	-0.00005	0.00007	2.55914
A2	2.61314	-0.00001	-0.00033	0.00012	-0.00021	2.61293
A3	2.56093	-0.00000	0.00011	-0.00005	0.00005	2.56098
A4	2.71622	-0.00000	0.00046	-0.00028	0.00018	2.71640
A5	2.61144	-0.00001	-0.00031	0.00015	-0.00016	2.61129
A6	2.84227	0.00002	-0.00036	0.00024	-0.00013	2.84214
A7	2.71731	-0.00001	0.00046	-0.00025	0.00021	2.71753
A8	2.84148	0.00002	-0.00034	0.00027	-0.00007	2.84141
A9	2.08551	-0.00001	-0.00002	-0.00002	-0.00004	2.08547
A10	2.10732	0.00001	-0.00004	0.00006	0.00002	2.10734
A11	2.08988	-0.00000	0.00006	-0.00003	0.00002	2.08991
A12	2.08556	-0.00000	-0.00000	-0.00003	-0.00003	2.08553
A13	2.08994	-0.00000	0.00007	-0.00005	0.00002	2.08996
A14	2.10722	0.00000	-0.00007	0.00008	0.00001	2.10722
A15	2.05601	0.00001	0.00009	-0.00006	0.00003	2.05604
A16	1.92779	-0.00000	-0.00016	0.00011	-0.00005	1.92774
A17	2.05651	0.00001	0.00014	-0.00012	0.00003	2.05654
A18	1.92800	0.00001	-0.00010	0.00006	-0.00004	1.92796
A19	2.01580	-0.00001	-0.00005	-0.00001	-0.00007	2.01573
A20	1.92469	-0.00000	0.00015	-0.00004	0.00011	1.92480
A21	1.88840	-0.00001	-0.00005	-0.00015	-0.00020	1.88820
A22	1.89732	0.00001	-0.00001	0.00001	-0.00000	1.89732
A23	1.84467	0.00002	-0.00010	0.00019	0.00009	1.84475
A24	1.88773	0.00001	0.00006	0.00001	0.00007	1.88780
A25	2.01572	-0.00001	-0.00007	0.00001	-0.00006	2.01566
A26	1.92473	-0.00000	0.00016	-0.00003	0.00012	1.92485
A27	1.88843	-0.00002	-0.00005	-0.00018	-0.00023	1.88820
A28	1.89733	0.00000	0.00000	-0.00002	-0.00002	1.89732
A29	1.84463	0.00002	-0.00010	0.00019	0.00010	1.84473
A30	1.88775	0.00001	0.00006	0.00004	0.00009	1.88785
A31	2.90653	-0.00000	0.00003	-0.00012	-0.00009	2.90644
A32	3.12627	0.00001	0.00013	0.00018	0.00031	3.12658
A33	2.90680	-0.00000	0.00009	0.00002	0.00012	2.90691
A34	3.12651	-0.00001	-0.00003	-0.00018	-0.00021	3.12630
A35	3.98381	0.00001	-0.00007	0.00005	-0.00002	3.98378
A36	3.98452	0.00002	0.00004	-0.00005	-0.00001	3.98450
A37	3.14554	-0.00001	-0.00007	-0.00001	-0.00008	3.14546
A38	3.13970	-0.00000	-0.00004	0.00002	-0.00002	3.13969
A39	3.14549	-0.00000	-0.00005	0.00003	-0.00003	3.14546

A40	3.13982	-0.00000	-0.00007	0.00011	0.00004	3.13986
A41	4.01577	0.00001	-0.00029	0.00027	-0.00002	4.01575
A42	4.01474	0.00002	-0.00023	0.00030	0.00007	4.01481
D1	0.01036	-0.00002	-0.00048	-0.00024	-0.00072	0.00964
D2	-0.00686	0.00002	0.00044	0.00028	0.00072	-0.00614
D3	-0.00484	0.00001	0.00048	0.00021	0.00069	-0.00415
D4	0.01036	-0.00002	-0.00052	-0.00019	-0.00071	0.00966
D5	-0.00346	-0.00002	-0.00045	-0.00029	-0.00074	-0.00420
D6	-0.00487	0.00002	0.00044	0.00028	0.00072	-0.00416
D7	-0.00084	0.00000	0.00014	0.00005	0.00019	-0.00065
D8	3.10524	0.00000	-0.00002	0.00015	0.00013	3.10537
D9	-0.00340	-0.00002	-0.00045	-0.00028	-0.00073	-0.00413
D10	-0.00084	0.00001	0.00018	0.00011	0.00029	-0.00055
D11	3.10548	0.00000	-0.00006	0.00018	0.00013	3.10561
D12	0.00716	0.00000	-0.00003	-0.00003	-0.00006	0.00710
D13	-3.10189	0.00000	0.00014	-0.00002	0.00011	-3.10178
D14	-3.10174	-0.00000	0.00008	-0.00012	-0.00004	-3.10178
D15	0.07240	0.00000	0.00025	-0.00012	0.00013	0.07253
D16	2.51364	0.00000	0.00037	-0.00017	0.00020	2.51384
D17	-0.66107	0.00001	0.00026	-0.00008	0.00018	-0.66089
D18	-0.66005	0.00000	0.00011	0.00009	0.00021	-0.65984
D19	2.51450	0.00000	0.00028	0.00010	0.00038	2.51488
D20	-1.15547	0.00000	0.00206	0.00002	0.00207	-1.15340
D21	1.00372	-0.00000	0.00213	-0.00001	0.00211	1.00583
D22	3.06515	-0.00000	0.00225	-0.00011	0.00214	3.06729
D23	-1.15646	0.00001	0.00217	0.00005	0.00221	-1.15424
D24	1.00273	0.00000	0.00224	0.00000	0.00224	1.00497
D25	3.06423	0.00000	0.00237	-0.00008	0.00229	3.06652

Item	Value	Threshold	Converged?
Maximum Force	0.000053	0.000450	YES
RMS Force	0.000016	0.000300	YES
Maximum Displacement	0.004556	0.001800	NO
RMS Displacement	0.001099	0.001200	YES

Predicted change in Energy=-1.019074D-07
Lowest energy point so far. Saving SCF results.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 09:21:38 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.013709	0.668811	0.047005
2	6	0	3.337785	1.693664	0.116019
3	6	0	4.013117	-0.668718	-0.045893

4	6	0	2.137726	2.286830	0.159901
5	6	0	3.338182	-1.694191	-0.115126
6	6	0	0.910673	2.329383	0.166498
7	6	0	2.137665	-2.286531	-0.159282
8	6	0	-0.383269	1.979576	0.145008
9	6	0	0.910660	-2.329589	-0.166245
10	6	0	-1.460574	1.393128	0.101701
11	6	0	-0.383227	-1.979358	-0.145094
12	6	0	-2.670510	0.710588	0.053913
13	6	0	-1.460606	-1.393092	-0.102107
14	6	0	-2.670537	-0.710377	-0.054420
15	6	0	-3.907208	1.412260	0.152347
16	6	0	-3.907106	-1.411985	-0.152962
17	7	0	-3.725626	2.875841	-0.049665
18	7	0	-3.725815	-2.875539	0.049121
19	1	0	-3.439658	3.160199	-0.996582
20	1	0	-4.575050	3.372967	0.196813
21	1	0	-3.440220	-3.159859	0.996155
22	1	0	-4.575206	-3.372590	-0.197629
23	1	0	-2.979509	3.193147	0.571250
24	1	0	-4.743449	1.049114	-0.436264
25	1	0	-4.743963	-1.048653	0.434593
26	1	0	-2.979472	-3.192949	-0.571483

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229618	0.000000			
3	C	1.340752	2.462345	0.000000		
4	C	2.479928	1.339370	3.506381	0.000000	
5	C	2.463006	3.395731	1.229603	4.167165	0.000000
6	C	3.521450	2.509494	4.319593	1.227809	4.707575
7	C	3.506585	4.166297	2.479414	4.584486	1.339425
8	C	4.589240	3.732134	5.135963	2.539693	5.235784
9	C	4.320277	4.707141	3.521110	4.787838	2.509823
10	C	5.522264	4.807783	5.851008	3.708080	5.710220
11	C	5.136413	5.234998	4.588622	4.964734	3.732439
12	C	6.684353	6.088506	6.825197	5.061117	6.474250
13	C	5.851650	5.709659	5.521732	5.153491	4.808243
14	C	6.825804	6.473670	6.683790	5.669972	6.089030
15	C	7.956427	7.250547	8.191539	6.107876	7.887791
16	C	8.192008	7.887069	7.955742	7.093597	7.250881
17	N	8.048455	7.163572	8.511877	5.896588	8.413493
18	N	8.512499	8.412879	8.047990	7.813030	7.163980
19	H	7.927721	7.022986	8.432572	5.762589	8.383387
20	H	9.005647	8.089471	9.494774	6.800178	9.401736
21	H	8.433306	8.382880	7.927413	7.840869	7.023522
22	H	9.495380	9.401103	9.005179	8.787510	8.089843

23	H	7.453335	6.508754	8.011971	5.213129	8.016883
24	H	8.778723	8.125688	8.932009	7.016974	8.540586
25	H	8.932901	8.540284	8.778478	7.652356	8.126499
26	H	8.012509	8.016195	7.452804	7.533168	6.509017

		6	7	8	9	10
6	C	0.000000				
7	C	4.787307	0.000000			
8	C	1.340564	4.964612	0.000000		
9	C	4.670840	1.227780	4.509993	0.000000	
10	C	2.550213	5.153186	1.227348	4.421897	0.000000
11	C	4.509603	2.539577	3.969549	1.340616	3.548978
12	C	3.931672	5.669808	2.617270	4.702757	1.389996
13	C	4.421757	3.707972	3.549171	2.550303	2.793664
14	C	4.702554	5.061034	3.536554	3.931835	2.431690
15	C	4.904415	7.093564	3.569320	6.108583	2.447232
16	C	6.108264	6.107710	4.899888	4.904389	3.730822
17	N	4.673394	7.812828	3.465911	6.971746	2.711422
18	N	6.971514	5.896673	5.895248	4.673472	4.832763
19	H	4.579125	7.840566	3.469670	7.053545	2.871505
20	H	5.584187	8.787335	4.417607	7.921109	3.691716
21	H	7.053395	5.762858	6.040132	4.579375	5.044674
22	H	7.920856	6.800267	6.807013	5.584224	5.701105
23	H	4.005424	7.532995	2.897395	6.795434	2.401605
24	H	5.828508	7.651991	4.496088	6.592229	3.344401
25	H	6.592262	7.017253	5.316924	5.828942	4.105332
26	H	6.795145	5.213118	5.831693	4.005338	4.877738

		11	12	13	14	15
11	C	0.000000				
12	C	3.536535	0.000000			
13	C	1.227315	2.431806	0.000000		
14	C	2.617313	1.425088	1.390075	0.000000	
15	C	4.899998	1.425291	3.731033	2.465297	0.000000
16	C	3.569271	2.465215	2.447101	1.425155	2.840700
17	N	5.895226	2.410875	4.832893	3.738207	1.488573
18	N	3.466086	3.738181	2.711399	2.410863	4.292875
19	H	6.040021	2.774117	5.044719	4.057163	2.143347
20	H	6.807031	3.276577	5.701266	4.512647	2.071802
21	H	3.470049	4.057170	2.871675	2.774181	4.672725
22	H	4.417754	4.512592	3.691649	3.276531	4.843913
23	H	5.831693	2.554646	4.877916	3.965403	2.051259
24	H	5.316762	2.156838	4.105251	2.745646	1.085190
25	H	4.496473	2.745734	3.344715	2.157002	2.614558
26	H	2.897430	3.965372	2.401406	2.554596	4.753165

		16	17	18	19	20
16	C	0.000000				
17	N	4.292908	0.000000			
18	N	1.488520	5.752228	0.000000		
19	H	4.672802	1.029218	6.132334	0.000000	

20	H	4.843993	1.014597	6.307681	1.660896	0.000000
21	H	2.143248	6.132280	1.029212	6.626774	6.678668
22	H	2.071793	6.307660	1.014599	6.678708	6.757080
23	H	4.753122	1.021229	6.136655	1.634295	1.648724
24	H	2.614716	2.126582	4.083390	2.543720	2.414423
25	H	1.085155	4.083279	2.126670	4.632916	4.431230
26	H	2.051218	6.136713	1.021237	6.383962	6.800544

		21	22	23	24	25
21	H	0.000000				
22	H	1.660894	0.000000			
23	H	6.383845	6.800465	0.000000		
24	H	4.633107	4.431334	2.953548	0.000000	
25	H	2.544069	2.414305	4.596177	2.271347	0.000000
26	H	1.634281	1.648759	6.487531	4.596194	2.953578

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=2 Diff= 1.21D-04
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.521296	-0.670158	-0.022842
2	6	0	3.845341	-1.696787	-0.055681
3	6	0	4.520745	0.669818	0.022745
4	6	0	2.645265	-2.291092	-0.078713
5	6	0	3.845842	1.697119	0.055631
6	6	0	1.418211	-2.333810	-0.083939
7	6	0	2.645342	2.290691	0.078700
8	6	0	0.124280	-1.983417	-0.074964
9	6	0	1.418338	2.334010	0.084001
10	6	0	-0.953008	-1.395769	-0.052522
11	6	0	0.124440	1.983294	0.075092
12	6	0	-2.162923	-0.711925	-0.029012
13	6	0	-0.952957	1.395912	0.052725
14	6	0	-2.162909	0.711979	0.029053
15	6	0	-3.399637	-1.416595	-0.102732
16	6	0	-3.399461	1.416674	0.102609
17	7	0	-3.218133	-2.872131	0.150881
18	7	0	-3.218092	2.872168	-0.151033
19	1	0	-2.932279	-3.122869	1.107285
20	1	0	-4.067548	-3.377626	-0.077974

```
    21        1        0     -2.932383    3.122843   -1.107490
    22        1        0     -4.067492    3.377655    0.077907
    23        1        0     -2.471959   -3.211201   -0.458354
    24        1        0     -4.235928   -1.032852    0.472589
    25        1        0     -4.236268    1.032839   -0.471836
    26        1        0     -2.471806    3.211280    0.458052
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6019542           0.2710791           0.1875814
 Leave Link  202 at Sat Sep 26 09:21:38 2026, MaxMem=    805306368 cpu:                  0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1010.2921804319 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.222036 cShort=  0.000000 cLong=
0.777964
  DFx  wShort=  0.000000 wLong=  0.200000 cFull=  0.000000 cShort=  0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0153853988 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1010.2767950331 Hartrees.
 Leave Link  301 at Sat Sep 26 09:21:38 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23224 LenP2D=   51951.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.85D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=         32
 NSgBfM=   683   683   683   683   683 MxSgAt=    26 MxSgA2=    26.
```

Supporting Information file

```
 Leave Link  302 at Sat Sep 26 09:21:39 2026, MaxMem=    805306368 cpu:                6.5 elap:
1.1
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Sat Sep 26 09:21:40 2026, MaxMem=    805306368 cpu:                0.7 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=    -0.000000   -0.000000   -0.000000
       Rot=    1.000000   -0.000001   -0.000001   -0.000034 Ang=  -0.00 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Leave Link  401 at Sat Sep 26 09:21:40 2026, MaxMem=    805306368 cpu:                3.5 elap:
0.6
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.413945097062
 DIIS: error= 7.51D-05 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -723.413945097062     IErMin= 1 ErrMin= 7.51D-05
 ErrMax= 7.51D-05  0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-06 BMatP= 2.41D-06
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.100D+01
 Coeff:      0.100D+01
 Gap=     0.704 Goal=   None    Shift=    0.000
 RMSDP=1.36D-05 MaxDP=5.65D-04              OVMax= 3.91D-04

 Cycle   2  Pass 1  IDiag  1:
 RMSU=  1.33D-05    CP:  1.00D+00
 E= -723.413947734973     Delta-E=       -0.000002637911 Rises=F Damp=F
 DIIS: error= 1.15D-05 at cycle   2 NSaved=   2.
 NSaved= 2 IEnMin= 2 EnMin= -723.413947734973     IErMin= 2 ErrMin= 1.15D-05
```

ErrMax= 1.15D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.20D-08 BMatP= 2.41D-06
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.122D+00 0.112D+01
Coeff: -0.122D+00 0.112D+01
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.62D-06 MaxDP=1.76D-04 DE=-2.64D-06 OVMax= 1.09D-04

Cycle 3 Pass 1 IDiag 1:
RMSU= 2.20D-06 CP: 1.00D+00 1.18D+00
E= -723.413947859413 Delta-E= -0.000000124440 Rises=F Damp=F
DIIS: error= 6.85D-06 at cycle 3 NSaved= 3.
NSaved= 3 IEnMin= 3 EnMin= -723.413947859413 IErMin= 3 ErrMin= 6.85D-06
ErrMax= 6.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.95D-08 BMatP= 6.20D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.585D-01 0.440D+00 0.618D+00
Coeff: -0.585D-01 0.440D+00 0.618D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.17D-06 MaxDP=5.43D-05 DE=-1.24D-07 OVMax= 7.94D-05

Cycle 4 Pass 1 IDiag 1:
RMSU= 9.20D-07 CP: 1.00D+00 1.19D+00 1.24D+00
E= -723.413947875037 Delta-E= -0.000000015624 Rises=F Damp=F
DIIS: error= 6.75D-06 at cycle 4 NSaved= 4.
NSaved= 4 IEnMin= 4 EnMin= -723.413947875037 IErMin= 4 ErrMin= 6.75D-06
ErrMax= 6.75D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.26D-09 BMatP= 1.95D-08
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.524D-02-0.117D+00 0.417D+00 0.694D+00
Coeff: 0.524D-02-0.117D+00 0.417D+00 0.694D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.19D-06 MaxDP=5.81D-05 DE=-1.56D-08 OVMax= 4.54D-05

Cycle 5 Pass 1 IDiag 1:
RMSU= 4.73D-07 CP: 1.00D+00 1.21D+00 1.57D+00 1.18D+00
E= -723.413947887340 Delta-E= -0.000000012303 Rises=F Damp=F
DIIS: error= 8.92D-07 at cycle 5 NSaved= 5.
NSaved= 5 IEnMin= 5 EnMin= -723.413947887340 IErMin= 5 ErrMin= 8.92D-07
ErrMax= 8.92D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.26D-10 BMatP= 9.26D-09
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.582D-02-0.792D-01 0.154D+00 0.313D+00 0.606D+00
Coeff: 0.582D-02-0.792D-01 0.154D+00 0.313D+00 0.606D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=3.42D-07 MaxDP=1.45D-05 DE=-1.23D-08 OVMax= 1.77D-05

Cycle 6 Pass 1 IDiag 1:
RMSU= 1.59D-07 CP: 1.00D+00 1.21D+00 1.65D+00 1.30D+00 1.22D+00
E= -723.413947888089 Delta-E= -0.000000000749 Rises=F Damp=F
DIIS: error= 6.37D-07 at cycle 6 NSaved= 6.
NSaved= 6 IEnMin= 6 EnMin= -723.413947888089 IErMin= 6 ErrMin= 6.37D-07

ErrMax= 6.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.40D-11 BMatP= 4.26D-10
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.140D-02-0.108D-01-0.138D-01-0.462D-02 0.242D+00 0.786D+00
Coeff: 0.140D-02-0.108D-01-0.138D-01-0.462D-02 0.242D+00 0.786D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=2.98D-07 MaxDP=1.48D-05 DE=-7.49D-10 OVMax= 1.03D-05

Cycle   7 Pass 1 IDiag 1:
RMSU= 5.30D-08   CP: 1.00D+00 1.22D+00 1.72D+00 1.41D+00 1.50D+00
               CP: 1.23D+00
E= -723.413947888388   Delta-E=   -0.000000000299 Rises=F Damp=F
DIIS: error= 3.98D-07 at cycle   7 NSaved=   7.
NSaved= 7 IEnMin= 7 EnMin= -723.413947888388   IErMin= 7 ErrMin= 3.98D-07
ErrMax= 3.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-11 BMatP= 7.40D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.102D-02 0.174D-01-0.483D-01-0.892D-01-0.652D-01 0.296D+00
Coeff-Com: 0.890D+00
Coeff: -0.102D-02 0.174D-01-0.483D-01-0.892D-01-0.652D-01 0.296D+00
Coeff: 0.890D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=2.31D-07 MaxDP=1.06D-05 DE=-2.99D-10 OVMax= 8.24D-06

Cycle   8 Pass 1 IDiag 1:
RMSU= 2.27D-08   CP: 1.00D+00 1.22D+00 1.78D+00 1.48D+00 1.71D+00
               CP: 1.53D+00 1.41D+00
E= -723.413947888523   Delta-E=   -0.000000000135 Rises=F Damp=F
DIIS: error= 2.01D-07 at cycle   8 NSaved=   8.
NSaved= 8 IEnMin= 8 EnMin= -723.413947888523   IErMin= 8 ErrMin= 2.01D-07
ErrMax= 2.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.05D-12 BMatP= 1.98D-11
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.811D-03 0.103D-01-0.162D-01-0.365D-01-0.973D-01-0.102D+00
Coeff-Com: 0.401D+00 0.841D+00
Coeff: -0.811D-03 0.103D-01-0.162D-01-0.365D-01-0.973D-01-0.102D+00
Coeff: 0.401D+00 0.841D+00
Gap=   0.179 Goal=   None   Shift=   0.000
RMSDP=1.14D-07 MaxDP=5.12D-06 DE=-1.35D-10 OVMax= 5.26D-06

Cycle   9 Pass 1 IDiag 1:
RMSU= 1.28D-08   CP: 1.00D+00 1.22D+00 1.80D+00 1.52D+00 1.81D+00
               CP: 1.68D+00 1.71D+00 1.73D+00
E= -723.413947888572   Delta-E=   -0.000000000049 Rises=F Damp=F
DIIS: error= 1.40D-07 at cycle   9 NSaved=   9.
NSaved= 9 IEnMin= 9 EnMin= -723.413947888572   IErMin= 9 ErrMin= 1.40D-07
ErrMax= 1.40D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.00D-12 BMatP= 7.05D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.142D-04-0.173D-02 0.102D-01 0.158D-01-0.179D-01-0.153D+00
Coeff-Com: -0.132D+00 0.358D+00 0.922D+00
Coeff: 0.142D-04-0.173D-02 0.102D-01 0.158D-01-0.179D-01-0.153D+00

Coeff: -0.132D+00 0.358D+00 0.922D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=4.52D-08 MaxDP=1.64D-06 DE=-4.89D-11 OVMax= 3.79D-06

Cycle 10 Pass 1 IDiag 1:
RMSU= 8.45D-09 CP: 1.00D+00 1.22D+00 1.81D+00 1.52D+00 1.85D+00
CP: 1.73D+00 1.91D+00 2.38D+00 1.77D+00
E= -723.413947888581 Delta-E= -0.000000000009 Rises=F Damp=F
DIIS: error= 5.15D-08 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -723.413947888581 IErMin=10 ErrMin= 5.15D-08
ErrMax= 5.15D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.13D-13 BMatP= 2.00D-12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.226D-03-0.370D-02 0.971D-02 0.183D-01 0.173D-01-0.566D-01
Coeff-Com: -0.172D+00-0.335D-01 0.474D+00 0.746D+00
Coeff: 0.226D-03-0.370D-02 0.971D-02 0.183D-01 0.173D-01-0.566D-01
Coeff: -0.172D+00-0.335D-01 0.474D+00 0.746D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.25D-08 MaxDP=7.32D-07 DE=-9.09D-12 OVMax= 1.54D-06

Cycle 11 Pass 1 IDiag 1:
RMSU= 4.18D-09 CP: 1.00D+00 1.22D+00 1.81D+00 1.52D+00 1.85D+00
CP: 1.73D+00 1.94D+00 2.69D+00 2.24D+00 1.59D+00
E= -723.413947888587 Delta-E= -0.000000000006 Rises=F Damp=F
DIIS: error= 2.55D-08 at cycle 11 NSaved= 11.
NSaved=11 IEnMin=11 EnMin= -723.413947888587 IErMin=11 ErrMin= 2.55D-08
ErrMax= 2.55D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-13 BMatP= 6.13D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.738D-04-0.850D-03 0.788D-03 0.251D-02 0.108D-01 0.161D-01
Coeff-Com: -0.255D-01-0.976D-01-0.668D-01 0.257D+00 0.903D+00
Coeff: 0.738D-04-0.850D-03 0.788D-03 0.251D-02 0.108D-01 0.161D-01
Coeff: -0.255D-01-0.976D-01-0.668D-01 0.257D+00 0.903D+00
Gap= 0.179 Goal= None Shift= 0.000
RMSDP=1.05D-08 MaxDP=5.49D-07 DE=-5.91D-12 OVMax= 7.45D-07

Cycle 12 Pass 1 IDiag 1:
RMSU= 1.69D-09 CP: 1.00D+00 1.22D+00 1.81D+00 1.52D+00 1.84D+00
CP: 1.72D+00 1.94D+00 2.84D+00 2.59D+00 2.07D+00
CP: 1.33D+00
E= -723.413947888591 Delta-E= -0.000000000004 Rises=F Damp=F
DIIS: error= 1.30D-08 at cycle 12 NSaved= 12.
NSaved=12 IEnMin=12 EnMin= -723.413947888591 IErMin=12 ErrMin= 1.30D-08
ErrMax= 1.30D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-14 BMatP= 1.01D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.105D-04 0.382D-03-0.186D-02-0.287D-02 0.234D-02 0.228D-01
Coeff-Com: 0.262D-01-0.485D-01-0.155D+00-0.345D-01 0.523D+00 0.668D+00
Coeff: -0.105D-04 0.382D-03-0.186D-02-0.287D-02 0.234D-02 0.228D-01
Coeff: 0.262D-01-0.485D-01-0.155D+00-0.345D-01 0.523D+00 0.668D+00
Gap= 0.179 Goal= None Shift= 0.000

Supporting Information file

RMSDP=5.08D-09 MaxDP=2.43D-07 DE=-3.87D-12 OVMax= 2.72D-07

SCF Done: E(RwB97XD) = -723.413947889 A.U. after 12 cycles
NFock= 12 Conv=0.51D-08 -V/T= 2.0047
KE= 7.200589625830D+02 PE=-3.701629051087D+03 EE= 1.247879345582D+03
Leave Link 502 at Sat Sep 26 09:37:48 2026, MaxMem= 805306368 cpu: 5803.7 elap: 967.6
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral first derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23224 LenP2D= 51951.
LDataN: DoStor=T MaxTD1= 7 Len= 274
Leave Link 701 at Sat Sep 26 09:37:48 2026, MaxMem= 805306368 cpu: 3.0 elap: 0.5
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 09:37:48 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral first derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 2527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 09:48:41 2026, MaxMem= 805306368 cpu: 3917.8 elap: 653.0
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.53856741D+00-4.34338794D-04 1.41939131D-04
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000013406	0.000040559	-0.000084104
2	6	0.000027888	-0.000037572	0.000097501
3	6	-0.000008342	-0.000043149	0.000083862
4	6	-0.000032393	0.000037810	-0.000114295
5	6	0.000023935	0.000041345	-0.000096850
6	6	0.000030287	-0.000026410	0.000090043
7	6	-0.000032862	-0.000039998	0.000114040

```
     8        6       -0.000022073    0.000001983   -0.000028268
     9        6        0.000030838    0.000028707   -0.000091359
    10        6        0.000012442    0.000004415    0.000004262
    11        6       -0.000027791   -0.000001809    0.000028340
    12        6        0.000004578    0.000006397   -0.000002608
    13        6        0.000022329   -0.000003150    0.000000102
    14        6       -0.000005508   -0.000007931   -0.000001163
    15        6       -0.000011664   -0.000011626   -0.000001607
    16        6       -0.000014044    0.000005035   -0.000000818
    17        7        0.000032334    0.000032424   -0.000023273
    18        7        0.000033920   -0.000031827    0.000020266
    19        1       -0.000010975   -0.000012547    0.000020261
    20        1       -0.000001667   -0.000005960   -0.000000848
    21        1       -0.000014214    0.000012308   -0.000018610
    22        1       -0.000000816    0.000004725   -0.000000333
    23        1       -0.000013053   -0.000009411    0.000003618
    24        1       -0.000001468    0.000000378    0.000005669
    25        1        0.000002824    0.000005293   -0.000000505
    26        1       -0.000011099    0.000010011   -0.000003321
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000114295 RMS     0.000036473
 Leave Link  716 at Sat Sep 26 09:48:41 2026, MaxMem=    805306368 cpu:                  0.2 elap:
0.0
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max     0.000024640 RMS     0.000010093
 Search for a local minimum.
 Step number  28 out of a maximum of  103
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 RMS Force = .10093D-04 SwitMx=.10000D-02 MixMth= 2
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points   18   19   20   21   22
                                     23   24   25   26   27
                                     28
 DE= -1.17D-07 DEPred=-1.02D-07 R= 1.15D+00
 Trust test= 1.15D+00 RLast= 5.76D-03 DXMaxT set to 8.06D-01
 ITU=  0  0  1  1  1  1  1  1  1  1  1  1  1  1 -1  1  1  1  1  1
 ITU=  1  1  1  1  0  0  1  0
    Eigenvalues ---    0.00251   0.00508   0.00942   0.01287   0.01698
    Eigenvalues ---    0.01768   0.01913   0.02674   0.02968   0.03072
    Eigenvalues ---    0.03243   0.03508   0.03780   0.04150   0.04338
    Eigenvalues ---    0.04461   0.05017   0.05423   0.05535   0.07909
    Eigenvalues ---    0.08151   0.10047   0.10265   0.11111   0.11207
```

```
     Eigenvalues ---    0.11436   0.11791   0.13632   0.15232   0.15581
     Eigenvalues ---    0.15898   0.15950   0.16001   0.16008   0.16711
     Eigenvalues ---    0.16882   0.21877   0.22442   0.24350   0.24976
     Eigenvalues ---    0.25000   0.25001   0.25003   0.25030   0.28466
     Eigenvalues ---    0.30019   0.31903   0.37244   0.37610   0.39414
     Eigenvalues ---    0.45851   0.45952   0.46897   0.47190   0.47646
     Eigenvalues ---    0.47691   0.47714   0.47891   0.48486   0.52111
     Eigenvalues ---    0.54974   0.55125   0.55637   0.55668   0.56238
     Eigenvalues ---    0.91017   0.93762   0.95032   0.95169   0.97893
     Eigenvalues ---    0.98635   1.37104
 En-DIIS/RFO-DIIS/Sim-DIIS IScMMF=       -3 using points:    28   27   26   25   24   23   22   21
20
 RFO step:  Lambda=-1.15496332D-07.
 NNeg= 0 NGDIIS= 9 SimSw=  2.50D-01 Rises=F DC= -1.17D-07 SmlDif=  1.00D-05
 NRisDI= 0 DoIntr=F SqrtH=F CThrHd= 10.0 CDAdj=  3.0
 RMS Error=  0.3310203011D-03 NUsed= 9 OKEnD=F EnDIS=F
 InvSVX:  RCond= 2.17D-08 Info=          0 Equed=N FErr=  1.51D-12 BErr=  6.91D-17
 DIIS inversion failure, remove point   9.
 InvSVX:  RCond= 3.09D-08 Info=          0 Equed=N FErr=  1.05D-12 BErr=  9.80D-17
 DIIS inversion failure, remove point   8.
 InvSVX:  RCond= 4.40D-08 Info=          0 Equed=N FErr=  3.79D-13 BErr=  5.15D-17
 DIIS inversion failure, remove point   7.
 InvSVX:  RCond= 5.41D-08 Info=          0 Equed=N FErr=  3.88D-13 BErr=  9.78D-17
 DIIS inversion failure, remove point   6.
 InvSVX:  RCond= 7.12D-08 Info=          0 Equed=N FErr=  8.01D-14 BErr=  8.94D-17
 DIIS inversion failure, remove point   5.
 InvSVX:  RCond= 9.55D-08 Info=          0 Equed=N FErr=  1.15D-13 BErr=  9.19D-17
 DIIS inversion failure, remove point   4.
 InvSVX:  RCond= 1.56D-07 Info=          0 Equed=N FErr=  1.47D-13 BErr=  4.72D-17
 RFO-DIIS uses    3 points instead of    9
 DidBck=F Rises=F RFO-DIIS coefs:    0.84003    0.36909   -0.20912    0.00000    0.00000
                  RFO-DIIS coefs:    0.00000    0.00000    0.00000    0.00000
 Iteration  1 RMS(Cart)=  0.00041744 RMS(Int)=  0.00000018
 Iteration  2 RMS(Cart)=  0.00000018 RMS(Int)=  0.00000006
  ITry=  1 IFail=0 DXMaxC=  1.72D-03 DCOld=  1.00D+10 DXMaxT=  8.06D-01 DXLimC=
3.00D+00 Rises=F
 Variable      Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                         (Linear)    (Quad)   (Total)
    R1        2.32364  -0.00002   0.00000  -0.00004  -0.00003   2.32361
    R2        2.53365   0.00002  -0.00001   0.00006   0.00005   2.53370
    R3        2.53104   0.00002   0.00000   0.00005   0.00006   2.53110
    R4        2.32361  -0.00002   0.00000  -0.00004  -0.00003   2.32358
    R5        2.32022  -0.00002  -0.00001  -0.00003  -0.00004   2.32019
    R6        2.53115   0.00002   0.00000   0.00006   0.00006   2.53121
    R7        2.53330   0.00001   0.00002   0.00002   0.00004   2.53334
    R8        2.32017  -0.00002  -0.00001  -0.00003  -0.00004   2.32013
    R9        2.31935  -0.00001  -0.00000  -0.00002  -0.00002   2.31933
   R10        2.53340   0.00001   0.00001   0.00004   0.00005   2.53344
```

R11	2.62671	0.00000	0.00002	0.00001	0.00003	2.62674
R12	2.31929	-0.00002	-0.00001	-0.00001	-0.00002	2.31926
R13	2.69303	-0.00000	-0.00005	0.00000	-0.00004	2.69298
R14	2.69341	0.00000	-0.00000	0.00002	0.00002	2.69343
R15	2.62686	0.00000	0.00002	0.00002	0.00004	2.62690
R16	2.69315	0.00000	-0.00002	0.00001	-0.00000	2.69315
R17	2.81300	0.00001	0.00003	0.00006	0.00009	2.81309
R18	2.05071	-0.00000	-0.00002	0.00001	-0.00001	2.05071
R19	2.81290	0.00001	0.00004	0.00006	0.00010	2.81299
R20	2.05065	-0.00000	-0.00002	0.00002	-0.00000	2.05064
R21	1.94494	-0.00002	-0.00002	-0.00007	-0.00009	1.94485
R22	1.91731	-0.00000	-0.00000	-0.00000	-0.00000	1.91731
R23	1.92984	-0.00001	0.00003	-0.00002	0.00001	1.92985
R24	1.94493	-0.00002	-0.00003	-0.00006	-0.00009	1.94484
R25	1.91731	-0.00000	-0.00000	0.00000	-0.00000	1.91731
R26	1.92986	-0.00001	0.00003	-0.00002	0.00001	1.92987
A1	2.55914	0.00000	0.00005	-0.00002	0.00004	2.55918
A2	2.61293	-0.00000	-0.00013	0.00004	-0.00010	2.61284
A3	2.56098	-0.00000	0.00004	-0.00003	0.00002	2.56099
A4	2.71640	-0.00002	0.00021	-0.00016	0.00005	2.71645
A5	2.61129	0.00000	-0.00014	0.00007	-0.00007	2.61122
A6	2.84214	0.00002	-0.00014	0.00015	0.00001	2.84215
A7	2.71753	-0.00002	0.00019	-0.00014	0.00005	2.71758
A8	2.84141	0.00002	-0.00016	0.00019	0.00003	2.84144
A9	2.08547	-0.00000	0.00001	-0.00003	-0.00002	2.08544
A10	2.10734	0.00001	-0.00003	0.00005	0.00002	2.10736
A11	2.08991	-0.00001	0.00002	-0.00002	0.00000	2.08991
A12	2.08553	-0.00001	-0.00000	-0.00002	-0.00003	2.08550
A13	2.08996	-0.00000	0.00003	-0.00002	0.00001	2.08997
A14	2.10722	0.00001	-0.00003	0.00004	0.00001	2.10724
A15	2.05604	0.00000	0.00003	-0.00003	-0.00000	2.05604
A16	1.92774	0.00000	-0.00011	0.00005	-0.00006	1.92768
A17	2.05654	-0.00001	0.00005	-0.00006	-0.00001	2.05653
A18	1.92796	0.00001	-0.00008	0.00008	-0.00000	1.92796
A19	2.01573	-0.00000	-0.00003	-0.00005	-0.00007	2.01566
A20	1.92480	-0.00001	0.00007	-0.00004	0.00003	1.92483
A21	1.88820	-0.00001	-0.00005	-0.00003	-0.00008	1.88812
A22	1.89732	0.00000	0.00000	0.00001	0.00001	1.89733
A23	1.84475	0.00001	-0.00003	0.00012	0.00009	1.84485
A24	1.88780	0.00000	0.00003	-0.00000	0.00003	1.88783
A25	2.01566	-0.00000	-0.00003	-0.00004	-0.00008	2.01558
A26	1.92485	-0.00001	0.00007	-0.00004	0.00004	1.92489
A27	1.88820	-0.00001	-0.00005	-0.00004	-0.00010	1.88811
A28	1.89732	0.00000	-0.00000	-0.00000	-0.00000	1.89732
A29	1.84473	0.00001	-0.00002	0.00012	0.00010	1.84483
A30	1.88785	0.00000	0.00003	0.00001	0.00004	1.88789
A31	2.90644	-0.00000	0.00006	-0.00011	-0.00004	2.90640
A32	3.12658	-0.00000	-0.00010	0.00019	0.00009	3.12667

A33	2.90691	-0.00000	-0.00004	0.00004	-0.00000	2.90691
A34	3.12630	0.00000	0.00014	-0.00017	-0.00003	3.12627
A35	3.98378	0.00000	-0.00008	0.00002	-0.00006	3.98372
A36	3.98450	0.00001	-0.00003	0.00002	-0.00001	3.98449
A37	3.14546	-0.00000	0.00001	-0.00005	-0.00004	3.14542
A38	3.13969	0.00000	-0.00000	0.00004	0.00004	3.13973
A39	3.14546	-0.00000	-0.00003	0.00000	-0.00003	3.14544
A40	3.13986	-0.00000	-0.00000	-0.00002	-0.00002	3.13984
A41	4.01575	0.00001	-0.00006	0.00010	0.00004	4.01579
A42	4.01481	0.00001	-0.00006	0.00010	0.00004	4.01486
D1	0.00964	-0.00002	-0.00019	-0.00045	-0.00064	0.00901
D2	-0.00614	0.00001	0.00019	0.00047	0.00066	-0.00549
D3	-0.00415	0.00002	0.00020	0.00047	0.00066	-0.00349
D4	0.00966	-0.00002	-0.00020	-0.00044	-0.00064	0.00901
D5	-0.00420	-0.00002	-0.00018	-0.00051	-0.00069	-0.00489
D6	-0.00416	0.00001	0.00018	0.00046	0.00064	-0.00351
D7	-0.00065	0.00000	0.00010	0.00016	0.00026	-0.00040
D8	3.10537	0.00000	-0.00001	0.00026	0.00025	3.10562
D9	-0.00413	-0.00002	-0.00018	-0.00052	-0.00070	-0.00483
D10	-0.00055	0.00000	0.00005	0.00020	0.00025	-0.00030
D11	3.10561	0.00000	0.00002	0.00012	0.00014	3.10575
D12	0.00710	0.00000	-0.00003	-0.00005	-0.00008	0.00702
D13	-3.10178	-0.00000	-0.00001	0.00002	0.00001	-3.10177
D14	-3.10178	0.00000	0.00008	-0.00013	-0.00005	-3.10183
D15	0.07253	-0.00000	0.00010	-0.00007	0.00003	0.07256
D16	2.51384	0.00000	0.00014	0.00003	0.00017	2.51400
D17	-0.66089	0.00000	0.00002	0.00012	0.00014	-0.66075
D18	-0.65984	0.00000	0.00002	0.00002	0.00004	-0.65980
D19	2.51488	-0.00000	0.00004	0.00009	0.00013	2.51501
D20	-1.15340	-0.00000	0.00095	-0.00019	0.00076	-1.15264
D21	1.00583	-0.00000	0.00099	-0.00025	0.00074	1.00657
D22	3.06729	-0.00001	0.00104	-0.00030	0.00074	3.06803
D23	-1.15424	0.00000	0.00100	-0.00011	0.00089	-1.15336
D24	1.00497	-0.00000	0.00103	-0.00017	0.00086	1.00583
D25	3.06652	-0.00001	0.00108	-0.00021	0.00087	3.06739

Item	Value	Threshold	Converged?
Maximum Force	0.000025	0.000450	YES
RMS Force	0.000010	0.000300	YES
Maximum Displacement	0.001719	0.001800	YES
RMS Displacement	0.000417	0.001200	YES

Predicted change in Energy=-5.124027D-08
Optimization completed.
-- Stationary point found.

! Optimized Parameters !			
! (Angstroms and Degrees) !			
! Name	Definition	Value	Derivative Info. !

Supporting Information file

```
--------------------------------------------------------------------------------
! R1    R(1,2)                1.2296       -DE/DX =    0.0              !
! R2    R(1,3)                1.3408       -DE/DX =    0.0              !
! R3    R(2,4)                1.3394       -DE/DX =    0.0              !
! R4    R(3,5)                1.2296       -DE/DX =    0.0              !
! R5    R(4,6)                1.2278       -DE/DX =    0.0              !
! R6    R(5,7)                1.3394       -DE/DX =    0.0              !
! R7    R(6,8)                1.3406       -DE/DX =    0.0              !
! R8    R(7,9)                1.2278       -DE/DX =    0.0              !
! R9    R(8,10)               1.2273       -DE/DX =    0.0              !
! R10   R(9,11)               1.3406       -DE/DX =    0.0              !
! R11   R(10,12)              1.39         -DE/DX =    0.0              !
! R12   R(11,13)              1.2273       -DE/DX =    0.0              !
! R13   R(12,14)              1.4251       -DE/DX =    0.0              !
! R14   R(12,15)              1.4253       -DE/DX =    0.0              !
! R15   R(13,14)              1.3901       -DE/DX =    0.0              !
! R16   R(14,16)              1.4252       -DE/DX =    0.0              !
! R17   R(15,17)              1.4886       -DE/DX =    0.0              !
! R18   R(15,24)              1.0852       -DE/DX =    0.0              !
! R19   R(16,18)              1.4885       -DE/DX =    0.0              !
! R20   R(16,25)              1.0852       -DE/DX =    0.0              !
! R21   R(17,19)              1.0292       -DE/DX =    0.0              !
! R22   R(17,20)              1.0146       -DE/DX =    0.0              !
! R23   R(17,23)              1.0212       -DE/DX =    0.0              !
! R24   R(18,21)              1.0292       -DE/DX =    0.0              !
! R25   R(18,22)              1.0146       -DE/DX =    0.0              !
! R26   R(18,26)              1.0212       -DE/DX =    0.0              !
! A1    A(2,1,3)            146.6279       -DE/DX =    0.0              !
! A2    A(1,2,4)            149.7101       -DE/DX =    0.0              !
! A3    A(1,3,5)            146.7332       -DE/DX =    0.0              !
! A4    A(2,4,6)            155.6385       -DE/DX =    0.0              !
! A5    A(3,5,7)            149.6158       -DE/DX =    0.0              !
! A6    A(4,6,8)            162.8426       -DE/DX =    0.0              !
! A7    A(5,7,9)            155.7028       -DE/DX =    0.0              !
! A8    A(7,9,11)           162.8008       -DE/DX =    0.0              !
! A9    A(10,12,14)         119.4884       -DE/DX =    0.0              !
! A10   A(10,12,15)         120.7417       -DE/DX =    0.0              !
! A11   A(14,12,15)         119.7429       -DE/DX =    0.0              !
! A12   A(12,14,13)         119.4922       -DE/DX =    0.0              !
! A13   A(12,14,16)         119.7458       -DE/DX =    0.0              !
! A14   A(13,14,16)         120.735        -DE/DX =    0.0              !
! A15   A(12,15,24)         117.8027       -DE/DX =    0.0              !
! A16   A(17,15,24)         110.4513       -DE/DX =    0.0              !
! A17   A(14,16,25)         117.8311       -DE/DX =    0.0              !
! A18   A(18,16,25)         110.4642       -DE/DX =    0.0              !
! A19   A(15,17,19)         115.4928       -DE/DX =    0.0              !
! A20   A(15,17,20)         110.2829       -DE/DX =    0.0              !
! A21   A(15,17,23)         108.1861       -DE/DX =    0.0              !
```

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! A22   A(19,17,20)          108.7082         -DE/DX =    0.0              !
! A23   A(19,17,23)          105.6966         -DE/DX =    0.0              !
! A24   A(20,17,23)          108.1631         -DE/DX =    0.0              !
! A25   A(16,18,21)          115.4887         -DE/DX =    0.0              !
! A26   A(16,18,22)          110.2859         -DE/DX =    0.0              !
! A27   A(16,18,26)          108.1861         -DE/DX =    0.0              !
! A28   A(21,18,22)          108.7083         -DE/DX =    0.0              !
! A29   A(21,18,26)          105.6952         -DE/DX =    0.0              !
! A30   A(22,18,26)          108.1656         -DE/DX =    0.0              !
! A31   L(6,8,10,7,-1)       166.5267         -DE/DX =    0.0              !
! A32   L(8,10,12,7,-1)      179.1399         -DE/DX =    0.0              !
! A33   L(9,11,13,4,-1)      166.5538         -DE/DX =    0.0              !
! A34   L(11,13,14,4,-1)     179.1237         -DE/DX =    0.0              !
! A35   L(12,15,17,24,-1)    228.2539         -DE/DX =    0.0              !
! A36   L(14,16,18,25,-1)    228.2953         -DE/DX =    0.0              !
! A37   L(6,8,10,7,-2)       180.2218         -DE/DX =    0.0              !
! A38   L(8,10,12,7,-2)      179.8907         -DE/DX =    0.0              !
! A39   L(9,11,13,4,-2)      180.2218         -DE/DX =    0.0              !
! A40   L(11,13,14,4,-2)     179.9006         -DE/DX =    0.0              !
! A41   L(12,15,17,24,-2)    230.0857         -DE/DX =    0.0              !
! A42   L(14,16,18,25,-2)    230.0317         -DE/DX =    0.0              !
! D1    D(3,1,2,4)            0.5525          -DE/DX =    0.0              !
! D2    D(2,1,3,5)           -0.3519          -DE/DX =    0.0              !
! D3    D(1,2,4,6)           -0.2377          -DE/DX =    0.0              !
! D4    D(1,3,5,7)            0.5534          -DE/DX =    0.0              !
! D5    D(2,4,6,8)           -0.2404          -DE/DX =    0.0              !
! D6    D(3,5,7,9)           -0.2381          -DE/DX =    0.0              !
! D7    D(4,6,12,14)          -0.0375         -DE/DX =    0.0              !
! D8    D(4,6,12,15)         177.9248         -DE/DX =    0.0              !
! D9    D(5,7,9,11)          -0.2367          -DE/DX =    0.0              !
! D10   D(7,9,14,12)          -0.0316         -DE/DX =    0.0              !
! D11   D(7,9,14,16)         177.9385         -DE/DX =    0.0              !
! D12   D(10,12,14,13)         0.4066         -DE/DX =    0.0              !
! D13   D(10,12,14,16)      -177.7189         -DE/DX =    0.0              !
! D14   D(15,12,14,13)      -177.719          -DE/DX =    0.0              !
! D15   D(15,12,14,16)         4.1555         -DE/DX =    0.0              !
! D16   D(10,12,15,24)       144.0322         -DE/DX =    0.0              !
! D17   D(14,12,15,24)       -37.8661         -DE/DX =    0.0              !
! D18   D(12,14,16,25)       -37.8062         -DE/DX =    0.0              !
! D19   D(13,14,16,25)       144.092          -DE/DX =    0.0              !
! D20   D(24,15,17,19)       -66.0849         -DE/DX =    0.0              !
! D21   D(24,15,17,20)        57.6297         -DE/DX =    0.0              !
! D22   D(24,15,17,23)       175.7427         -DE/DX =    0.0              !
! D23   D(25,16,18,21)       -66.1333         -DE/DX =    0.0              !
! D24   D(25,16,18,22)        57.5808         -DE/DX =    0.0              !
! D25   D(25,16,18,26)       175.6986         -DE/DX =    0.0              !
--------------------------------------------------------------------------------
Lowest energy point so far.  Saving SCF results.
```

Supporting Information file

Largest change from initial coordinates is atom 20 2.066 Angstoms.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Sep 26 09:48:42 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l202.exe)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.013709	0.668811	0.047005
2	6	0	3.337785	1.693664	0.116019
3	6	0	4.013117	-0.668718	-0.045893
4	6	0	2.137726	2.286830	0.159901
5	6	0	3.338182	-1.694191	-0.115126
6	6	0	0.910673	2.329383	0.166498
7	6	0	2.137665	-2.286531	-0.159282
8	6	0	-0.383269	1.979576	0.145008
9	6	0	0.910660	-2.329589	-0.166245
10	6	0	-1.460574	1.393128	0.101701
11	6	0	-0.383227	-1.979358	-0.145094
12	6	0	-2.670510	0.710588	0.053913
13	6	0	-1.460606	-1.393092	-0.102107
14	6	0	-2.670537	-0.710377	-0.054420
15	6	0	-3.907208	1.412260	0.152347
16	6	0	-3.907106	-1.411985	-0.152962
17	7	0	-3.725626	2.875841	-0.049665
18	7	0	-3.725815	-2.875539	0.049121
19	1	0	-3.439658	3.160199	-0.996582
20	1	0	-4.575050	3.372967	0.196813
21	1	0	-3.440220	-3.159859	0.996155
22	1	0	-4.575206	-3.372590	-0.197629
23	1	0	-2.979509	3.193147	0.571250
24	1	0	-4.743449	1.049114	-0.436264
25	1	0	-4.743963	-1.048653	0.434593
26	1	0	-2.979472	-3.192949	-0.571483

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229618	0.000000			
3	C	1.340752	2.462345	0.000000		
4	C	2.479928	1.339370	3.506381	0.000000	
5	C	2.463006	3.395731	1.229603	4.167165	0.000000
6	C	3.521450	2.509494	4.319593	1.227809	4.707575
7	C	3.506585	4.166297	2.479414	4.584486	1.339425
8	C	4.589240	3.732134	5.135963	2.539693	5.235784

9	C	4.320277	4.707141	3.521110	4.787838	2.509823
10	C	5.522264	4.807783	5.851008	3.708080	5.710220
11	C	5.136413	5.234998	4.588622	4.964734	3.732439
12	C	6.684353	6.088506	6.825197	5.061117	6.474250
13	C	5.851650	5.709659	5.521732	5.153491	4.808243
14	C	6.825804	6.473670	6.683790	5.669972	6.089030
15	C	7.956427	7.250547	8.191539	6.107876	7.887791
16	C	8.192008	7.887069	7.955742	7.093597	7.250881
17	N	8.048455	7.163572	8.511877	5.896588	8.413493
18	N	8.512499	8.412879	8.047990	7.813030	7.163980
19	H	7.927721	7.022986	8.432572	5.762589	8.383387
20	H	9.005647	8.089471	9.494774	6.800178	9.401736
21	H	8.433306	8.382880	7.927413	7.840869	7.023522
22	H	9.495380	9.401103	9.005179	8.787510	8.089843
23	H	7.453335	6.508754	8.011971	5.213129	8.016883
24	H	8.778723	8.125688	8.932009	7.016974	8.540586
25	H	8.932901	8.540284	8.778478	7.652356	8.126499
26	H	8.012509	8.016195	7.452804	7.533168	6.509017

		6	7	8	9	10
6	C	0.000000				
7	C	4.787307	0.000000			
8	C	1.340564	4.964612	0.000000		
9	C	4.670840	1.227780	4.509993	0.000000	
10	C	2.550213	5.153186	1.227348	4.421897	0.000000
11	C	4.509603	2.539577	3.969549	1.340616	3.548978
12	C	3.931672	5.669808	2.617270	4.702757	1.389996
13	C	4.421757	3.707972	3.549171	2.550303	2.793664
14	C	4.702554	5.061034	3.536554	3.931835	2.431690
15	C	4.904415	7.093564	3.569320	6.108583	2.447232
16	C	6.108264	6.107710	4.899888	4.904389	3.730822
17	N	4.673394	7.812828	3.465911	6.971746	2.711422
18	N	6.971514	5.896673	5.895248	4.673472	4.832763
19	H	4.579125	7.840566	3.469670	7.053545	2.871505
20	H	5.584187	8.787335	4.417607	7.921109	3.691716
21	H	7.053395	5.762858	6.040132	4.579375	5.044674
22	H	7.920856	6.800267	6.807013	5.584224	5.701105
23	H	4.005424	7.532995	2.897395	6.795434	2.401605
24	H	5.828508	7.651991	4.496088	6.592229	3.344401
25	H	6.592262	7.017253	5.316924	5.828942	4.105332
26	H	6.795145	5.213118	5.831693	4.005338	4.877738

		11	12	13	14	15
11	C	0.000000				
12	C	3.536535	0.000000			
13	C	1.227315	2.431806	0.000000		
14	C	2.617313	1.425088	1.390075	0.000000	
15	C	4.899998	1.425291	3.731033	2.465297	0.000000
16	C	3.569271	2.465215	2.447101	1.425155	2.840700
17	N	5.895226	2.410875	4.832893	3.738207	1.488573

18	N	3.466086	3.738181	2.711399	2.410863	4.292875
19	H	6.040021	2.774117	5.044719	4.057163	2.143347
20	H	6.807031	3.276577	5.701266	4.512647	2.071802
21	H	3.470049	4.057170	2.871675	2.774181	4.672725
22	H	4.417754	4.512592	3.691649	3.276531	4.843913
23	H	5.831693	2.554646	4.877916	3.965403	2.051259
24	H	5.316762	2.156838	4.105251	2.745646	1.085190
25	H	4.496473	2.745734	3.344715	2.157002	2.614558
26	H	2.897430	3.965372	2.401406	2.554596	4.753165

		16	17	18	19	20
16	C	0.000000				
17	N	4.292908	0.000000			
18	N	1.488520	5.752228	0.000000		
19	H	4.672802	1.029218	6.132334	0.000000	
20	H	4.843993	1.014597	6.307681	1.660896	0.000000
21	H	2.143248	6.132280	1.029212	6.626774	6.678668
22	H	2.071793	6.307660	1.014599	6.678708	6.757080
23	H	4.753122	1.021229	6.136655	1.634295	1.648724
24	H	2.614716	2.126582	4.083390	2.543720	2.414423
25	H	1.085155	4.083279	2.126670	4.632916	4.431230
26	H	2.051218	6.136713	1.021237	6.383962	6.800544

		21	22	23	24	25
21	H	0.000000				
22	H	1.660894	0.000000			
23	H	6.383845	6.800465	0.000000		
24	H	4.633107	4.431334	2.953548	0.000000	
25	H	2.544069	2.414305	4.596177	2.271347	0.000000
26	H	1.634281	1.648759	6.487531	4.596194	2.953578

		26
26	H	0.000000

Stoichiometry C16H8N2
Framework group C1[X(C16H8N2)]
Deg. of freedom 72
Full point group C1 NOp 1
RotChk: IX=2 Diff= 6.63D-16
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.521296	-0.670158	-0.022842
2	6	0	3.845341	-1.696787	-0.055681
3	6	0	4.520745	0.669818	0.022745
4	6	0	2.645265	-2.291092	-0.078713
5	6	0	3.845842	1.697119	0.055631
6	6	0	1.418211	-2.333810	-0.083939

7	6	0	2.645342	2.290691	0.078700
8	6	0	0.124280	-1.983417	-0.074964
9	6	0	1.418338	2.334010	0.084001
10	6	0	-0.953008	-1.395769	-0.052522
11	6	0	0.124440	1.983294	0.075092
12	6	0	-2.162923	-0.711925	-0.029012
13	6	0	-0.952957	1.395912	0.052725
14	6	0	-2.162909	0.711979	0.029053
15	6	0	-3.399637	-1.416595	-0.102732
16	6	0	-3.399461	1.416674	0.102609
17	7	0	-3.218133	-2.872131	0.150881
18	7	0	-3.218092	2.872168	-0.151033
19	1	0	-2.932279	-3.122869	1.107285
20	1	0	-4.067548	-3.377626	-0.077974
21	1	0	-2.932383	3.122843	-1.107490
22	1	0	-4.067492	3.377655	0.077907
23	1	0	-2.471959	-3.211201	-0.458354
24	1	0	-4.235928	-1.032852	0.472589
25	1	0	-4.236268	1.032839	-0.471836
26	1	0	-2.471806	3.211280	0.458052

Rotational constants (GHZ): 0.6019542 0.2710791 0.1875814

Leave Link 202 at Sat Sep 26 09:48:42 2026, MaxMem= 805306368 cpu: 0.0 elap: 0.0

(Enter /home/user/gauss16/g16/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

****

Population analysis using the SCF Density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Alpha occ. eigenvalues --	-0.39347	-0.38751	-0.36617	-0.31868	-0.30721
Alpha occ. eigenvalues --	-0.30418	-0.25990	-0.25032	-0.18984	
Alpha virt. eigenvalues --	-0.01086	0.00687	0.00981	0.04375	0.05856
Alpha virt. eigenvalues --	0.06494	0.09536	0.10546	0.11693	0.11868
Alpha virt. eigenvalues --	0.12793	0.12821	0.14787	0.15683	0.15933
Alpha virt. eigenvalues --	0.16155	0.17554	0.18043	0.18325	0.18646
Alpha virt. eigenvalues --	0.20128	0.20460	0.21357	0.22549	0.23912
Alpha virt. eigenvalues --	0.24549	0.26553	0.26963	0.27633	0.28154
Alpha virt. eigenvalues --	0.28657	0.28798	0.28972	0.30491	0.31236
Alpha virt. eigenvalues --	0.31908	0.32215	0.32600	0.33384	0.34759
Alpha virt. eigenvalues --	0.35348	0.35888	0.36145	0.36711	0.37400
Alpha virt. eigenvalues --	0.37913	0.38321	0.39300	0.39506	0.39998
Alpha virt. eigenvalues --	0.40696	0.40900	0.41563	0.41793	0.42924
Alpha virt. eigenvalues --	0.43059	0.43281	0.44455	0.45130	0.45411
Alpha virt. eigenvalues --	0.46238	0.46448	0.46913	0.48238	0.48503
Alpha virt. eigenvalues --	0.48695	0.48800	0.50134	0.50183	0.50496
Alpha virt. eigenvalues --	0.50892	0.52009	0.52207	0.53502	0.53975
Alpha virt. eigenvalues --	0.54043	0.54457	0.54501	0.54589	0.56820
Alpha virt. eigenvalues --	0.57004	0.57555	0.57780	0.59273	0.59453
Alpha virt. eigenvalues --	0.59805	0.60455	0.61277	0.61762	0.61885
Alpha virt. eigenvalues --	0.62184	0.62906	0.63057	0.63893	0.64810
Alpha virt. eigenvalues --	0.64855	0.65825	0.66090	0.66788	0.67550
Alpha virt. eigenvalues --	0.67824	0.68313	0.69793	0.70645	0.70732
Alpha virt. eigenvalues --	0.71511	0.71850	0.72518	0.74333	0.74645
Alpha virt. eigenvalues --	0.75200	0.76762	0.77604	0.77685	0.78484
Alpha virt. eigenvalues --	0.79449	0.81581	0.81713	0.83162	0.83176
Alpha virt. eigenvalues --	0.83795	0.86609	0.88856	0.89093	0.89616
Alpha virt. eigenvalues --	0.91220	0.91981	0.93847	0.94546	0.94983
Alpha virt. eigenvalues --	0.96473	0.97785	0.97848	0.98397	0.98475
Alpha virt. eigenvalues --	0.99573	1.00774	1.02010	1.02052	1.04872
Alpha virt. eigenvalues --	1.07355	1.07801	1.09140	1.09375	1.09523
Alpha virt. eigenvalues --	1.10303	1.11520	1.14044	1.14935	1.15817
Alpha virt. eigenvalues --	1.17824	1.18346	1.21995	1.22201	1.23168
Alpha virt. eigenvalues --	1.25236	1.25323	1.26322	1.27177	1.27998
Alpha virt. eigenvalues --	1.29486	1.30209	1.31574	1.32902	1.33415
Alpha virt. eigenvalues --	1.34014	1.34476	1.35556	1.37547	1.38190
Alpha virt. eigenvalues --	1.38370	1.40379	1.40909	1.41149	1.42962
Alpha virt. eigenvalues --	1.43192	1.43734	1.44322	1.45264	1.46239
Alpha virt. eigenvalues --	1.46778	1.48697	1.49102	1.49242	1.50827
Alpha virt. eigenvalues --	1.51621	1.51955	1.52315	1.53390	1.54186
Alpha virt. eigenvalues --	1.54609	1.54764	1.55953	1.56096	1.56263
Alpha virt. eigenvalues --	1.56926	1.57890	1.58186	1.60179	1.60458
Alpha virt. eigenvalues --	1.61123	1.62528	1.64400	1.64485	1.66249
Alpha virt. eigenvalues --	1.66282	1.69291	1.70741	1.71894	1.72625
Alpha virt. eigenvalues --	1.73383	1.73792	1.73798	1.74858	1.75304
Alpha virt. eigenvalues --	1.76743	1.77046	1.78297	1.79604	1.80312
Alpha virt. eigenvalues --	1.80600	1.81122	1.82209	1.83674	1.83911
Alpha virt. eigenvalues --	1.84434	1.85091	1.85634	1.86238	1.87093

Alpha virt. eigenvalues --	1.87511	1.88473	1.89659	1.90410	1.92461
Alpha virt. eigenvalues --	1.92495	1.95591	1.96491	1.98409	1.98429
Alpha virt. eigenvalues --	1.99951	2.02463	2.02906	2.03978	2.04984
Alpha virt. eigenvalues --	2.06132	2.07344	2.09280	2.09396	2.09971
Alpha virt. eigenvalues --	2.14792	2.15557	2.17065	2.18142	2.19888
Alpha virt. eigenvalues --	2.20277	2.22191	2.23363	2.25082	2.26129
Alpha virt. eigenvalues --	2.27808	2.30334	2.32042	2.33814	2.35278
Alpha virt. eigenvalues --	2.37564	2.38837	2.41048	2.41301	2.41327
Alpha virt. eigenvalues --	2.45085	2.46483	2.46609	2.47554	2.48857
Alpha virt. eigenvalues --	2.49173	2.49743	2.49921	2.51085	2.51602
Alpha virt. eigenvalues --	2.52111	2.53324	2.53680	2.53900	2.56318
Alpha virt. eigenvalues --	2.58490	2.58673	2.59063	2.59406	2.60205
Alpha virt. eigenvalues --	2.60529	2.61774	2.62660	2.64638	2.65058
Alpha virt. eigenvalues --	2.66223	2.66606	2.67608	2.68326	2.69233
Alpha virt. eigenvalues --	2.69976	2.70835	2.71211	2.73613	2.74950
Alpha virt. eigenvalues --	2.75151	2.75908	2.76607	2.78141	2.78193
Alpha virt. eigenvalues --	2.79460	2.79874	2.81492	2.81507	2.83475
Alpha virt. eigenvalues --	2.84428	2.85532	2.86014	2.86855	2.87260
Alpha virt. eigenvalues --	2.87816	2.88509	2.88784	2.89314	2.89533
Alpha virt. eigenvalues --	2.90614	2.91113	2.91200	2.91538	2.91889
Alpha virt. eigenvalues --	2.93294	2.94272	2.94821	2.95645	2.96002
Alpha virt. eigenvalues --	2.96725	2.97272	2.98718	2.99245	2.99463
Alpha virt. eigenvalues --	2.99619	2.99783	3.00873	3.02983	3.03176
Alpha virt. eigenvalues --	3.03540	3.04076	3.04712	3.05131	3.06695
Alpha virt. eigenvalues --	3.06883	3.07896	3.08669	3.09484	3.10102
Alpha virt. eigenvalues --	3.10324	3.10957	3.11956	3.13013	3.13765
Alpha virt. eigenvalues --	3.14129	3.15514	3.15687	3.17155	3.17811
Alpha virt. eigenvalues --	3.17958	3.20315	3.20884	3.22911	3.23716
Alpha virt. eigenvalues --	3.23997	3.24469	3.25231	3.26268	3.26620
Alpha virt. eigenvalues --	3.28562	3.29641	3.30456	3.31112	3.31481
Alpha virt. eigenvalues --	3.32269	3.33200	3.33379	3.35339	3.36821
Alpha virt. eigenvalues --	3.37600	3.38365	3.39652	3.39871	3.40453
Alpha virt. eigenvalues --	3.41216	3.42523	3.43128	3.44080	3.46398
Alpha virt. eigenvalues --	3.46511	3.46587	3.48015	3.49695	3.49813
Alpha virt. eigenvalues --	3.50751	3.51245	3.51571	3.53074	3.53490
Alpha virt. eigenvalues --	3.54852	3.57053	3.57466	3.59569	3.59635
Alpha virt. eigenvalues --	3.63147	3.63464	3.65097	3.66886	3.67442
Alpha virt. eigenvalues --	3.68467	3.69988	3.70616	3.72890	3.73677
Alpha virt. eigenvalues --	3.75964	3.76176	3.79093	3.80517	3.82171
Alpha virt. eigenvalues --	3.85404	3.85699	3.86704	3.91633	3.92304
Alpha virt. eigenvalues --	3.94621	3.95461	3.96831	3.96887	3.98500
Alpha virt. eigenvalues --	4.02212	4.02973	4.06064	4.06434	4.07490
Alpha virt. eigenvalues --	4.10423	4.10595	4.11955	4.16011	4.20057
Alpha virt. eigenvalues --	4.20347	4.23628	4.23934	4.24863	4.26665
Alpha virt. eigenvalues --	4.28600	4.31904	4.36867	4.38480	4.38561
Alpha virt. eigenvalues --	4.39820	4.40964	4.44891	4.45664	4.47988
Alpha virt. eigenvalues --	4.50696	4.51696	4.53425	4.60901	4.61930
Alpha virt. eigenvalues --	4.63649	4.65329	4.68904	4.74381	4.77441

Alpha virt. eigenvalues --	4.77744	4.78620	4.81160	4.81463	4.82301
Alpha virt. eigenvalues --	4.84978	4.86439	4.87524	4.87859	4.89583
Alpha virt. eigenvalues --	4.90330	4.94508	4.94696	4.94784	4.98329
Alpha virt. eigenvalues --	5.00766	5.01302	5.01368	5.01653	5.04562
Alpha virt. eigenvalues --	5.06596	5.09430	5.11625	5.13209	5.14641
Alpha virt. eigenvalues --	5.16643	5.17485	5.21866	5.22138	5.22635
Alpha virt. eigenvalues --	5.24772	5.26446	5.27575	5.28714	5.30005
Alpha virt. eigenvalues --	5.31037	5.34863	5.36737	5.37780	5.41064
Alpha virt. eigenvalues --	5.43469	5.43480	5.49282	5.49693	5.50597
Alpha virt. eigenvalues --	5.57121	5.57325	5.59770	5.65891	5.71752
Alpha virt. eigenvalues --	5.76075	5.77990	5.89884	5.94474	6.03632
Alpha virt. eigenvalues --	6.08301	6.09607	6.15741	6.29101	22.50101
Alpha virt. eigenvalues --	22.61095	22.67070	22.95393	22.99955	23.26336
Alpha virt. eigenvalues --	23.27543	23.48236	23.58702	23.71953	23.77030
Alpha virt. eigenvalues --	23.96298	24.16572	24.28179	24.32210	24.57413
Alpha virt. eigenvalues --	31.91726	31.95392			

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	5.355464	0.773331	0.725210	-0.232743	-0.191768	-0.220552
2	C	0.773331	5.352710	-0.192414	0.716852	-0.198324	-0.294061
3	C	0.725210	-0.192414	5.356682	-0.060923	0.773286	-0.038924
4	C	-0.232743	0.716852	-0.060923	5.556113	-0.036180	0.631701
5	C	-0.191768	-0.198324	0.773286	-0.036180	5.351011	-0.022540
6	C	-0.220552	-0.294061	-0.038924	0.631701	-0.022540	5.740743
7	C	-0.060680	-0.036171	-0.232530	-0.013924	0.716864	-0.005715
8	C	-0.041681	-0.086192	-0.005157	-0.260272	-0.004498	0.838060
9	C	-0.038880	-0.022579	-0.221167	-0.005645	-0.293084	-0.011010
10	C	-0.012959	-0.044455	-0.000154	-0.315114	0.000846	-0.298431
11	C	-0.005142	-0.004497	-0.041686	-0.004460	-0.085492	-0.019845
12	C	-0.000403	-0.002686	-0.000017	-0.033747	0.000220	-0.095968
13	C	-0.000151	0.000874	-0.013009	0.017250	-0.044237	0.017559
14	C	-0.000018	0.000222	-0.000405	0.002635	-0.002671	0.008062
15	C	0.000021	0.000122	-0.000004	0.002828	-0.000017	0.016267
16	C	-0.000004	-0.000017	0.000021	-0.000254	0.000122	-0.001628
17	N	0.000000	-0.000000	-0.000000	-0.000048	-0.000000	0.000064
18	N	-0.000000	-0.000000	0.000000	-0.000002	-0.000000	-0.000014
19	H	-0.000003	-0.000028	-0.000000	-0.000822	0.000000	-0.005159
20	H	0.000000	0.000000	0.000000	0.000021	-0.000000	0.000186
21	H	-0.000000	0.000000	-0.000003	0.000004	-0.000028	0.000022
22	H	0.000000	-0.000000	0.000000	-0.000000	0.000000	-0.000001
23	H	0.000003	0.000031	0.000000	0.000642	-0.000000	0.002840
24	H	0.000000	0.000002	-0.000000	0.000062	-0.000000	0.000716
25	H	-0.000000	-0.000000	0.000000	-0.000011	0.000002	-0.000125
26	H	0.000000	-0.000000	0.000003	-0.000003	0.000031	-0.000010

		7	8	9	10	11	12
1	C	-0.060680	-0.041681	-0.038880	-0.012959	-0.005142	-0.000403
2	C	-0.036171	-0.086192	-0.022579	-0.044455	-0.004497	-0.002686
3	C	-0.232530	-0.005157	-0.221167	-0.000154	-0.041686	-0.000017

4	C	-0.013924	-0.260272	-0.005645	-0.315114	-0.004460	-0.033747
5	C	0.716864	-0.004498	-0.293084	0.000846	-0.085492	0.000220
6	C	-0.005715	0.838060	-0.011010	-0.298431	-0.019845	-0.095968
7	C	5.559932	-0.004359	0.628459	0.017276	-0.260458	0.002653
8	C	-0.004359	5.694805	-0.019669	0.289078	-0.062302	-0.536464
9	C	0.628459	-0.019669	5.740660	0.017361	0.838294	0.008010
10	C	0.017276	0.289078	0.017361	6.434007	0.033281	0.449335
11	C	-0.260458	-0.062302	0.838294	0.033281	5.696174	0.007068
12	C	0.002653	-0.536464	0.008010	0.449335	0.007068	5.654137
13	C	-0.316259	0.033118	-0.296932	-0.106441	0.287003	-0.100433
14	C	-0.033843	0.007074	-0.095632	-0.100241	-0.537618	0.487528
15	C	-0.000253	0.074122	-0.001612	-0.233459	-0.016406	0.317372
16	C	0.002838	-0.016454	0.016275	-0.005314	0.074553	-0.005937
17	N	-0.000002	0.002873	-0.000015	0.028684	-0.000401	-0.108774
18	N	-0.000049	-0.000399	0.000042	-0.002730	0.002749	-0.007344
19	H	0.000004	-0.007446	0.000022	0.028157	0.000363	0.038848
20	H	-0.000000	0.001817	-0.000001	-0.002122	-0.000012	0.000642
21	H	-0.000822	0.000362	-0.005146	0.001539	-0.007434	0.001217
22	H	0.000021	-0.000012	0.000186	-0.000059	0.001822	0.000960
23	H	-0.000003	0.008725	-0.000010	0.006060	-0.000193	-0.026531
24	H	-0.000011	0.009072	-0.000125	0.023160	-0.002008	-0.105048
25	H	0.000062	-0.002004	0.000713	-0.005740	0.009066	-0.004767
26	H	0.000644	-0.000193	0.002827	-0.000709	0.008707	-0.002659

		13	14	15	16	17	18
1	C	-0.000151	-0.000018	0.000021	-0.000004	0.000000	-0.000000
2	C	0.000874	0.000222	0.000122	-0.000017	-0.000000	-0.000000
3	C	-0.013009	-0.000405	-0.000004	0.000021	-0.000000	0.000000
4	C	0.017250	0.002635	0.002828	-0.000254	-0.000048	-0.000002
5	C	-0.044237	-0.002671	-0.000017	0.000122	-0.000000	-0.000000
6	C	0.017559	0.008062	0.016267	-0.001628	0.000064	-0.000014
7	C	-0.316259	-0.033843	-0.000253	0.002838	-0.000002	-0.000049
8	C	0.033118	0.007074	0.074122	-0.016454	0.002873	-0.000399
9	C	-0.296932	-0.095632	-0.001612	0.016275	-0.000015	0.000042
10	C	-0.106441	-0.100241	-0.233459	-0.005314	0.028684	-0.002730
11	C	0.287003	-0.537618	-0.016406	0.074553	-0.000401	0.002749
12	C	-0.100433	0.487528	0.317372	-0.005937	-0.108774	-0.007344
13	C	6.436981	0.448645	-0.005169	-0.232929	-0.002741	0.028596
14	C	0.448645	5.654700	-0.006092	0.316893	-0.007351	-0.108588
15	C	-0.005169	-0.006092	5.819082	-0.054201	0.223321	-0.000689
16	C	-0.232929	0.316893	-0.054201	5.818361	-0.000692	0.223455
17	N	-0.002741	-0.007351	0.223321	-0.000692	6.133081	-0.000015
18	N	0.028596	-0.108588	-0.000689	0.223455	-0.000015	6.132940
19	H	0.001539	0.001229	-0.093008	0.001197	0.329070	0.000009
20	H	-0.000059	0.000961	-0.038846	-0.000137	0.373945	-0.000002
21	H	0.028170	0.038753	0.001192	-0.092936	0.000009	0.329093
22	H	-0.002116	0.000637	-0.000136	-0.038861	-0.000002	0.373936
23	H	-0.000710	-0.002666	-0.009276	-0.000159	0.362287	0.000000
24	H	-0.005751	-0.004757	0.459533	0.002232	-0.028433	-0.000596

25	H	0.023188	-0.104989	0.002248	0.459531	-0.000597	-0.028442
26	H	0.006070	-0.026480	-0.000159	-0.009333	0.000000	0.362289

		19	20	21	22	23	24
1	C	-0.000003	0.000000	-0.000000	0.000000	0.000003	0.000000
2	C	-0.000028	0.000000	0.000000	-0.000000	0.000031	0.000002
3	C	-0.000000	0.000000	-0.000003	0.000000	0.000000	-0.000000
4	C	-0.000822	0.000021	0.000004	-0.000000	0.000642	0.000062
5	C	0.000000	-0.000000	-0.000028	0.000000	-0.000000	-0.000000
6	C	-0.005159	0.000186	0.000022	-0.000001	0.002840	0.000716
7	C	0.000004	-0.000000	-0.000822	0.000021	-0.000003	-0.000011
8	C	-0.007446	0.001817	0.000362	-0.000012	0.008725	0.009072
9	C	0.000022	-0.000001	-0.005146	0.000186	-0.000010	-0.000125
10	C	0.028157	-0.002122	0.001539	-0.000059	0.006060	0.023160
11	C	0.000363	-0.000012	-0.007434	0.001822	-0.000193	-0.002008
12	C	0.038848	0.000642	0.001217	0.000960	-0.026531	-0.105048
13	C	0.001539	-0.000059	0.028170	-0.002116	-0.000710	-0.005751
14	C	0.001229	0.000961	0.038753	0.000637	-0.002666	-0.004757
15	C	-0.093008	-0.038846	0.001192	-0.000136	-0.009276	0.459533
16	C	0.001197	-0.000137	-0.092936	-0.038861	-0.000159	0.002232
17	N	0.329070	0.373945	0.000009	-0.000002	0.362287	-0.028433
18	N	0.000009	-0.000002	0.329093	0.373936	0.000000	-0.000596
19	H	0.501318	-0.032246	-0.000004	0.000000	-0.035762	-0.006557
20	H	-0.032246	0.404607	0.000000	-0.000000	-0.008550	-0.002872
21	H	-0.000004	0.000000	0.501248	-0.032245	-0.000001	0.000668
22	H	0.000000	-0.000000	-0.032245	0.404611	-0.000000	-0.000156
23	H	-0.035762	-0.008550	-0.000001	-0.000000	0.387839	0.004381
24	H	-0.006557	-0.002872	0.000668	-0.000156	0.004381	0.537369
25	H	0.000668	-0.000156	-0.006544	-0.002868	-0.000221	-0.016107
26	H	-0.000001	-0.000000	-0.035778	-0.008538	0.000000	-0.000221

		25	26
1	C	-0.000000	0.000000
2	C	-0.000000	-0.000000
3	C	0.000000	0.000003
4	C	-0.000011	-0.000003
5	C	0.000002	0.000031
6	C	-0.000125	-0.000010
7	C	0.000062	0.000644
8	C	-0.002004	-0.000193
9	C	0.000713	0.002827
10	C	-0.005740	-0.000709
11	C	0.009066	0.008707
12	C	-0.004767	-0.002659
13	C	0.023188	0.006070
14	C	-0.104989	-0.026480
15	C	0.002248	-0.000159
16	C	0.459531	-0.009333
17	N	-0.000597	0.000000
18	N	-0.028442	0.362289

19	H	0.000668	-0.000001
20	H	-0.000156	-0.000000
21	H	-0.006544	-0.035778
22	H	-0.002868	-0.008538
23	H	-0.000221	0.000000
24	H	-0.016107	-0.000221
25	H	0.537164	0.004378
26	H	0.004378	0.387840

Mulliken charges:

		1
1	C	-0.049045
2	C	0.037279
3	C	-0.048810
4	C	0.036037
5	C	0.036456
6	C	-0.242238
7	C	0.036328
8	C	0.087994
9	C	-0.241343
10	C	-0.200860
11	C	0.088874
12	C	0.062790
13	C	-0.202056
14	C	0.064011
15	C	-0.456780
16	C	-0.456624
17	N	-0.304263
18	N	-0.304239
19	H	0.278611
20	H	0.302823
21	H	0.278664
22	H	0.302822
23	H	0.311273
24	H	0.135449
25	H	0.135552
26	H	0.311295

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.049045
2	C	0.037279
3	C	-0.048810
4	C	0.036037
5	C	0.036456
6	C	-0.242238
7	C	0.036328
8	C	0.087994
9	C	-0.241343

10 C -0.200860
11 C 0.088874
12 C 0.062790
13 C -0.202056
14 C 0.064011
15 C -0.321331
16 C -0.321071
17 N 0.588445
18 N 0.588542
Electronic spatial extent (au): <R**2>= 5315.4160
Charge= -0.0000 electrons
Dipole moment (field-independent basis, Debye):
X= -11.5359 Y= -0.0011 Z= 0.0004 Tot= 11.5359
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -92.8947 YY= -62.8241 ZZ= -106.7165
XY= -0.0191 XZ= -0.0039 YZ= -5.8659
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= -5.4163 YY= 24.6544 ZZ= -19.2381
XY= -0.0191 XZ= -0.0039 YZ= -5.8659
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= -198.6885 YYY= -0.0156 ZZZ= -0.0007 XYY= -205.9495
XXY= 0.0129 XXZ= 0.0193 XZZ= -15.6657 YZZ= 0.0036
YYZ= -0.0079 XYZ= 20.6220
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -5142.4329 YYYY= -1804.4017 ZZZZ= -141.2675 XXXY= -0.3050
XXXZ= -0.0909 YYYX= -0.1465 YYYZ= -30.9323 ZZZX= -0.0023
ZZZY= -26.3663 XXYY= -713.8275 XXZZ= -938.0678 YYZZ= -394.5455
XXYZ= -80.1466 YYXZ= 0.0138 ZZXY= -0.0141
N-N= 1.010276795033D+03 E-N=-3.701629051216D+03 KE= 7.200589625830D+02
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Sat Sep 26 09:48:42 2026, MaxMem= 805306368 cpu: 3.1 elap: 0.6
(Enter /home/user/gauss16/g16/l9999.exe)
Unable to Open any file for archive entry.
1\1\GINC-MAKCLUS\FOpt\RwB97XD\def2TZVP\C16H8N2\USER\26-Sep-2026\0\\#p
opt freq wb97xd def2tzvp\\title card\\0,1\C,4.0137088258,0.6688108827,
0.0470052293\C,3.3377849565,1.6936644054,0.1160191688\C,4.0131169456,-
0.6687183695,-0.0458929281\C,2.1377261836,2.2868300676,0.1599009531\C,
3.3381823741,-1.6941907488,-0.115125913\C,0.9106728464,2.3293834356,0.
1664983357\C,2.1376649086,-2.2865308665,-0.1592824689\C,-0.3832688114,
1.979576007,0.1450081559\C,0.910659667,-2.3295892976,-0.1662453224\C,-
1.4605741781,1.3931280207,0.1017014283\C,-0.3832267059,-1.9793580864,-
0.1450935175\C,-2.6705098007,0.710587852,0.053913335\C,-1.4606063402,-
1.3930921072,-0.1021074088\C,-2.6705374656,-0.7103765391,-0.0544203895
\C,-3.9072075584,1.4122599542,0.152347149\C,-3.9071056435,-1.411985494
5,-0.1529620402\N,-3.7256258515,2.8758406787,-0.049664922\N,-3.7258147

845,-2.8755387333,0.0491205516\H,-3.4396575376,3.1601994972,-0.9965821
711\H,-4.5750497931,3.3729672969,0.1968126105\H,-3.4402200236,-3.15985
85793,0.9961551389\H,-4.5752064273,-3.3725901656,-0.1976285588\H,-2.97
95088706,3.1931471397,0.5712497023\H,-4.7434486038,1.0491141743,-0.436
2639254\H,-4.7439630628,-1.0486530027,0.4345930825\H,-2.9794722888,-3.
1929490817,-0.5714830351\\Version=ES64L-G16RevC.01\State=1-A\HF=-723.4
139479\RMSD=5.079e-09\RMSF=3.647e-05\Dipole=-4.5385673,0.0006114,-0.00
06245\Quadrupole=-4.0268643,18.5971342,-14.5702699,0.0152961,0.004439,
-3.198071\PG=C01 [X(C16H8N2)]\\@
The archive entry for this job was punched.

IF IT'S NOT TRUE, IT'S WELL INVENTED -- DANTE
Leave Link 9999 at Sat Sep 26 09:48:42 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
Job cpu time: 4 days 0 hours 51 minutes 20.2 seconds.
Elapsed time: 0 days 16 hours 8 minutes 49.5 seconds.
File lengths (MBytes): RWF= 229 Int= 0 D2E= 0 Chk= 27 Scr= 1
Normal termination of Gaussian 16 at Sat Sep 26 09:48:42 2026.
(Enter /home/user/gauss16/g16/l1.exe)
Link1: Proceeding to internal job step number 2.

#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RwB97XD/def2TZVP Freq
---
1/10=4,29=7,30=1,38=1,40=1/1,3;
2/12=2,40=1/2;
3/5=44,7=101,11=2,14=-4,25=1,30=1,70=2,71=2,74=-58,116=1,140=1/1,2,3;
4/5=101/1;
5/5=2,38=6,98=1/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
Leave Link 1 at Sat Sep 26 09:48:42 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.1
(Enter /home/user/gauss16/g16/l101.exe)
Structure from the checkpoint file: "cdca-n2-b-4h2.chk"
---
title card

Charge = 0 Multiplicity = 1
Redundant internal coordinates found in file. (old form).
C,0,4.0137088258,0.6688108827,0.0470052293
C,0,3.3377849565,1.6936644054,0.1160191688
C,0,4.0131169456,-0.6687183695,-0.0458929281

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C,0,2.1377261836,2.2868300676,0.1599009531
C,0,3.3381823741,-1.6941907488,-0.115125913
C,0,0.9106728464,2.3293834356,0.1664983357
C,0,2.1376649086,-2.2865308665,-0.1592824689
C,0,-0.3832688114,1.979576007,0.1450081559
C,0,0.910659667,-2.3295892976,-0.1662453224
C,0,-1.4605741781,1.3931280207,0.1017014283
C,0,-0.3832267059,-1.9793580864,-0.1450935175
C,0,-2.6705098007,0.710587852,0.053913335
C,0,-1.4606063402,-1.3930921072,-0.1021074088
C,0,-2.6705374656,-0.7103765391,-0.0544203895
C,0,-3.9072075584,1.4122599542,0.152347149
C,0,-3.9071056435,-1.4119854945,-0.1529620402
N,0,-3.7256258515,2.8758406787,-0.049664922
N,0,-3.7258147845,-2.8755387333,0.0491205516
H,0,-3.4396575376,3.1601994972,-0.9965821711
H,0,-4.5750497931,3.3729672969,0.1968126105
H,0,-3.4402200236,-3.1598585793,0.9961551389
H,0,-4.5752064273,-3.3725901656,-0.1976285588
H,0,-2.9795088706,3.1931471397,0.5712497023
H,0,-4.7434486038,1.0491141743,-0.4362639254
H,0,-4.7439630628,-1.0486530027,0.4345930825
H,0,-2.9794722888,-3.1929490817,-0.5714830351
Recover connectivity data from disk.
ITRead= 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
ITRead= 0 0 0 0 0 0
MicOpt= -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
MicOpt= -1 -1 -1 -1 -1 -1
NAtoms= 26 NQM= 26 NQMF= 0 NMMI= 0 NMMIF= 0
NMic= 0 NMicF= 0.
Isotopes and Nuclear Properties:
(Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic moments (NMagM)
in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10
IAtWgt= 12 12 12 12 12 12 12 12 12 12
AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000
NucSpn= 0 0 0 0 0 0 0 0 0 0
AtZEff= 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000 3.6000000
NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

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```
 Atom       11        12        13        14        15        16        17        18        19        20
 IAtWgt=        12        12        12        12        12        12        14        14         1         1
 AtmWgt=    12.0000000    12.0000000    12.0000000    12.0000000    12.0000000    12.0000000
14.0030740  14.0030740   1.0078250   1.0078250
 NucSpn=          0         0         0         0         0         0         2         2         1         1
 AtZEff=    3.6000000    3.6000000    3.6000000    3.6000000    3.6000000    3.6000000    4.5500000
4.5500000   1.0000000   1.0000000
 NQMom=     0.0000000    0.0000000    0.0000000    0.0000000    0.0000000    0.0000000    2.0440000
2.0440000   0.0000000   0.0000000
 NMagM=     0.0000000    0.0000000    0.0000000    0.0000000    0.0000000    0.0000000    0.4037610
0.4037610   2.7928460   2.7928460
 AtZNuc=    6.0000000    6.0000000    6.0000000    6.0000000    6.0000000    6.0000000    7.0000000
7.0000000   1.0000000   1.0000000

 Atom       21        22        23        24        25        26
 IAtWgt=          1         1         1         1         1         1
 AtmWgt=    1.0078250   1.0078250   1.0078250   1.0078250   1.0078250   1.0078250
 NucSpn=          1         1         1         1         1         1
 AtZEff=    1.0000000   1.0000000   1.0000000   1.0000000   1.0000000   1.0000000
 NQMom=     0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000
 NMagM=     2.7928460   2.7928460   2.7928460   2.7928460   2.7928460   2.7928460
 AtZNuc=    1.0000000   1.0000000   1.0000000   1.0000000   1.0000000   1.0000000
 Leave Link  101 at Sat Sep 26 09:48:43 2026, MaxMem=    805306368 cpu:                2.2 elap:
0.4
 (Enter /home/user/gauss16/g16/l103.exe)

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.
                      ----------------------------
                      !    Initial Parameters    !
                      ! (Angstroms and Degrees)  !
 --------------------------                     --------------------------
 ! Name  Definition              Value          Derivative Info.                !
 --------------------------------------------------------------------------------
 ! R1    R(1,2)                  1.2296         calculate D2E/DX2 analytically  !
 ! R2    R(1,3)                  1.3408         calculate D2E/DX2 analytically  !
 ! R3    R(2,4)                  1.3394         calculate D2E/DX2 analytically  !
 ! R4    R(3,5)                  1.2296         calculate D2E/DX2 analytically  !
 ! R5    R(4,6)                  1.2278         calculate D2E/DX2 analytically  !
 ! R6    R(5,7)                  1.3394         calculate D2E/DX2 analytically  !
 ! R7    R(6,8)                  1.3406         calculate D2E/DX2 analytically  !
 ! R8    R(7,9)                  1.2278         calculate D2E/DX2 analytically  !
 ! R9    R(8,10)                 1.2273         calculate D2E/DX2 analytically  !
 ! R10   R(9,11)                 1.3406         calculate D2E/DX2 analytically  !
 ! R11   R(10,12)                1.39           calculate D2E/DX2 analytically  !
 ! R12   R(11,13)                1.2273         calculate D2E/DX2 analytically  !
 ! R13   R(12,14)                1.4251         calculate D2E/DX2 analytically  !
```

```
! R14   R(12,15)            1.4253       calculate D2E/DX2 analytically  !
! R15   R(13,14)            1.3901       calculate D2E/DX2 analytically  !
! R16   R(14,16)            1.4252       calculate D2E/DX2 analytically  !
! R17   R(15,17)            1.4886       calculate D2E/DX2 analytically  !
! R18   R(15,24)            1.0852       calculate D2E/DX2 analytically  !
! R19   R(16,18)            1.4885       calculate D2E/DX2 analytically  !
! R20   R(16,25)            1.0852       calculate D2E/DX2 analytically  !
! R21   R(17,19)            1.0292       calculate D2E/DX2 analytically  !
! R22   R(17,20)            1.0146       calculate D2E/DX2 analytically  !
! R23   R(17,23)            1.0212       calculate D2E/DX2 analytically  !
! R24   R(18,21)            1.0292       calculate D2E/DX2 analytically  !
! R25   R(18,22)            1.0146       calculate D2E/DX2 analytically  !
! R26   R(18,26)            1.0212       calculate D2E/DX2 analytically  !
! A1    A(2,1,3)          146.6279       calculate D2E/DX2 analytically  !
! A2    A(1,2,4)          149.7101       calculate D2E/DX2 analytically  !
! A3    A(1,3,5)          146.7332       calculate D2E/DX2 analytically  !
! A4    A(2,4,6)          155.6385       calculate D2E/DX2 analytically  !
! A5    A(3,5,7)          149.6158       calculate D2E/DX2 analytically  !
! A6    A(4,6,8)          162.8426       calculate D2E/DX2 analytically  !
! A7    A(5,7,9)          155.7028       calculate D2E/DX2 analytically  !
! A8    A(7,9,11)          162.8008       calculate D2E/DX2 analytically  !
! A9    A(10,12,14)        119.4884       calculate D2E/DX2 analytically  !
! A10   A(10,12,15)        120.7417       calculate D2E/DX2 analytically  !
! A11   A(14,12,15)        119.7429       calculate D2E/DX2 analytically  !
! A12   A(12,14,13)        119.4922       calculate D2E/DX2 analytically  !
! A13   A(12,14,16)        119.7458       calculate D2E/DX2 analytically  !
! A14   A(13,14,16)        120.735        calculate D2E/DX2 analytically  !
! A15   A(12,15,24)        117.8027       calculate D2E/DX2 analytically  !
! A16   A(17,15,24)        110.4513       calculate D2E/DX2 analytically  !
! A17   A(14,16,25)        117.8311       calculate D2E/DX2 analytically  !
! A18   A(18,16,25)        110.4642       calculate D2E/DX2 analytically  !
! A19   A(15,17,19)        115.4928       calculate D2E/DX2 analytically  !
! A20   A(15,17,20)        110.2829       calculate D2E/DX2 analytically  !
! A21   A(15,17,23)        108.1861       calculate D2E/DX2 analytically  !
! A22   A(19,17,20)        108.7082       calculate D2E/DX2 analytically  !
! A23   A(19,17,23)        105.6966       calculate D2E/DX2 analytically  !
! A24   A(20,17,23)        108.1631       calculate D2E/DX2 analytically  !
! A25   A(16,18,21)        115.4887       calculate D2E/DX2 analytically  !
! A26   A(16,18,22)        110.2859       calculate D2E/DX2 analytically  !
! A27   A(16,18,26)        108.1861       calculate D2E/DX2 analytically  !
! A28   A(21,18,22)        108.7083       calculate D2E/DX2 analytically  !
! A29   A(21,18,26)        105.6952       calculate D2E/DX2 analytically  !
! A30   A(22,18,26)        108.1656       calculate D2E/DX2 analytically  !
! A31   L(6,8,10,7,-1)     166.5267       calculate D2E/DX2 analytically  !
! A32   L(8,10,12,7,-1)     179.1399       calculate D2E/DX2 analytically  !
! A33   L(9,11,13,4,-1)     166.5538       calculate D2E/DX2 analytically  !
! A34   L(11,13,14,4,-1)    179.1237       calculate D2E/DX2 analytically  !
! A35   L(12,15,17,24,-1)   228.2539       calculate D2E/DX2 analytically  !
```

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 ! A36   L(14,16,18,25,-1)     228.2953        calculate D2E/DX2 analytically  !
 ! A37   L(6,8,10,7,-2)        180.2218        calculate D2E/DX2 analytically  !
 ! A38   L(8,10,12,7,-2)       179.8907        calculate D2E/DX2 analytically  !
 ! A39   L(9,11,13,4,-2)       180.2218        calculate D2E/DX2 analytically  !
 ! A40   L(11,13,14,4,-2)      179.9006        calculate D2E/DX2 analytically  !
 ! A41   L(12,15,17,24,-2)     230.0857        calculate D2E/DX2 analytically  !
 ! A42   L(14,16,18,25,-2)     230.0317        calculate D2E/DX2 analytically  !
 ! D1    D(3,1,2,4)             0.5525         calculate D2E/DX2 analytically  !
 ! D2    D(2,1,3,5)            -0.3519         calculate D2E/DX2 analytically  !
 ! D3    D(1,2,4,6)            -0.2377         calculate D2E/DX2 analytically  !
 ! D4    D(1,3,5,7)             0.5534         calculate D2E/DX2 analytically  !
 ! D5    D(2,4,6,8)            -0.2404         calculate D2E/DX2 analytically  !
 ! D6    D(3,5,7,9)            -0.2381         calculate D2E/DX2 analytically  !
 ! D7    D(4,6,12,14)           -0.0375        calculate D2E/DX2 analytically  !
 ! D8    D(4,6,12,15)          177.9248         calculate D2E/DX2 analytically  !
 ! D9    D(5,7,9,11)           -0.2367         calculate D2E/DX2 analytically  !
 ! D10   D(7,9,14,12)           -0.0316        calculate D2E/DX2 analytically  !
 ! D11   D(7,9,14,16)          177.9385         calculate D2E/DX2 analytically  !
 ! D12   D(10,12,14,13)          0.4066         calculate D2E/DX2 analytically  !
 ! D13   D(10,12,14,16)       -177.7189         calculate D2E/DX2 analytically  !
 ! D14   D(15,12,14,13)       -177.719          calculate D2E/DX2 analytically  !
 ! D15   D(15,12,14,16)          4.1555         calculate D2E/DX2 analytically  !
 ! D16   D(10,12,15,24)        144.0322         calculate D2E/DX2 analytically  !
 ! D17   D(14,12,15,24)        -37.8661         calculate D2E/DX2 analytically  !
 ! D18   D(12,14,16,25)        -37.8062         calculate D2E/DX2 analytically  !
 ! D19   D(13,14,16,25)        144.092          calculate D2E/DX2 analytically  !
 ! D20   D(24,15,17,19)        -66.0849         calculate D2E/DX2 analytically  !
 ! D21   D(24,15,17,20)         57.6297         calculate D2E/DX2 analytically  !
 ! D22   D(24,15,17,23)        175.7427         calculate D2E/DX2 analytically  !
 ! D23   D(25,16,18,21)        -66.1333         calculate D2E/DX2 analytically  !
 ! D24   D(25,16,18,22)         57.5808         calculate D2E/DX2 analytically  !
 ! D25   D(25,16,18,26)        175.6986         calculate D2E/DX2 analytically  !
 ---------------------------------------------------------------------------
  Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07 EigMax=2.50D+02 EigMin=1.00D-
04
 Number of steps in this run=      2 maximum allowed number of steps=      2.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

  Leave Link  103 at Sat Sep 26 09:48:43 2026, MaxMem=    805306368 cpu:                0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l202.exe)
                      Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1          6           0        4.013709    0.668811    0.047005
     2          6           0        3.337785    1.693664    0.116019
```

3	6	0	4.013117	-0.668718	-0.045893
4	6	0	2.137726	2.286830	0.159901
5	6	0	3.338182	-1.694191	-0.115126
6	6	0	0.910673	2.329383	0.166498
7	6	0	2.137665	-2.286531	-0.159282
8	6	0	-0.383269	1.979576	0.145008
9	6	0	0.910660	-2.329589	-0.166245
10	6	0	-1.460574	1.393128	0.101701
11	6	0	-0.383227	-1.979358	-0.145094
12	6	0	-2.670510	0.710588	0.053913
13	6	0	-1.460606	-1.393092	-0.102107
14	6	0	-2.670537	-0.710377	-0.054420
15	6	0	-3.907208	1.412260	0.152347
16	6	0	-3.907106	-1.411985	-0.152962
17	7	0	-3.725626	2.875841	-0.049665
18	7	0	-3.725815	-2.875539	0.049121
19	1	0	-3.439658	3.160199	-0.996582
20	1	0	-4.575050	3.372967	0.196813
21	1	0	-3.440220	-3.159859	0.996155
22	1	0	-4.575206	-3.372590	-0.197629
23	1	0	-2.979509	3.193147	0.571250
24	1	0	-4.743449	1.049114	-0.436264
25	1	0	-4.743963	-1.048653	0.434593
26	1	0	-2.979472	-3.192949	-0.571483

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.229618	0.000000			
3	C	1.340752	2.462345	0.000000		
4	C	2.479928	1.339370	3.506381	0.000000	
5	C	2.463006	3.395731	1.229603	4.167165	0.000000
6	C	3.521450	2.509494	4.319593	1.227809	4.707575
7	C	3.506585	4.166297	2.479414	4.584486	1.339425
8	C	4.589240	3.732134	5.135963	2.539693	5.235784
9	C	4.320277	4.707141	3.521110	4.787838	2.509823
10	C	5.522264	4.807783	5.851008	3.708080	5.710220
11	C	5.136413	5.234998	4.588622	4.964734	3.732439
12	C	6.684353	6.088506	6.825197	5.061117	6.474250
13	C	5.851650	5.709659	5.521732	5.153491	4.808243
14	C	6.825804	6.473670	6.683790	5.669972	6.089030
15	C	7.956427	7.250547	8.191539	6.107876	7.887791
16	C	8.192008	7.887069	7.955742	7.093597	7.250881
17	N	8.048455	7.163572	8.511877	5.896588	8.413493
18	N	8.512499	8.412879	8.047990	7.813030	7.163980
19	H	7.927721	7.022986	8.432572	5.762589	8.383387
20	H	9.005647	8.089471	9.494774	6.800178	9.401736
21	H	8.433306	8.382880	7.927413	7.840869	7.023522

22	H	9.495380	9.401103	9.005179	8.787510	8.089843
23	H	7.453335	6.508754	8.011971	5.213129	8.016883
24	H	8.778723	8.125688	8.932009	7.016974	8.540586
25	H	8.932901	8.540284	8.778478	7.652356	8.126499
26	H	8.012509	8.016195	7.452804	7.533168	6.509017

		6	7	8	9	10
6	C	0.000000				
7	C	4.787307	0.000000			
8	C	1.340564	4.964612	0.000000		
9	C	4.670840	1.227780	4.509993	0.000000	
10	C	2.550213	5.153186	1.227348	4.421897	0.000000
11	C	4.509603	2.539577	3.969549	1.340616	3.548978
12	C	3.931672	5.669808	2.617270	4.702757	1.389996
13	C	4.421757	3.707972	3.549171	2.550303	2.793664
14	C	4.702554	5.061034	3.536554	3.931835	2.431690
15	C	4.904415	7.093564	3.569320	6.108583	2.447232
16	C	6.108264	6.107710	4.899888	4.904389	3.730822
17	N	4.673394	7.812828	3.465911	6.971746	2.711422
18	N	6.971514	5.896673	5.895248	4.673472	4.832763
19	H	4.579125	7.840566	3.469670	7.053545	2.871505
20	H	5.584187	8.787335	4.417607	7.921109	3.691716
21	H	7.053395	5.762858	6.040132	4.579375	5.044674
22	H	7.920856	6.800267	6.807013	5.584224	5.701105
23	H	4.005424	7.532995	2.897395	6.795434	2.401605
24	H	5.828508	7.651991	4.496088	6.592229	3.344401
25	H	6.592262	7.017253	5.316924	5.828942	4.105332
26	H	6.795145	5.213118	5.831693	4.005338	4.877738

		11	12	13	14	15
11	C	0.000000				
12	C	3.536535	0.000000			
13	C	1.227315	2.431806	0.000000		
14	C	2.617313	1.425088	1.390075	0.000000	
15	C	4.899998	1.425291	3.731033	2.465297	0.000000
16	C	3.569271	2.465215	2.447101	1.425155	2.840700
17	N	5.895226	2.410875	4.832893	3.738207	1.488573
18	N	3.466086	3.738181	2.711399	2.410863	4.292875
19	H	6.040021	2.774117	5.044719	4.057163	2.143347
20	H	6.807031	3.276577	5.701266	4.512647	2.071802
21	H	3.470049	4.057170	2.871675	2.774181	4.672725
22	H	4.417754	4.512592	3.691649	3.276531	4.843913
23	H	5.831693	2.554646	4.877916	3.965403	2.051259
24	H	5.316762	2.156838	4.105251	2.745646	1.085190
25	H	4.496473	2.745734	3.344715	2.157002	2.614558
26	H	2.897430	3.965372	2.401406	2.554596	4.753165

		16	17	18	19	20
16	C	0.000000				
17	N	4.292908	0.000000			
18	N	1.488520	5.752228	0.000000		

```
 19  H    4.672802   1.029218   6.132334   0.000000
 20  H    4.843993   1.014597   6.307681   1.660896   0.000000
 21  H    2.143248   6.132280   1.029212   6.626774   6.678668
 22  H    2.071793   6.307660   1.014599   6.678708   6.757080
 23  H    4.753122   1.021229   6.136655   1.634295   1.648724
 24  H    2.614716   2.126582   4.083390   2.543720   2.414423
 25  H    1.085155   4.083279   2.126670   4.632916   4.431230
 26  H    2.051218   6.136713   1.021237   6.383962   6.800544
            21         22         23         24         25
 21  H    0.000000
 22  H    1.660894   0.000000
 23  H    6.383845   6.800465   0.000000
 24  H    4.633107   4.431334   2.953548   0.000000
 25  H    2.544069   2.414305   4.596177   2.271347   0.000000
 26  H    1.634281   1.648759   6.487531   4.596194   2.953578
            26
 26  H    0.000000
Stoichiometry    C16H8N2
Framework group  C1[X(C16H8N2)]
Deg. of freedom    72
Full point group                 C1      NOp   1
RotChk:  IX=2 Diff= 6.62D-16
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0        4.521296   -0.670158   -0.022842
    2          6           0        3.845341   -1.696787   -0.055681
    3          6           0        4.520745    0.669818    0.022745
    4          6           0        2.645265   -2.291092   -0.078713
    5          6           0        3.845842    1.697119    0.055631
    6          6           0        1.418211   -2.333810   -0.083939
    7          6           0        2.645342    2.290691    0.078700
    8          6           0        0.124280   -1.983417   -0.074964
    9          6           0        1.418338    2.334010    0.084001
   10          6           0       -0.953008   -1.395769   -0.052522
   11          6           0        0.124440    1.983294    0.075092
   12          6           0       -2.162923   -0.711925   -0.029012
   13          6           0       -0.952957    1.395912    0.052725
   14          6           0       -2.162909    0.711979    0.029053
   15          6           0       -3.399637   -1.416595   -0.102732
   16          6           0       -3.399461    1.416674    0.102609
   17          7           0       -3.218133   -2.872131    0.150881
   18          7           0       -3.218092    2.872168   -0.151033
   19          1           0       -2.932279   -3.122869    1.107285
```

```
    20        1        0     -4.067548   -3.377626   -0.077974
    21        1        0     -2.932383    3.122843   -1.107490
    22        1        0     -4.067492    3.377655    0.077907
    23        1        0     -2.471959   -3.211201   -0.458354
    24        1        0     -4.235928   -1.032852    0.472589
    25        1        0     -4.236268    1.032839   -0.471836
    26        1        0     -2.471806    3.211280    0.458052
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6019542           0.2710791           0.1875814
 Leave Link  202 at Sat Sep 26 09:48:43 2026, MaxMem=    805306368 cpu:                  0.1 elap:
0.0
 (Enter /home/user/gauss16/g16/l301.exe)
 Standard basis: def2TZVP (5D, 7F)
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are   696 symmetry adapted cartesian basis functions of A   symmetry.
 There are   606 symmetry adapted basis functions of A   symmetry.
   606 basis functions,   982 primitive gaussians,   696 cartesian basis functions
    59 alpha electrons       59 beta electrons
       nuclear repulsion energy      1010.2921804319 Hartrees.
 IExCor= 4639 DFT=T Ex+Corr=wB97XD ExCW=0 ScaHFX=  1.000000
 ScaDFX=  1.000000  1.000000  1.000000  1.000000 ScalE2=  1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=           0 ICorTp=0 IEmpDi=121
  HFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.222036 cShort=    0.000000 cLong=
0.777964
  DFx    wShort=    0.000000 wLong=    0.200000 cFull=    0.000000 cShort=    0.000000 cLong=
1.000000
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 R6Disp:  Grimme-D2 Dispersion energy=       -0.0153853988 Hartrees.
 Nuclear repulsion after empirical dispersion term =     1010.2767950331 Hartrees.
 Leave Link  301 at Sat Sep 26 09:48:43 2026, MaxMem=    805306368 cpu:                  0.3 elap:
0.0
 (Enter /home/user/gauss16/g16/l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1 NCelD=      1
       NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=     0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   26565 NPrTT=   83856 LenC2=   23224 LenP2D=   51951.
 LDataN:  DoStor=T MaxTD1= 6 Len=  172
 NBasis=   606 RedAO= T EigKep=  1.85D-06  NBF=   606
 NBsUse=   606 1.00D-06 EigRej= -1.00D+00 NBFU=   606
 Precomputing XC quadrature grid using
 IXCGrd= 4 IRadAn=          5 IRanWt=         -1 IRanGd=          0 AccXCQ= 0.00D+00.
 Generated NRdTot=       0 NPtTot=          0 NUsed=          0 NTot=         32
 NSgBfM=   683   683   683   683   683 MxSgAt=    26 MxSgA2=    26.
```

Supporting Information file

```
 Leave Link  302 at Sat Sep 26 09:48:44 2026, MaxMem=    805306368 cpu:                6.5 elap:
1.1
 (Enter /home/user/gauss16/g16/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Sat Sep 26 09:48:44 2026, MaxMem=    805306368 cpu:                0.8 elap:
0.1
 (Enter /home/user/gauss16/g16/l401.exe)
 Initial guess from the checkpoint file:  "cdca-n2-b-4h2.chk"
 B after Tr=     0.000000    0.000000   -0.000000
       Rot=    1.000000    0.000000    0.000000   -0.000000 Ang=   0.00 deg.
 Guess basis will be translated and rotated to current coordinates.
 JPrj=2 DoOrth=T DoCkMO=T.
 Leave Link  401 at Sat Sep 26 09:48:45 2026, MaxMem=    805306368 cpu:                4.3 elap:
0.7
 (Enter /home/user/gauss16/g16/l502.exe)
 Integral symmetry usage will be decided dynamically.
 Closed shell SCF:
 Using DIIS extrapolation, IDIIS=  1040.
 NGot=   805306368 LenX=   804326778 LenY=   803841666
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFJK:  IHMeth= 1 ICntrl=       0 DoSepK=T KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
       NFxFlg=           0 DoJE=T BraDBF=F KetDBF=F FulRan=T
       wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=           0 NGrid=           0
       NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
 Symmetry not used in FoFCou.
 E= -723.413947888582
 DIIS: error= 4.13D-09 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -723.413947888582     IErMin= 1 ErrMin= 4.13D-09
 ErrMax= 4.13D-09  0.00D+00 EMaxC= 1.00D-01 BMatC= 4.38D-15 BMatP= 4.38D-15
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.100D+01
 Coeff:      0.100D+01
 Gap=     0.179 Goal=   None    Shift=    0.000
 RMSDP=1.00D-09 MaxDP=4.85D-08             OVMax= 6.50D-08

 SCF Done:  E(RwB97XD) =  -723.413947889     A.U. after    1 cycles
          NFock=  1  Conv=0.10D-08     -V/T= 2.0047
 KE= 7.200589625989D+02 PE=-3.701629051232D+03 EE= 1.247879345711D+03
 Leave Link  502 at Sat Sep 26 09:50:10 2026, MaxMem=    805306368 cpu:              512.3 elap:
85.4
```

Supporting Information file

(Enter /home/user/gauss16/g16/l801.exe)
DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000
Range of M.O.s used for correlation: 1 606
NBasis= 606 NAE= 59 NBE= 59 NFC= 0 NFV= 0
NROrb= 606 NOA= 59 NOB= 59 NVA= 547 NVB= 547

**** Warning!!: The largest alpha MO coefficient is 0.60170250D+02

Leave Link 801 at Sat Sep 26 09:50:10 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l1101.exe)
Using compressed storage, NAtomX= 26.
Will process 27 centers per pass.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23224 LenP2D= 51951.
LDataN: DoStor=T MaxTD1= 7 Len= 274
R6Disp: Adding Grimme-D2 dispersion energy 1st derivatives to the gradient.
Leave Link 1101 at Sat Sep 26 09:50:12 2026, MaxMem= 805306368 cpu: 11.1 elap: 1.8
(Enter /home/user/gauss16/g16/l1102.exe)
Symmetrizing basis deriv contribution to polar:
IMax=3 JMax=2 DiffMx= 0.00D+00
Leave Link 1102 at Sat Sep 26 09:50:12 2026, MaxMem= 805306368 cpu: 0.6 elap: 0.1
(Enter /home/user/gauss16/g16/l1110.exe)
Forming Gx(P) for the SCF density, NAtomX= 26.
Integral derivatives from FoFJK, PRISM(SPDF).
Do as many integral derivatives as possible in FoFJK.
G2DrvN: MDV= 805303554.
G2DrvN: will do 27 centers at a time, making 1 passes.
Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.
FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 3507 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
End of G2Drv F.D. properties file 721 does not exist.
End of G2Drv F.D. properties file 722 does not exist.
End of G2Drv F.D. properties file 788 does not exist.
Leave Link 1110 at Sat Sep 26 10:17:14 2026, MaxMem= 805306368 cpu: 9728.0 elap: 1621.6
(Enter /home/user/gauss16/g16/l1002.exe)
Minotr: Closed shell wavefunction.
IDoAtm=11111111111111111111111111
Direct CPHF calculation.
Differentiating once with respect to electric field.

with respect to dipole field.
Differentiating once with respect to nuclear coordinates.
Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.
Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.
NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.
7847 words used for storage of precomputed grid.
Two-electron integrals replicated using symmetry.
MDV= 805306368 using IRadAn= 1.
Solving linear equations simultaneously, MaxMat= 384.
FoF2E skips out because all densities are zero.
CalDSu exits because no D1Ps are significant.
FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 78 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2 IDoP0=3 IntGTp=3.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 78 NMatS0= 78 NMatT0= 0 NMatD0= 78 NMtDS0= 0 NMtDT0= 0
Integrals replicated using symmetry in FoFCou.
There are 81 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.
78 vectors produced by pass 0 Test12= 3.98D-14 1.23D-09 XBig12= 6.49D+02 1.76D+01.
AX will form 78 AO Fock derivatives at one time.
78 vectors produced by pass 1 Test12= 3.98D-14 1.23D-09 XBig12= 1.32D+02 1.99D+00.
78 vectors produced by pass 2 Test12= 3.98D-14 1.23D-09 XBig12= 5.74D+00 4.30D-01.
78 vectors produced by pass 3 Test12= 3.98D-14 1.23D-09 XBig12= 1.70D-01 7.10D-02.
78 vectors produced by pass 4 Test12= 3.98D-14 1.23D-09 XBig12= 2.61D-03 6.92D-03.
78 vectors produced by pass 5 Test12= 3.98D-14 1.23D-09 XBig12= 2.60D-05 7.08D-04.
78 vectors produced by pass 6 Test12= 3.98D-14 1.23D-09 XBig12= 2.33D-07 5.19D-05.
57 vectors produced by pass 7 Test12= 3.98D-14 1.23D-09 XBig12= 1.65D-09 4.26D-06.
19 vectors produced by pass 8 Test12= 3.98D-14 1.23D-09 XBig12= 1.24D-11 4.22D-07.
3 vectors produced by pass 9 Test12= 3.98D-14 1.23D-09 XBig12= 1.36D-13 4.44D-08.
2 vectors produced by pass 10 Test12= 3.98D-14 1.23D-09 XBig12= 1.73D-14 2.43D-08.
1 vectors produced by pass 11 Test12= 3.98D-14 1.23D-09 XBig12= 1.16D-16 1.51D-09.
InvSVY: IOpt=1 It= 1 EMax= 1.07D-14
Solved reduced A of dimension 628 with 81 vectors.
FullF1: Do perturbations 1 to 3.
Isotropic polarizability for W= 0.000000 300.53 Bohr**3.
End of Minotr F.D. properties file 721 does not exist.
End of Minotr F.D. properties file 722 does not exist.
End of Minotr F.D. properties file 788 does not exist.
Leave Link 1002 at Sat Sep 26 12:05:25 2026, MaxMem= 805306368 cpu: 38934.8 elap: 6490.4
(Enter /home/user/gauss16/g16/l601.exe)
Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

****

Population analysis using the SCF Density.

Supporting Information file

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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(A) (A) (A) (A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -14.56781 -14.56778 -10.30326 -10.30282 -10.30086
Alpha occ. eigenvalues -- -10.30032 -10.29858 -10.29834 -10.29807 -10.29797
Alpha occ. eigenvalues -- -10.29567 -10.29565 -10.29261 -10.29257 -10.29039
Alpha occ. eigenvalues -- -10.29036 -10.27870 -10.27865 -1.11228 -1.11161
Alpha occ. eigenvalues -- -0.93721 -0.92087 -0.90358 -0.87859 -0.87048
Alpha occ. eigenvalues -- -0.82842 -0.82769 -0.79209 -0.76178 -0.72895
Alpha occ. eigenvalues -- -0.72196 -0.69291 -0.69055 -0.67726 -0.67652
Alpha occ. eigenvalues -- -0.66757 -0.65685 -0.62380 -0.62287 -0.60382
Alpha occ. eigenvalues -- -0.54007 -0.52211 -0.50454 -0.47972 -0.46644
Alpha occ. eigenvalues -- -0.46540 -0.44728 -0.44711 -0.44042 -0.41243
Alpha occ. eigenvalues -- -0.39347 -0.38751 -0.36617 -0.31868 -0.30721
Alpha occ. eigenvalues -- -0.30418 -0.25990 -0.25032 -0.18984
Alpha virt. eigenvalues -- -0.01086 0.00687 0.00981 0.04375 0.05856
Alpha virt. eigenvalues -- 0.06494 0.09536 0.10546 0.11693 0.11868
Alpha virt. eigenvalues -- 0.12793 0.12821 0.14787 0.15683 0.15933
Alpha virt. eigenvalues -- 0.16155 0.17554 0.18043 0.18325 0.18646
Alpha virt. eigenvalues -- 0.20128 0.20460 0.21357 0.22549 0.23912
Alpha virt. eigenvalues -- 0.24549 0.26553 0.26963 0.27633 0.28154
Alpha virt. eigenvalues -- 0.28657 0.28798 0.28972 0.30491 0.31236
Alpha virt. eigenvalues -- 0.31908 0.32215 0.32600 0.33384 0.34759
Alpha virt. eigenvalues -- 0.35348 0.35888 0.36145 0.36711 0.37400
Alpha virt. eigenvalues -- 0.37913 0.38321 0.39300 0.39506 0.39998
Alpha virt. eigenvalues -- 0.40696 0.40900 0.41563 0.41793 0.42924
Alpha virt. eigenvalues -- 0.43059 0.43281 0.44455 0.45130 0.45411
Alpha virt. eigenvalues -- 0.46238 0.46448 0.46913 0.48238 0.48503
Alpha virt. eigenvalues -- 0.48695 0.48800 0.50134 0.50183 0.50496
Alpha virt. eigenvalues -- 0.50892 0.52009 0.52207 0.53502 0.53975
Alpha virt. eigenvalues -- 0.54043 0.54457 0.54501 0.54589 0.56820
Alpha virt. eigenvalues -- 0.57004 0.57555 0.57780 0.59273 0.59453
Alpha virt. eigenvalues -- 0.59805 0.60455 0.61277 0.61762 0.61885
Alpha virt. eigenvalues -- 0.62184 0.62906 0.63057 0.63893 0.64810
Alpha virt. eigenvalues -- 0.64855 0.65825 0.66090 0.66788 0.67550
Alpha virt. eigenvalues -- 0.67824 0.68313 0.69793 0.70645 0.70732
Alpha virt. eigenvalues -- 0.71511 0.71850 0.72518 0.74333 0.74645
Alpha virt. eigenvalues -- 0.75200 0.76762 0.77604 0.77685 0.78484
Alpha virt. eigenvalues -- 0.79449 0.81581 0.81713 0.83162 0.83176
Alpha virt. eigenvalues -- 0.83795 0.86609 0.88856 0.89093 0.89616
Alpha virt. eigenvalues -- 0.91220 0.91981 0.93847 0.94546 0.94983
Alpha virt. eigenvalues -- 0.96473 0.97785 0.97848 0.98397 0.98475
Alpha virt. eigenvalues -- 0.99573 1.00774 1.02010 1.02052 1.04872
Alpha virt. eigenvalues -- 1.07355 1.07801 1.09140 1.09375 1.09523

Alpha virt. eigenvalues --	1.10303	1.11520	1.14044	1.14935	1.15817
Alpha virt. eigenvalues --	1.17824	1.18346	1.21995	1.22201	1.23168
Alpha virt. eigenvalues --	1.25236	1.25323	1.26322	1.27177	1.27998
Alpha virt. eigenvalues --	1.29486	1.30209	1.31574	1.32902	1.33415
Alpha virt. eigenvalues --	1.34014	1.34476	1.35556	1.37547	1.38190
Alpha virt. eigenvalues --	1.38370	1.40379	1.40909	1.41149	1.42962
Alpha virt. eigenvalues --	1.43192	1.43734	1.44322	1.45264	1.46239
Alpha virt. eigenvalues --	1.46778	1.48697	1.49102	1.49242	1.50827
Alpha virt. eigenvalues --	1.51621	1.51955	1.52315	1.53390	1.54186
Alpha virt. eigenvalues --	1.54609	1.54764	1.55953	1.56096	1.56263
Alpha virt. eigenvalues --	1.56926	1.57890	1.58186	1.60179	1.60458
Alpha virt. eigenvalues --	1.61123	1.62528	1.64400	1.64485	1.66249
Alpha virt. eigenvalues --	1.66282	1.69291	1.70741	1.71894	1.72625
Alpha virt. eigenvalues --	1.73383	1.73792	1.73798	1.74858	1.75304
Alpha virt. eigenvalues --	1.76743	1.77046	1.78297	1.79604	1.80312
Alpha virt. eigenvalues --	1.80600	1.81122	1.82209	1.83674	1.83911
Alpha virt. eigenvalues --	1.84434	1.85091	1.85634	1.86238	1.87093
Alpha virt. eigenvalues --	1.87511	1.88473	1.89659	1.90410	1.92461
Alpha virt. eigenvalues --	1.92495	1.95591	1.96491	1.98409	1.98429
Alpha virt. eigenvalues --	1.99951	2.02463	2.02906	2.03978	2.04984
Alpha virt. eigenvalues --	2.06132	2.07344	2.09280	2.09396	2.09971
Alpha virt. eigenvalues --	2.14792	2.15557	2.17065	2.18142	2.19888
Alpha virt. eigenvalues --	2.20277	2.22191	2.23363	2.25082	2.26129
Alpha virt. eigenvalues --	2.27808	2.30334	2.32042	2.33814	2.35278
Alpha virt. eigenvalues --	2.37564	2.38837	2.41048	2.41301	2.41327
Alpha virt. eigenvalues --	2.45085	2.46483	2.46609	2.47554	2.48857
Alpha virt. eigenvalues --	2.49173	2.49743	2.49921	2.51085	2.51602
Alpha virt. eigenvalues --	2.52111	2.53324	2.53680	2.53900	2.56318
Alpha virt. eigenvalues --	2.58490	2.58673	2.59063	2.59406	2.60205
Alpha virt. eigenvalues --	2.60529	2.61774	2.62660	2.64638	2.65058
Alpha virt. eigenvalues --	2.66223	2.66606	2.67608	2.68326	2.69233
Alpha virt. eigenvalues --	2.69976	2.70835	2.71211	2.73613	2.74950
Alpha virt. eigenvalues --	2.75151	2.75908	2.76607	2.78141	2.78193
Alpha virt. eigenvalues --	2.79460	2.79874	2.81492	2.81507	2.83475
Alpha virt. eigenvalues --	2.84428	2.85532	2.86014	2.86855	2.87260
Alpha virt. eigenvalues --	2.87816	2.88509	2.88784	2.89314	2.89533
Alpha virt. eigenvalues --	2.90614	2.91113	2.91200	2.91538	2.91889
Alpha virt. eigenvalues --	2.93294	2.94272	2.94821	2.95645	2.96002
Alpha virt. eigenvalues --	2.96725	2.97272	2.98718	2.99245	2.99463
Alpha virt. eigenvalues --	2.99619	2.99783	3.00873	3.02983	3.03176
Alpha virt. eigenvalues --	3.03540	3.04076	3.04712	3.05131	3.06695
Alpha virt. eigenvalues --	3.06883	3.07896	3.08669	3.09484	3.10102
Alpha virt. eigenvalues --	3.10324	3.10957	3.11956	3.13013	3.13765
Alpha virt. eigenvalues --	3.14129	3.15514	3.15687	3.17155	3.17811
Alpha virt. eigenvalues --	3.17958	3.20315	3.20884	3.22911	3.23716
Alpha virt. eigenvalues --	3.23997	3.24469	3.25231	3.26268	3.26620
Alpha virt. eigenvalues --	3.28562	3.29641	3.30456	3.31112	3.31481
Alpha virt. eigenvalues --	3.32269	3.33200	3.33379	3.35339	3.36821

Alpha virt. eigenvalues --	3.37600	3.38365	3.39652	3.39871	3.40453
Alpha virt. eigenvalues --	3.41216	3.42523	3.43128	3.44080	3.46398
Alpha virt. eigenvalues --	3.46511	3.46587	3.48015	3.49695	3.49813
Alpha virt. eigenvalues --	3.50751	3.51245	3.51571	3.53074	3.53490
Alpha virt. eigenvalues --	3.54852	3.57053	3.57466	3.59569	3.59635
Alpha virt. eigenvalues --	3.63147	3.63464	3.65097	3.66886	3.67442
Alpha virt. eigenvalues --	3.68467	3.69988	3.70616	3.72890	3.73677
Alpha virt. eigenvalues --	3.75964	3.76176	3.79093	3.80518	3.82171
Alpha virt. eigenvalues --	3.85404	3.85699	3.86704	3.91633	3.92304
Alpha virt. eigenvalues --	3.94621	3.95461	3.96831	3.96887	3.98500
Alpha virt. eigenvalues --	4.02212	4.02973	4.06064	4.06434	4.07490
Alpha virt. eigenvalues --	4.10423	4.10595	4.11955	4.16011	4.20057
Alpha virt. eigenvalues --	4.20347	4.23628	4.23934	4.24863	4.26665
Alpha virt. eigenvalues --	4.28600	4.31904	4.36867	4.38480	4.38561
Alpha virt. eigenvalues --	4.39820	4.40964	4.44891	4.45664	4.47988
Alpha virt. eigenvalues --	4.50696	4.51696	4.53425	4.60901	4.61930
Alpha virt. eigenvalues --	4.63649	4.65329	4.68904	4.74381	4.77441
Alpha virt. eigenvalues --	4.77744	4.78620	4.81160	4.81463	4.82301
Alpha virt. eigenvalues --	4.84978	4.86439	4.87524	4.87859	4.89583
Alpha virt. eigenvalues --	4.90330	4.94508	4.94696	4.94784	4.98329
Alpha virt. eigenvalues --	5.00766	5.01302	5.01368	5.01653	5.04562
Alpha virt. eigenvalues --	5.06596	5.09430	5.11625	5.13209	5.14641
Alpha virt. eigenvalues --	5.16643	5.17485	5.21866	5.22138	5.22635
Alpha virt. eigenvalues --	5.24772	5.26446	5.27575	5.28714	5.30005
Alpha virt. eigenvalues --	5.31037	5.34863	5.36737	5.37780	5.41064
Alpha virt. eigenvalues --	5.43469	5.43480	5.49282	5.49693	5.50597
Alpha virt. eigenvalues --	5.57121	5.57325	5.59770	5.65891	5.71752
Alpha virt. eigenvalues --	5.76075	5.77990	5.89884	5.94474	6.03632
Alpha virt. eigenvalues --	6.08301	6.09607	6.15741	6.29101	22.50101
Alpha virt. eigenvalues --	22.61095	22.67070	22.95393	22.99955	23.26336
Alpha virt. eigenvalues --	23.27543	23.48236	23.58702	23.71953	23.77030
Alpha virt. eigenvalues --	23.96298	24.16572	24.28179	24.32210	24.57413
Alpha virt. eigenvalues --	31.91726	31.95392			

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	5.355464	0.773331	0.725210	-0.232743	-0.191768	-0.220552
2	C	0.773331	5.352710	-0.192414	0.716852	-0.198324	-0.294061
3	C	0.725210	-0.192414	5.356683	-0.060923	0.773286	-0.038924
4	C	-0.232743	0.716852	-0.060923	5.556113	-0.036180	0.631701
5	C	-0.191768	-0.198324	0.773286	-0.036180	5.351011	-0.022540
6	C	-0.220552	-0.294061	-0.038924	0.631701	-0.022540	5.740743
7	C	-0.060680	-0.036171	-0.232530	-0.013924	0.716864	-0.005715
8	C	-0.041681	-0.086192	-0.005157	-0.260272	-0.004498	0.838060
9	C	-0.038880	-0.022579	-0.221167	-0.005645	-0.293084	-0.011010
10	C	-0.012959	-0.044455	-0.000154	-0.315114	0.000846	-0.298431
11	C	-0.005142	-0.004497	-0.041686	-0.004460	-0.085492	-0.019845
12	C	-0.000403	-0.002686	-0.000017	-0.033747	0.000220	-0.095968
13	C	-0.000151	0.000874	-0.013009	0.017250	-0.044237	0.017559

14	C	-0.000018	0.000222	-0.000405	0.002635	-0.002671	0.008062
15	C	0.000021	0.000122	-0.000004	0.002828	-0.000017	0.016267
16	C	-0.000004	-0.000017	0.000021	-0.000254	0.000122	-0.001628
17	N	0.000000	-0.000000	-0.000000	-0.000048	-0.000000	0.000064
18	N	-0.000000	-0.000000	0.000000	-0.000002	-0.000000	-0.000014
19	H	-0.000003	-0.000028	-0.000000	-0.000822	0.000000	-0.005159
20	H	0.000000	0.000000	0.000000	0.000021	-0.000000	0.000186
21	H	-0.000000	0.000000	-0.000003	0.000004	-0.000028	0.000022
22	H	0.000000	-0.000000	0.000000	-0.000000	0.000000	-0.000001
23	H	0.000003	0.000031	0.000000	0.000642	-0.000000	0.002840
24	H	0.000000	0.000002	-0.000000	0.000062	-0.000000	0.000716
25	H	-0.000000	-0.000000	0.000000	-0.000011	0.000002	-0.000125
26	H	0.000000	-0.000000	0.000003	-0.000003	0.000031	-0.000010

		7	8	9	10	11	12
1	C	-0.060680	-0.041681	-0.038880	-0.012959	-0.005142	-0.000403
2	C	-0.036171	-0.086192	-0.022579	-0.044455	-0.004497	-0.002686
3	C	-0.232530	-0.005157	-0.221167	-0.000154	-0.041686	-0.000017
4	C	-0.013924	-0.260272	-0.005645	-0.315114	-0.004460	-0.033747
5	C	0.716864	-0.004498	-0.293084	0.000846	-0.085492	0.000220
6	C	-0.005715	0.838060	-0.011010	-0.298431	-0.019845	-0.095968
7	C	5.559932	-0.004359	0.628459	0.017276	-0.260458	0.002653
8	C	-0.004359	5.694805	-0.019669	0.289078	-0.062302	-0.536464
9	C	0.628459	-0.019669	5.740660	0.017361	0.838294	0.008010
10	C	0.017276	0.289078	0.017361	6.434007	0.033281	0.449335
11	C	-0.260458	-0.062302	0.838294	0.033281	5.696174	0.007068
12	C	0.002653	-0.536464	0.008010	0.449335	0.007068	5.654137
13	C	-0.316259	0.033118	-0.296932	-0.106441	0.287003	-0.100433
14	C	-0.033843	0.007074	-0.095632	-0.100241	-0.537618	0.487528
15	C	-0.000253	0.074122	-0.001612	-0.233459	-0.016406	0.317372
16	C	0.002838	-0.016454	0.016275	-0.005314	0.074553	-0.005937
17	N	-0.000002	0.002873	-0.000015	0.028684	-0.000401	-0.108774
18	N	-0.000049	-0.000399	0.000042	-0.002730	0.002749	-0.007344
19	H	0.000004	-0.007446	0.000022	0.028157	0.000363	0.038848
20	H	-0.000000	0.001817	-0.000001	-0.002122	-0.000012	0.000642
21	H	-0.000822	0.000362	-0.005146	0.001539	-0.007434	0.001217
22	H	0.000021	-0.000012	0.000186	-0.000059	0.001822	0.000960
23	H	-0.000003	0.008725	-0.000010	0.006060	-0.000193	-0.026531
24	H	-0.000011	0.009072	-0.000125	0.023160	-0.002008	-0.105048
25	H	0.000062	-0.002004	0.000713	-0.005740	0.009066	-0.004767
26	H	0.000644	-0.000193	0.002827	-0.000709	0.008707	-0.002659

		13	14	15	16	17	18
1	C	-0.000151	-0.000018	0.000021	-0.000004	0.000000	-0.000000
2	C	0.000874	0.000222	0.000122	-0.000017	-0.000000	-0.000000
3	C	-0.013009	-0.000405	-0.000004	0.000021	-0.000000	0.000000
4	C	0.017250	0.002635	0.002828	-0.000254	-0.000048	-0.000002
5	C	-0.044237	-0.002671	-0.000017	0.000122	-0.000000	-0.000000
6	C	0.017559	0.008062	0.016267	-0.001628	0.000064	-0.000014
7	C	-0.316259	-0.033843	-0.000253	0.002838	-0.000002	-0.000049

8	C	0.033118	0.007074	0.074122	-0.016454	0.002873	-0.000399
9	C	-0.296932	-0.095632	-0.001612	0.016275	-0.000015	0.000042
10	C	-0.106441	-0.100241	-0.233459	-0.005314	0.028684	-0.002730
11	C	0.287003	-0.537618	-0.016406	0.074553	-0.000401	0.002749
12	C	-0.100433	0.487528	0.317372	-0.005937	-0.108774	-0.007344
13	C	6.436981	0.448645	-0.005169	-0.232929	-0.002741	0.028596
14	C	0.448645	5.654701	-0.006092	0.316893	-0.007351	-0.108588
15	C	-0.005169	-0.006092	5.819082	-0.054201	0.223321	-0.000689
16	C	-0.232929	0.316893	-0.054201	5.818361	-0.000692	0.223455
17	N	-0.002741	-0.007351	0.223321	-0.000692	6.133081	-0.000015
18	N	0.028596	-0.108588	-0.000689	0.223455	-0.000015	6.132940
19	H	0.001539	0.001229	-0.093008	0.001197	0.329070	0.000009
20	H	-0.000059	0.000961	-0.038846	-0.000137	0.373945	-0.000002
21	H	0.028170	0.038753	0.001192	-0.092936	0.000009	0.329093
22	H	-0.002116	0.000637	-0.000136	-0.038861	-0.000002	0.373936
23	H	-0.000710	-0.002666	-0.009276	-0.000159	0.362287	0.000000
24	H	-0.005751	-0.004757	0.459533	0.002232	-0.028433	-0.000596
25	H	0.023188	-0.104989	0.002248	0.459531	-0.000597	-0.028442
26	H	0.006070	-0.026480	-0.000159	-0.009333	0.000000	0.362289

		19	20	21	22	23	24
1	C	-0.000003	0.000000	-0.000000	0.000000	0.000003	0.000000
2	C	-0.000028	0.000000	0.000000	-0.000000	0.000031	0.000002
3	C	-0.000000	0.000000	-0.000003	0.000000	0.000000	-0.000000
4	C	-0.000822	0.000021	0.000004	-0.000000	0.000642	0.000062
5	C	0.000000	-0.000000	-0.000028	0.000000	-0.000000	-0.000000
6	C	-0.005159	0.000186	0.000022	-0.000001	0.002840	0.000716
7	C	0.000004	-0.000000	-0.000822	0.000021	-0.000003	-0.000011
8	C	-0.007446	0.001817	0.000362	-0.000012	0.008725	0.009072
9	C	0.000022	-0.000001	-0.005146	0.000186	-0.000010	-0.000125
10	C	0.028157	-0.002122	0.001539	-0.000059	0.006060	0.023160
11	C	0.000363	-0.000012	-0.007434	0.001822	-0.000193	-0.002008
12	C	0.038848	0.000642	0.001217	0.000960	-0.026531	-0.105048
13	C	0.001539	-0.000059	0.028170	-0.002116	-0.000710	-0.005751
14	C	0.001229	0.000961	0.038753	0.000637	-0.002666	-0.004757
15	C	-0.093008	-0.038846	0.001192	-0.000136	-0.009276	0.459533
16	C	0.001197	-0.000137	-0.092936	-0.038861	-0.000159	0.002232
17	N	0.329070	0.373945	0.000009	-0.000002	0.362287	-0.028433
18	N	0.000009	-0.000002	0.329093	0.373936	0.000000	-0.000596
19	H	0.501318	-0.032246	-0.000004	0.000000	-0.035762	-0.006557
20	H	-0.032246	0.404607	0.000000	-0.000000	-0.008550	-0.002872
21	H	-0.000004	0.000000	0.501248	-0.032245	-0.000001	0.000668
22	H	0.000000	-0.000000	-0.032245	0.404611	-0.000000	-0.000156
23	H	-0.035762	-0.008550	-0.000001	-0.000000	0.387839	0.004381
24	H	-0.006557	-0.002872	0.000668	-0.000156	0.004381	0.537369
25	H	0.000668	-0.000156	-0.006544	-0.002868	-0.000221	-0.016107
26	H	-0.000001	-0.000000	-0.035778	-0.008538	0.000000	-0.000221

		25	26
1	C	-0.000000	0.000000

2	C	-0.000000	-0.000000
3	C	0.000000	0.000003
4	C	-0.000011	-0.000003
5	C	0.000002	0.000031
6	C	-0.000125	-0.000010
7	C	0.000062	0.000644
8	C	-0.002004	-0.000193
9	C	0.000713	0.002827
10	C	-0.005740	-0.000709
11	C	0.009066	0.008707
12	C	-0.004767	-0.002659
13	C	0.023188	0.006070
14	C	-0.104989	-0.026480
15	C	0.002248	-0.000159
16	C	0.459531	-0.009333
17	N	-0.000597	0.000000
18	N	-0.028442	0.362289
19	H	0.000668	-0.000001
20	H	-0.000156	-0.000000
21	H	-0.006544	-0.035778
22	H	-0.002868	-0.008538
23	H	-0.000221	0.000000
24	H	-0.016107	-0.000221
25	H	0.537164	0.004378
26	H	0.004378	0.387840

Mulliken charges:

		1
1	C	-0.049045
2	C	0.037279
3	C	-0.048810
4	C	0.036037
5	C	0.036456
6	C	-0.242238
7	C	0.036328
8	C	0.087994
9	C	-0.241343
10	C	-0.200860
11	C	0.088874
12	C	0.062790
13	C	-0.202056
14	C	0.064011
15	C	-0.456780
16	C	-0.456624
17	N	-0.304263
18	N	-0.304239
19	H	0.278611
20	H	0.302823
21	H	0.278664

22 H 0.302822
23 H 0.311273
24 H 0.135449
25 H 0.135552
26 H 0.311295
Sum of Mulliken charges = -0.00000
Mulliken charges with hydrogens summed into heavy atoms:
1
1 C -0.049045
2 C 0.037279
3 C -0.048810
4 C 0.036037
5 C 0.036456
6 C -0.242238
7 C 0.036328
8 C 0.087994
9 C -0.241343
10 C -0.200860
11 C 0.088874
12 C 0.062790
13 C -0.202056
14 C 0.064011
15 C -0.321331
16 C -0.321071
17 N 0.588445
18 N 0.588542
APT charges:
1
1 C -0.153975
2 C 0.198324
3 C -0.148953
4 C -0.421321
5 C 0.193731
6 C 0.471890
7 C -0.417533
8 C -0.616469
9 C 0.468672
10 C 0.463428
11 C -0.613815
12 C 0.254870
13 C 0.461459
14 C 0.256785
15 C -0.789529
16 C -0.790147
17 N -0.007331
18 N -0.007265
19 H 0.078269
20 H 0.248870

```
   21  H    0.078302
   22  H    0.248882
   23  H    0.228519
   24  H    0.042810
   25  H    0.043005
   26  H    0.228522
 Sum of APT charges =  -0.00000
 APT charges with hydrogens summed into heavy atoms:
                1
    1  C   -0.153975
    2  C    0.198324
    3  C   -0.148953
    4  C   -0.421321
    5  C    0.193731
    6  C    0.471890
    7  C   -0.417533
    8  C   -0.616469
    9  C    0.468672
   10  C    0.463428
   11  C   -0.613815
   12  C    0.254870
   13  C    0.461459
   14  C    0.256785
   15  C   -0.746719
   16  C   -0.747142
   17  N    0.548326
   18  N    0.548440
 Electronic spatial extent (au):  <R**2>=          5315.4160
 Charge=           0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=          -11.5359    Y=           -0.0011    Z=            0.0004  Tot=           11.5359
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=          -92.8947   YY=          -62.8241   ZZ=         -106.7165
   XY=           -0.0191   XZ=           -0.0039   YZ=           -5.8659
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -5.4163   YY=           24.6544   ZZ=          -19.2381
   XY=           -0.0191   XZ=           -0.0039   YZ=           -5.8659
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=         -198.6885  YYY=           -0.0156  ZZZ=           -0.0007  XYY=         -205.9495
  XXY=            0.0129  XXZ=            0.0193  XZZ=          -15.6657  YZZ=            0.0036
  YYZ=           -0.0079  XYZ=           20.6220
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=         -5142.4333 YYYY=         -1804.4017 ZZZZ=          -141.2675 XXXY=           -
0.3050
 XXXZ=           -0.0909 YYYX=           -0.1465 YYYZ=          -30.9323 ZZZX=           -0.0023
 ZZZY=          -26.3663 XXYY=          -713.8274 XXZZ=          -938.0678 YYZZ=           -
394.5455
 XXYZ=          -80.1466 YYXZ=            0.0138 ZZXY=           -0.0141
```

N-N= 1.010276795033D+03 E-N=-3.701629051183D+03 KE= 7.200589625989D+02
Exact polarizability: 496.115 -0.033 299.643 -0.004 4.404 105.836
Approx polarizability: 693.425 -0.063 401.489 -0.010 11.785 131.974
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Sat Sep 26 12:05:25 2026, MaxMem= 805306368 cpu: 3.6 elap: 0.7
(Enter /home/user/gauss16/g16/l701.exe)
... and contract with generalized density number 0.
Compute integral second derivatives.
R6Disp: Adding Grimme-D2 dispersion energy 2nd derivatives to the Hessian.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 26565 NPrTT= 83856 LenC2= 23224 LenP2D= 51951.
LDataN: DoStor=T MaxTD1= 8 Len= 415
Leave Link 701 at Sat Sep 26 12:05:26 2026, MaxMem= 805306368 cpu: 4.9 elap: 0.8
(Enter /home/user/gauss16/g16/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Sat Sep 26 12:05:26 2026, MaxMem= 805306368 cpu: 0.2 elap: 0.0
(Enter /home/user/gauss16/g16/l703.exe)
Integral derivatives from FoFJK, PRISM(SPDF).
Compute integral second derivatives, UseDBF=F ICtDFT= 0.
Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=T KAlg= 0 I1Cent= 0 FoldK=F
IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800
NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T
wScrn= 0.000000 ICntrl= 100527 IOpCl= 0 I1Cent= 0 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Sat Sep 26 13:47:50 2026, MaxMem= 805306368 cpu: 36854.2 elap: 6143.7
(Enter /home/user/gauss16/g16/l716.exe)
Dipole =-4.53856779D+00-4.34363684D-04 1.41846677D-04
Polarizability= 4.96114833D+02-3.33392007D-02 2.99642617D+02
-3.96350732D-03 4.40425124D+00 1.05835535D+02
Full mass-weighted force constant matrix:
Low frequencies --- -2.7337 -0.0005 0.0001 0.0006 1.6816 2.8737
Low frequencies --- 39.5028 51.0957 57.5709
Diagonal vibrational polarizability:
190.4942101 203.4538427 211.0787944
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:

1	2	3
A	A	A

Supporting Information file

Frequencies --		39.3765			51.0955			57.5650		
Red. masses --		1.9524			5.6445			4.9977		
Frc consts --		0.0018			0.0087			0.0098		
IR Inten --		2.2353			0.4329			12.7322		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.11	0.04	0.02	0.00	0.00	-0.08	-0.03	0.03	-0.18
2	6	0.09	-0.08	0.01	0.00	0.01	-0.16	0.02	-0.00	-0.10
3	6	0.11	0.04	0.02	-0.00	-0.00	0.08	0.03	0.03	-0.18
4	6	0.00	0.06	-0.00	-0.00	0.01	-0.21	0.00	0.03	0.04
5	6	-0.09	-0.08	0.01	0.00	-0.01	0.16	-0.02	-0.00	-0.10
6	6	0.01	-0.05	-0.02	-0.00	0.00	-0.16	0.00	-0.02	0.13
7	6	-0.00	0.06	-0.00	-0.00	-0.01	0.21	-0.00	0.03	0.04
8	6	0.02	0.02	-0.03	-0.00	0.00	-0.09	0.00	-0.01	0.20
9	6	-0.01	-0.05	-0.02	-0.00	-0.00	0.16	-0.00	-0.02	0.13
10	6	0.01	-0.02	-0.04	-0.00	0.00	-0.01	-0.00	-0.02	0.17
11	6	-0.02	0.02	-0.03	-0.00	-0.00	0.09	-0.00	-0.01	0.20
12	6	-0.00	-0.00	-0.01	-0.00	-0.00	0.04	-0.00	-0.01	0.08
13	6	-0.01	-0.02	-0.04	-0.00	0.00	0.01	0.00	-0.02	0.17
14	6	0.00	-0.00	-0.01	-0.00	0.00	-0.04	0.00	-0.01	0.08
15	6	0.03	0.00	0.02	-0.00	-0.01	0.13	0.01	0.01	-0.09
16	6	-0.03	0.00	0.02	-0.00	0.01	-0.13	-0.01	0.01	-0.09
17	7	-0.02	0.01	0.05	0.00	0.02	0.27	-0.06	-0.01	-0.16
18	7	0.02	0.01	0.05	0.00	-0.02	-0.26	0.06	-0.01	-0.16
19	1	-0.37	0.01	0.15	0.01	0.11	0.29	-0.28	-0.08	-0.12
20	1	0.09	-0.03	-0.27	0.00	-0.01	0.32	-0.00	0.01	-0.40
21	1	0.38	0.01	0.15	0.01	-0.11	-0.29	0.28	-0.08	-0.12
22	1	-0.09	-0.03	-0.28	0.01	0.01	-0.32	0.00	0.01	-0.40
23	1	0.24	0.07	0.33	0.00	-0.04	0.29	0.09	0.05	-0.02
24	1	-0.07	0.05	-0.18	0.02	0.05	0.12	-0.09	-0.01	-0.22
25	1	0.07	0.05	-0.18	0.02	-0.05	-0.12	0.09	-0.01	-0.22
26	1	-0.24	0.07	0.33	0.00	0.04	-0.30	-0.09	0.05	-0.02
		4			5			6		
		A			A			A		
Frequencies --		69.3790			102.1015			115.9525		
Red. masses --		6.0086			10.6504			3.9215		
Frc consts --		0.0170			0.0654			0.0311		
IR Inten --		0.9603			0.5691			43.2503		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.13	0.02	-0.28	0.00	-0.00	0.06	-0.02	-0.10
2	6	-0.07	0.17	0.01	-0.14	-0.09	-0.01	-0.03	0.03	-0.02
3	6	0.02	0.13	0.02	-0.28	-0.00	0.00	-0.06	-0.02	-0.10
4	6	-0.04	0.10	-0.01	-0.05	-0.27	-0.01	0.02	-0.04	0.07
5	6	0.07	0.17	0.01	-0.14	0.09	0.01	0.03	0.03	-0.02
6	6	-0.03	0.00	-0.02	-0.04	-0.36	-0.01	0.01	0.02	0.10
7	6	0.04	0.10	-0.01	-0.05	0.27	0.01	-0.02	-0.04	0.07
8	6	-0.06	-0.11	-0.03	-0.01	-0.26	-0.00	0.01	-0.01	0.06
9	6	0.03	0.00	-0.02	-0.04	0.36	0.01	-0.01	0.02	0.10
10	6	-0.10	-0.17	-0.03	0.09	-0.06	0.00	0.01	0.01	-0.04

11	6	0.06	-0.11	-0.03	-0.01	0.26	0.00	-0.01	-0.01	0.06
12	6	-0.06	-0.11	-0.01	0.13	0.00	0.00	0.01	-0.01	-0.15
13	6	0.10	-0.17	-0.03	0.09	0.06	-0.00	-0.01	0.01	-0.04
14	6	0.06	-0.11	-0.01	0.13	-0.00	-0.00	-0.01	-0.01	-0.15
15	6	-0.12	0.00	0.00	0.12	0.01	0.01	0.01	-0.02	-0.18
16	6	0.12	0.00	0.00	0.12	-0.01	-0.01	-0.01	-0.02	-0.18
17	7	-0.25	-0.01	0.04	0.11	0.01	-0.01	0.01	0.03	0.18
18	7	0.25	-0.01	0.04	0.11	-0.01	0.01	-0.01	0.03	0.18
19	1	-0.27	-0.01	0.04	0.16	0.00	-0.03	-0.05	0.26	0.25
20	1	-0.30	0.06	0.05	0.09	0.03	0.04	0.02	-0.03	0.24
21	1	0.27	-0.01	0.04	0.16	-0.00	0.02	0.05	0.26	0.25
22	1	0.30	0.06	0.05	0.09	-0.03	-0.04	-0.02	-0.03	0.24
23	1	-0.29	-0.09	0.04	0.07	-0.00	-0.05	0.04	-0.12	0.30
24	1	-0.08	0.09	0.01	0.13	0.02	0.03	-0.00	0.08	-0.26
25	1	0.08	0.09	0.01	0.13	-0.02	-0.03	0.00	0.08	-0.26
26	1	0.29	-0.09	0.04	0.07	0.00	0.05	-0.04	-0.12	0.30

	7	8	9
	A	A	A
Frequencies --	134.4832	155.5463	160.5524
Red. masses --	1.0721	10.2003	2.5740
Frc consts --	0.0114	0.1454	0.0391
IR Inten --	0.1866	3.5378	29.4147

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	-0.00	-0.01	-0.01	0.18	-0.13	0.05	-0.07
2	6	-0.00	0.00	0.01	-0.00	-0.01	0.31	0.08	-0.08	0.00
3	6	0.00	-0.00	0.00	-0.01	0.01	-0.18	0.13	0.05	-0.07
4	6	-0.00	0.01	0.00	-0.00	-0.01	0.18	-0.01	0.07	0.08
5	6	-0.00	-0.00	-0.01	-0.01	0.01	-0.31	-0.08	-0.08	0.00
6	6	-0.00	0.01	-0.00	-0.00	0.00	-0.15	-0.00	-0.06	0.08
7	6	-0.00	-0.01	-0.00	-0.00	0.01	-0.18	0.01	0.07	0.08
8	6	-0.00	0.00	-0.01	-0.00	0.01	-0.37	0.01	0.01	0.01
9	6	-0.00	-0.01	-0.00	-0.00	-0.00	0.15	0.00	-0.06	0.08
10	6	-0.01	-0.00	-0.00	0.00	0.01	-0.28	-0.01	-0.03	-0.06
11	6	-0.00	-0.00	0.01	-0.00	-0.01	0.37	-0.01	0.01	0.01
12	6	-0.01	-0.00	0.00	-0.00	0.00	-0.07	-0.01	-0.00	-0.07
13	6	-0.01	0.00	0.00	0.00	-0.01	0.28	0.01	-0.03	-0.06
14	6	-0.01	0.00	-0.00	-0.00	-0.00	0.07	0.01	-0.00	-0.07
15	6	-0.01	-0.00	0.04	-0.01	0.00	-0.02	-0.00	0.02	0.04
16	6	-0.01	0.00	-0.04	-0.01	0.00	0.02	0.00	0.01	0.04
17	7	0.02	-0.01	-0.01	0.02	0.02	0.11	0.01	0.01	-0.01
18	7	0.02	0.01	0.01	0.02	-0.02	-0.11	-0.01	0.01	-0.01
19	1	0.41	-0.00	-0.12	0.00	0.12	0.14	0.37	0.02	-0.11
20	1	-0.11	0.05	0.35	0.04	-0.02	0.14	-0.12	0.07	0.34
21	1	0.41	0.00	0.12	-0.00	-0.12	-0.14	-0.37	0.02	-0.11
22	1	-0.11	-0.05	-0.35	0.04	0.03	-0.13	0.11	0.06	0.33
23	1	-0.26	-0.08	-0.31	0.04	-0.02	0.15	-0.25	-0.05	-0.29
24	1	0.02	-0.02	0.10	0.04	0.03	0.04	0.02	0.02	0.07
25	1	0.02	0.02	-0.10	0.04	-0.03	-0.04	-0.01	0.01	0.06

26	1	-0.26	0.08	0.31	0.05	0.01	-0.16	0.24	-0.05	-0.28

	10	11	12
	A	A	A
Frequencies --	163.0300	174.2165	206.3597
Red. masses --	3.5754	6.3576	3.8595
Frc consts --	0.0560	0.1137	0.0968
IR Inten --	22.8090	1.4693	32.0132

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	0.00	-0.00	-0.13	0.08	-0.02	0.09	-0.04	-0.14
2	6	-0.04	0.00	-0.01	-0.20	0.13	0.00	-0.03	0.03	0.04
3	6	-0.04	0.00	0.00	0.13	0.08	-0.02	-0.09	-0.04	-0.14
4	6	-0.05	0.02	0.00	-0.15	0.03	0.03	0.01	-0.04	0.17
5	6	-0.04	-0.01	0.01	0.20	0.13	0.00	0.03	0.03	0.04
6	6	-0.05	0.04	0.01	-0.14	-0.18	0.02	0.01	0.07	0.09
7	6	-0.05	-0.02	0.00	0.15	0.03	0.03	-0.01	-0.04	0.17
8	6	-0.04	0.06	0.01	-0.13	-0.15	-0.00	-0.00	0.02	-0.08
9	6	-0.05	-0.05	-0.00	0.14	-0.18	0.02	-0.01	0.07	0.09
10	6	-0.04	0.07	0.01	-0.02	0.03	-0.02	-0.01	0.01	-0.15
11	6	-0.04	-0.06	-0.01	0.13	-0.15	-0.00	0.00	0.02	-0.08
12	6	-0.07	0.00	-0.00	-0.00	0.06	-0.02	-0.01	-0.00	-0.03
13	6	-0.03	-0.07	-0.01	0.02	0.03	-0.02	0.01	0.01	-0.15
14	6	-0.07	-0.00	0.00	0.00	0.06	-0.02	0.01	-0.00	-0.03
15	6	0.01	-0.13	-0.02	0.04	-0.01	0.01	-0.03	0.00	0.15
16	6	0.01	0.13	0.02	-0.04	-0.01	0.01	0.03	0.00	0.15
17	7	0.22	-0.11	0.01	0.17	0.00	-0.00	-0.02	-0.03	-0.04
18	7	0.22	0.11	-0.01	-0.18	0.00	-0.00	0.02	-0.03	-0.04
19	1	0.20	-0.05	0.03	0.06	0.01	0.03	-0.25	-0.19	-0.02
20	1	0.33	-0.26	-0.04	0.28	-0.11	-0.15	0.08	-0.05	-0.35
21	1	0.19	0.05	-0.03	-0.06	0.01	0.03	0.25	-0.19	-0.02
22	1	0.33	0.26	0.06	-0.28	-0.11	-0.15	-0.08	-0.05	-0.35
23	1	0.33	0.02	0.06	0.33	0.13	0.11	0.17	0.14	0.08
24	1	-0.06	-0.23	-0.06	0.01	-0.08	0.02	0.06	-0.04	0.29
25	1	-0.06	0.23	0.06	-0.01	-0.08	0.02	-0.05	-0.04	0.29
26	1	0.34	-0.02	-0.07	-0.33	0.13	0.11	-0.17	0.14	0.08

	13	14	15
	A	A	A
Frequencies --	217.9422	275.7195	283.4780
Red. masses --	3.2304	11.4246	6.9851
Frc consts --	0.0904	0.5117	0.3307
IR Inten --	23.5435	2.1321	16.2954

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	-0.00	-0.01	0.30	-0.01	0.01	-0.02	-0.10	0.04
2	6	-0.00	0.00	-0.06	-0.08	0.24	0.01	0.01	-0.11	-0.03
3	6	-0.00	0.00	0.01	0.30	0.01	-0.00	0.01	-0.10	0.04
4	6	-0.00	-0.01	0.01	-0.11	0.32	0.01	-0.11	0.16	-0.05
5	6	-0.00	-0.00	0.06	-0.08	-0.24	-0.01	-0.01	-0.11	-0.03
6	6	0.00	0.00	0.03	-0.09	-0.14	-0.01	-0.11	0.25	0.02
7	6	-0.00	0.01	-0.01	-0.10	-0.31	-0.01	0.11	0.16	-0.05

8	6	-0.00	-0.00	0.05	-0.16	-0.37	-0.01	-0.11	0.11	0.07
9	6	0.00	-0.00	-0.03	-0.09	0.14	0.01	0.11	0.25	0.02
10	6	0.00	0.00	-0.04	-0.03	-0.12	-0.01	-0.20	-0.07	0.00
11	6	-0.00	0.00	-0.05	-0.16	0.37	0.01	0.12	0.10	0.07
12	6	0.00	0.01	-0.10	0.04	-0.00	-0.01	-0.13	-0.04	-0.04
13	6	0.00	-0.00	0.04	-0.03	0.12	0.01	0.20	-0.08	0.00
14	6	0.00	-0.01	0.10	0.04	0.00	0.01	0.13	-0.04	-0.04
15	6	0.00	-0.00	-0.27	0.03	0.00	-0.01	-0.13	-0.08	-0.04
16	6	0.00	0.00	0.27	0.03	-0.01	0.01	0.12	-0.08	-0.04
17	7	0.01	0.04	0.08	0.06	0.01	0.00	0.11	-0.07	0.01
18	7	0.01	-0.04	-0.08	0.06	-0.01	-0.00	-0.11	-0.07	0.01
19	1	0.13	0.31	0.11	0.04	0.02	0.01	0.11	0.02	0.03
20	1	-0.05	0.02	0.34	0.09	-0.03	-0.03	0.22	-0.25	-0.02
21	1	0.13	-0.31	-0.11	0.04	-0.02	-0.01	-0.11	0.02	0.03
22	1	-0.05	-0.02	-0.34	0.09	0.02	0.03	-0.22	-0.25	-0.02
23	1	-0.10	-0.16	0.07	0.11	0.03	0.04	0.22	0.06	0.07
24	1	-0.02	0.03	-0.33	0.04	-0.01	0.01	-0.12	-0.18	0.04
25	1	-0.02	-0.03	0.33	0.04	0.00	-0.01	0.12	-0.18	0.04
26	1	-0.10	0.16	-0.07	0.10	-0.03	-0.04	-0.22	0.06	0.07

	16	17	18
	A	A	A
Frequencies --	313.8299	315.8128	356.8477
Red. masses --	8.9808	6.6147	3.7269
Frc consts --	0.5211	0.3887	0.2796
IR Inten --	3.9178	5.5896	52.8561

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.01	-0.24	0.03	0.00	0.15	-0.04	0.00	0.04
2	6	-0.00	0.01	-0.26	0.01	0.03	-0.14	-0.03	-0.00	0.03
3	6	-0.00	-0.01	0.23	-0.03	0.00	0.17	-0.04	-0.00	-0.04
4	6	-0.01	0.00	0.22	0.03	-0.03	-0.19	-0.03	0.03	-0.04
5	6	-0.00	-0.01	0.27	-0.01	0.03	-0.13	-0.03	0.00	-0.03
6	6	-0.01	-0.00	0.27	0.03	-0.04	0.13	-0.03	0.05	-0.02
7	6	-0.01	0.00	-0.21	-0.04	-0.03	-0.20	-0.03	-0.03	0.04
8	6	-0.00	0.01	-0.13	0.02	-0.04	0.25	-0.01	0.05	0.05
9	6	-0.01	0.00	-0.27	-0.03	-0.04	0.12	-0.03	-0.05	0.02
10	6	-0.01	0.01	-0.28	0.03	-0.01	-0.13	-0.02	0.02	0.02
11	6	-0.00	-0.01	0.11	-0.02	-0.04	0.26	-0.01	-0.05	-0.05
12	6	0.00	0.01	-0.05	0.02	0.01	-0.21	0.02	0.03	-0.02
13	6	-0.01	-0.01	0.29	-0.03	-0.01	-0.12	-0.02	-0.02	-0.02
14	6	0.00	-0.01	0.07	-0.02	0.00	-0.21	0.02	-0.03	0.02
15	6	-0.02	0.04	0.10	-0.02	0.04	0.14	-0.03	0.17	0.01
16	6	-0.03	-0.05	-0.11	0.01	0.03	0.14	-0.03	-0.17	-0.01
17	7	0.03	0.04	0.01	-0.01	0.02	-0.02	0.11	0.22	-0.02
18	7	0.03	-0.04	-0.00	0.01	0.02	-0.02	0.11	-0.22	0.02
19	1	0.00	-0.02	-0.00	-0.09	-0.12	-0.03	0.14	0.25	-0.02
20	1	0.08	-0.01	-0.07	0.03	0.02	-0.18	0.22	0.07	-0.06
21	1	-0.00	0.02	0.00	0.09	-0.11	-0.03	0.14	-0.25	0.02
22	1	0.08	0.01	0.08	-0.03	0.02	-0.17	0.22	-0.07	0.06

23	1	0.09	0.14	0.02	0.07	0.14	0.00	0.20	0.37	0.00
24	1	0.10	0.05	0.27	0.16	0.06	0.38	0.09	0.18	0.19
25	1	0.11	-0.05	-0.30	-0.15	0.06	0.37	0.09	-0.18	-0.19
26	1	0.09	-0.15	-0.02	-0.06	0.14	0.00	0.20	-0.37	-0.00

	19	20	21
	A	A	A
Frequencies --	366.7473	380.1698	408.1047
Red. masses --	11.5524	6.1275	3.5836
Frc consts --	0.9155	0.5218	0.3517
IR Inten --	0.0074	34.8401	223.6451

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.02	0.53	-0.18	0.04	0.03	0.10	-0.07	0.04
2	6	0.00	0.01	-0.39	-0.15	0.03	-0.04	0.02	-0.02	-0.07
3	6	0.00	0.02	-0.52	0.18	0.04	0.03	-0.10	-0.07	0.04
4	6	0.00	-0.01	0.18	-0.06	-0.14	-0.02	-0.05	0.15	0.00
5	6	0.00	-0.01	0.38	0.15	0.03	-0.04	-0.02	-0.02	-0.07
6	6	0.00	0.00	-0.10	-0.05	0.01	0.04	-0.04	0.03	0.06
7	6	0.00	0.01	-0.18	0.06	-0.14	-0.02	0.05	0.15	0.00
8	6	0.00	-0.00	0.08	0.05	0.25	0.02	-0.07	-0.09	-0.02
9	6	0.00	-0.00	0.10	0.05	0.01	0.04	0.04	0.03	0.06
10	6	0.00	-0.00	-0.04	0.01	0.14	-0.06	0.03	0.07	-0.07
11	6	0.00	0.00	-0.08	-0.05	0.26	0.02	0.07	-0.09	-0.02
12	6	-0.00	-0.00	-0.01	-0.02	-0.00	0.00	0.03	0.05	0.04
13	6	0.00	0.00	0.04	-0.01	0.14	-0.06	-0.03	0.07	-0.07
14	6	-0.00	0.00	0.01	0.02	-0.00	0.00	-0.03	0.05	0.04
15	6	-0.01	-0.00	0.06	0.04	-0.11	0.02	0.16	-0.04	0.05
16	6	-0.01	0.00	-0.06	-0.04	-0.12	0.02	-0.16	-0.04	0.05
17	7	-0.01	-0.02	-0.01	-0.09	-0.15	0.01	-0.04	-0.05	-0.00
18	7	-0.01	0.02	0.01	0.09	-0.15	0.01	0.04	-0.05	-0.00
19	1	-0.00	-0.08	-0.02	-0.10	-0.20	0.00	-0.04	-0.12	-0.02
20	1	-0.01	-0.00	-0.03	-0.20	-0.00	0.05	-0.16	0.13	0.05
21	1	-0.00	0.08	0.02	0.10	-0.20	0.00	0.04	-0.12	-0.02
22	1	-0.01	0.00	0.03	0.20	-0.00	0.06	0.16	0.13	0.05
23	1	-0.01	0.02	-0.03	-0.19	-0.28	-0.03	-0.16	-0.21	-0.06
24	1	0.02	-0.00	0.10	-0.10	-0.10	-0.21	-0.15	0.01	-0.47
25	1	0.02	0.00	-0.10	0.10	-0.10	-0.21	0.16	0.01	-0.47
26	1	-0.01	-0.02	0.03	0.19	-0.28	-0.03	0.16	-0.21	-0.06

	22	23	24
	A	A	A
Frequencies --	422.5913	427.2834	436.4875
Red. masses --	9.7087	10.2691	10.7921
Frc consts --	1.0215	1.1046	1.2114
IR Inten --	7.5203	26.4088	32.3530

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.01	0.15	0.03	-0.03	-0.23	0.16	-0.02	0.02
2	6	0.05	-0.04	0.13	-0.01	-0.02	0.41	-0.28	0.29	0.02
3	6	0.00	0.01	-0.15	-0.03	-0.03	-0.23	0.16	0.02	-0.02
4	6	0.03	-0.01	-0.33	-0.04	0.08	-0.12	-0.06	-0.08	-0.05

5	6	0.05	0.04	-0.12	0.01	-0.02	0.41	-0.28	-0.29	-0.02
6	6	0.02	-0.00	0.18	-0.03	0.02	-0.24	-0.06	-0.22	0.03
7	6	0.03	0.01	0.33	0.04	0.08	-0.12	-0.07	0.08	0.05
8	6	-0.01	-0.05	0.24	-0.03	-0.02	0.25	0.10	0.27	0.03
9	6	0.02	0.00	-0.18	0.03	0.02	-0.24	-0.06	0.22	-0.03
10	6	-0.02	-0.03	-0.36	0.03	0.08	0.01	0.13	0.28	-0.04
11	6	-0.01	0.05	-0.23	0.03	-0.02	0.26	0.10	-0.27	-0.03
12	6	-0.02	-0.01	-0.11	0.02	0.03	-0.15	0.03	0.03	-0.01
13	6	-0.02	0.03	0.36	-0.03	0.08	0.00	0.13	-0.29	0.04
14	6	-0.02	0.01	0.11	-0.02	0.03	-0.15	0.03	-0.03	0.01
15	6	-0.04	-0.03	0.06	0.08	-0.04	0.08	0.06	0.01	0.02
16	6	-0.04	0.03	-0.06	-0.08	-0.04	0.08	0.06	-0.01	-0.02
17	7	-0.02	-0.06	0.02	-0.05	-0.06	0.00	-0.05	0.01	0.00
18	7	-0.01	0.06	-0.02	0.05	-0.06	0.00	-0.05	-0.01	-0.00
19	1	-0.04	-0.10	0.01	-0.09	-0.16	-0.01	-0.06	-0.04	-0.01
20	1	0.00	-0.07	-0.03	-0.11	0.06	-0.03	-0.11	0.11	0.01
21	1	-0.04	0.09	-0.01	0.09	-0.16	-0.01	-0.06	0.04	0.01
22	1	0.01	0.08	0.03	0.11	0.06	-0.03	-0.11	-0.11	-0.01
23	1	0.01	-0.02	0.02	-0.09	-0.12	-0.02	-0.11	-0.07	-0.03
24	1	0.10	-0.03	0.27	0.02	0.01	-0.05	0.07	0.05	0.00
25	1	0.10	0.03	-0.28	-0.03	0.01	-0.05	0.07	-0.05	-0.00
26	1	0.02	0.01	-0.02	0.09	-0.12	-0.02	-0.11	0.07	0.03

	25	26	27
	A	A	A
Frequencies --	462.5588	467.5733	467.7922
Red. masses --	11.9232	10.1280	2.8148
Frc consts --	1.5031	1.3046	0.3629
IR Inten --	2.4145	5.1288	247.8109

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	0.01	-0.09	0.07	-0.01	-0.20	0.03	-0.03	0.01
2	6	0.00	-0.01	0.26	-0.03	0.06	0.05	0.02	-0.02	-0.03
3	6	0.00	0.01	-0.10	0.07	0.01	0.19	-0.03	-0.03	0.02
4	6	0.00	0.01	-0.41	0.04	-0.15	0.20	-0.04	0.12	0.03
5	6	0.00	-0.01	0.26	-0.03	-0.05	-0.04	-0.02	-0.03	-0.03
6	6	0.00	-0.01	0.43	0.03	0.03	-0.37	-0.03	-0.07	0.00
7	6	-0.01	0.01	-0.41	0.04	0.13	-0.22	0.04	0.13	0.02
8	6	0.00	0.01	-0.26	-0.00	-0.03	0.34	0.00	0.01	-0.04
9	6	-0.00	-0.01	0.42	0.03	-0.02	0.38	0.04	-0.08	0.02
10	6	-0.01	-0.01	0.06	-0.03	-0.04	-0.17	0.06	0.13	0.09
11	6	-0.00	0.01	-0.25	-0.00	0.03	-0.34	-0.00	0.01	-0.06
12	6	-0.00	-0.00	0.03	-0.04	-0.00	-0.06	0.03	-0.01	-0.06
13	6	0.01	-0.01	0.06	-0.02	0.02	0.16	-0.06	0.13	0.09
14	6	0.00	-0.00	0.03	-0.03	0.00	0.07	-0.04	-0.01	-0.06
15	6	-0.01	0.00	-0.02	-0.07	-0.00	0.03	-0.07	-0.02	-0.06
16	6	0.01	0.00	-0.02	-0.08	0.01	-0.02	0.07	-0.02	-0.06
17	7	0.01	0.01	-0.00	0.01	-0.02	0.00	-0.05	-0.07	0.02
18	7	-0.01	0.01	-0.00	0.00	0.03	-0.01	0.05	-0.07	0.02
19	1	0.01	0.03	0.00	0.02	-0.03	-0.00	-0.10	-0.05	0.03

20	1	0.02	-0.01	-0.00	0.05	-0.07	-0.02	-0.04	-0.06	-0.03
21	1	-0.01	0.03	0.00	0.00	0.04	-0.00	0.10	-0.04	0.03
22	1	-0.02	-0.01	-0.00	0.04	0.08	0.03	0.04	-0.06	-0.03
23	1	0.02	0.01	0.01	0.04	0.06	-0.00	-0.02	-0.07	0.06
24	1	-0.03	-0.00	-0.04	0.05	-0.01	0.21	0.30	-0.06	0.55
25	1	0.02	-0.00	-0.03	0.09	0.02	-0.29	-0.30	-0.06	0.54
26	1	-0.02	0.01	0.01	0.04	-0.05	-0.01	0.02	-0.07	0.06

	28	29	30
	A	A	A
Frequencies --	475.8789	495.1822	495.7561
Red. masses --	9.6272	7.6747	8.4951
Frc consts --	1.2845	1.1088	1.2301
IR Inten --	1.0977	139.8037	22.8095

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.19	0.04	-0.05	0.08	-0.00	0.00	-0.23	0.08	0.01
2	6	0.11	-0.17	0.01	0.13	-0.07	-0.01	0.02	-0.07	-0.02
3	6	-0.19	-0.04	0.05	0.10	0.01	-0.00	0.22	0.08	0.01
4	6	-0.11	0.40	0.06	0.05	0.04	0.00	0.04	-0.15	0.01
5	6	0.11	0.17	-0.01	0.13	0.06	0.00	-0.04	-0.08	-0.02
6	6	-0.08	-0.14	-0.10	0.03	-0.35	-0.00	0.03	0.36	0.01
7	6	-0.11	-0.40	-0.06	0.04	-0.05	-0.00	-0.04	-0.15	0.01
8	6	0.03	0.09	0.12	0.09	0.14	-0.02	-0.13	-0.28	-0.06
9	6	-0.08	0.14	0.11	0.03	0.39	0.00	-0.03	0.32	0.01
10	6	0.09	0.16	-0.09	-0.10	-0.15	0.04	0.07	0.10	0.11
11	6	0.03	-0.09	-0.12	0.11	-0.17	0.02	0.12	-0.26	-0.06
12	6	0.08	0.01	-0.02	-0.14	-0.03	-0.01	0.07	0.04	-0.10
13	6	0.09	-0.15	0.09	-0.11	0.16	-0.03	-0.06	0.08	0.11
14	6	0.08	-0.01	0.02	-0.14	0.03	-0.00	-0.05	0.04	-0.10
15	6	0.14	-0.01	0.03	-0.20	-0.00	-0.02	0.07	-0.01	0.01
16	6	0.14	0.01	-0.04	-0.20	0.00	0.02	-0.05	-0.01	0.00
17	7	-0.04	-0.01	0.00	0.03	0.01	-0.00	-0.03	-0.03	0.01
18	7	-0.04	0.01	-0.00	0.03	-0.01	0.00	0.03	-0.03	0.01
19	1	-0.07	-0.07	-0.00	0.13	0.11	-0.01	-0.12	-0.09	0.02
20	1	-0.14	0.14	0.02	0.15	-0.21	0.03	-0.08	0.08	-0.05
21	1	-0.07	0.07	0.00	0.14	-0.12	0.01	0.11	-0.08	0.02
22	1	-0.14	-0.14	-0.02	0.16	0.22	-0.04	0.07	0.06	-0.05
23	1	-0.11	-0.13	-0.02	0.11	0.19	-0.01	-0.05	-0.12	0.03
24	1	0.05	0.05	-0.16	-0.17	-0.07	0.07	0.24	0.02	0.24
25	1	0.04	-0.05	0.17	-0.20	0.07	-0.05	-0.22	0.01	0.25
26	1	-0.11	0.12	0.02	0.11	-0.20	0.01	0.04	-0.09	0.03

	31	32	33
	A	A	A
Frequencies --	520.5818	551.4453	617.6772
Red. masses --	7.4487	6.0843	1.7546
Frc consts --	1.1893	1.0901	0.3944
IR Inten --	188.0008	156.7874	496.5390

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.05	-0.03	0.02	0.06	-0.03	-0.00	0.04	-0.01	0.00

2	6	-0.04	0.03	-0.05	0.14	-0.08	-0.00	0.03	-0.02	-0.00
3	6	-0.05	-0.03	0.02	0.06	0.03	0.00	0.04	0.01	-0.00
4	6	-0.02	-0.00	0.05	0.02	-0.04	0.00	0.01	-0.04	-0.00
5	6	0.04	0.03	-0.05	0.14	0.08	0.00	0.03	0.02	0.00
6	6	-0.01	-0.04	-0.02	0.02	-0.04	0.00	-0.00	-0.01	-0.00
7	6	0.02	-0.00	0.05	0.02	0.04	-0.00	0.01	0.04	0.00
8	6	0.03	0.10	-0.13	-0.10	-0.15	-0.03	-0.03	-0.03	0.02
9	6	0.01	-0.03	-0.02	0.02	0.04	-0.00	-0.00	0.01	0.00
10	6	-0.05	-0.10	0.31	0.13	0.32	0.06	-0.00	0.05	-0.06
11	6	-0.03	0.10	-0.13	-0.10	0.15	0.03	-0.03	0.03	-0.02
12	6	-0.03	0.01	-0.31	-0.10	0.04	-0.04	-0.05	0.00	0.09
13	6	0.05	-0.10	0.31	0.13	-0.32	-0.07	-0.00	-0.05	0.06
14	6	0.03	0.01	-0.31	-0.10	-0.04	0.04	-0.05	-0.00	-0.10
15	6	0.10	-0.02	0.17	-0.16	0.01	-0.04	0.02	-0.01	0.05
16	6	-0.10	-0.02	0.17	-0.16	-0.01	0.04	0.02	0.01	-0.05
17	7	0.01	0.03	-0.01	-0.02	-0.00	0.00	0.00	0.07	-0.01
18	7	-0.01	0.03	-0.01	-0.02	0.00	-0.00	0.00	-0.07	0.01
19	1	0.00	-0.11	-0.03	0.02	0.04	-0.00	0.06	0.04	-0.03
20	1	-0.01	0.08	-0.05	0.04	-0.11	0.02	0.01	0.05	0.02
21	1	-0.00	-0.11	-0.03	0.02	-0.04	0.00	0.06	-0.04	0.03
22	1	0.01	0.08	-0.05	0.04	0.11	-0.02	0.01	-0.05	-0.02
23	1	-0.01	0.04	-0.04	-0.00	0.08	-0.02	-0.01	0.08	-0.04
24	1	-0.18	0.10	-0.37	0.16	-0.00	0.47	-0.37	-0.02	-0.56
25	1	0.18	0.10	-0.38	0.16	0.00	-0.47	-0.37	0.02	0.56
26	1	0.01	0.04	-0.04	-0.00	-0.08	0.02	-0.01	-0.08	0.04

	34	35	36
	A	A	A
Frequencies --	678.3617	709.8037	761.1933
Red. masses --	3.1425	6.7155	5.5791
Frc consts --	0.8520	1.9934	1.9046
IR Inten --	10.9693	313.8164	14.6439

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	0.05	0.00	-0.04	0.01	0.00	0.07	0.09	0.00
2	6	0.08	0.01	-0.00	-0.02	0.02	-0.00	0.13	0.01	0.00
3	6	-0.03	0.05	0.00	-0.04	-0.01	-0.00	-0.07	0.09	0.00
4	6	0.05	-0.05	0.00	-0.01	0.04	0.00	0.07	-0.09	-0.00
5	6	-0.08	0.01	-0.00	-0.02	-0.02	0.00	-0.13	0.01	0.00
6	6	0.02	-0.05	-0.00	0.02	0.01	0.00	0.00	-0.09	-0.00
7	6	-0.05	-0.05	0.00	-0.01	-0.04	-0.00	-0.07	-0.09	-0.00
8	6	-0.06	-0.06	-0.01	0.03	0.00	0.02	-0.10	0.02	-0.00
9	6	-0.02	-0.05	-0.00	0.02	-0.01	-0.00	-0.00	-0.09	-0.00
10	6	0.03	0.16	0.02	0.03	-0.01	-0.12	-0.19	-0.06	0.01
11	6	0.06	-0.06	-0.01	0.03	-0.00	-0.02	0.10	0.02	-0.00
12	6	-0.12	0.01	-0.03	0.04	-0.00	0.44	-0.04	0.27	-0.00
13	6	-0.03	0.16	0.02	0.03	0.01	0.12	0.19	-0.06	0.01
14	6	0.12	0.01	-0.03	0.04	0.00	-0.44	0.04	0.27	-0.00
15	6	-0.16	-0.03	0.05	-0.08	0.06	-0.18	0.03	0.06	-0.05
16	6	0.16	-0.03	0.05	-0.08	-0.06	0.18	-0.03	0.06	-0.05

17	7	-0.02	-0.02	0.00	0.01	-0.05	-0.00	0.02	-0.15	0.02
18	7	0.02	-0.02	0.00	0.01	0.05	0.00	-0.02	-0.15	0.02
19	1	0.12	0.00	-0.03	-0.01	0.12	0.03	-0.15	-0.14	0.06
20	1	0.08	-0.21	0.04	0.01	-0.08	0.06	-0.12	0.10	-0.01
21	1	-0.12	0.00	-0.03	-0.01	-0.12	-0.03	0.15	-0.14	0.06
22	1	-0.08	-0.21	0.04	0.02	0.08	-0.06	0.12	0.10	-0.01
23	1	0.02	0.16	-0.05	0.01	-0.10	0.04	-0.04	-0.35	0.07
24	1	-0.43	-0.05	-0.35	0.21	-0.07	0.40	0.10	-0.18	0.24
25	1	0.43	-0.05	-0.35	0.20	0.07	-0.40	-0.10	-0.18	0.24
26	1	-0.02	0.16	-0.05	0.01	0.10	-0.03	0.04	-0.35	0.07

	37	38	39
	A	A	A
Frequencies --	783.1226	935.5951	958.7307
Red. masses --	4.5280	3.1932	2.3563
Frc consts --	1.6361	1.6468	1.2761
IR Inten --	3.2355	1.4687	0.1639

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.15	-0.09	-0.00	-0.04	-0.05	-0.00	-0.04	0.04	0.00
2	6	0.09	-0.13	-0.00	-0.07	-0.00	-0.00	0.00	0.05	0.00
3	6	0.15	0.09	0.00	0.04	-0.05	-0.00	-0.04	-0.04	-0.00
4	6	-0.09	-0.10	-0.00	-0.00	0.05	0.00	0.05	0.02	0.00
5	6	0.09	0.13	0.00	0.07	-0.00	-0.00	0.00	-0.05	-0.00
6	6	-0.12	-0.04	-0.00	0.04	0.03	0.00	0.05	-0.02	-0.00
7	6	-0.09	0.10	0.00	0.00	0.05	0.00	0.05	-0.02	-0.00
8	6	-0.12	0.09	0.00	0.08	-0.03	-0.00	0.00	-0.01	0.00
9	6	-0.12	0.04	0.00	-0.04	0.03	0.00	0.05	0.02	0.00
10	6	-0.13	-0.01	-0.00	0.06	-0.06	0.00	-0.02	0.00	0.00
11	6	-0.12	-0.09	-0.00	-0.08	-0.03	-0.00	0.00	0.01	-0.00
12	6	0.03	0.06	0.04	0.06	0.08	-0.01	-0.09	-0.00	0.01
13	6	-0.13	0.01	0.00	-0.06	-0.06	0.00	-0.02	-0.00	-0.00
14	6	0.03	-0.06	-0.04	-0.06	0.08	-0.01	-0.09	0.00	-0.01
15	6	0.14	0.02	-0.03	-0.06	0.17	-0.02	0.03	-0.15	0.01
16	6	0.14	-0.02	0.03	0.06	0.17	-0.02	0.03	0.15	-0.01
17	7	0.03	-0.00	-0.00	-0.02	-0.15	0.05	0.03	0.12	-0.04
18	7	0.03	0.00	0.00	0.02	-0.15	0.05	0.03	-0.12	0.04
19	1	-0.15	-0.06	0.04	0.16	-0.24	-0.05	-0.18	0.19	0.05
20	1	-0.13	0.29	-0.05	0.12	-0.36	-0.01	-0.13	0.37	0.01
21	1	-0.15	0.06	-0.04	-0.16	-0.24	-0.04	-0.18	-0.19	-0.05
22	1	-0.13	-0.29	0.05	-0.12	-0.36	-0.01	-0.13	-0.37	-0.01
23	1	-0.05	-0.25	0.05	0.03	0.20	-0.09	-0.03	-0.25	0.09
24	1	0.30	0.00	0.23	-0.14	0.27	-0.20	0.14	-0.25	0.25
25	1	0.30	-0.00	-0.23	0.13	0.26	-0.20	0.14	0.25	-0.25
26	1	-0.05	0.25	-0.05	-0.03	0.20	-0.09	-0.03	0.25	-0.09

	40	41	42
	A	A	A
Frequencies --	1023.5302	1030.0236	1054.2966
Red. masses --	1.5323	2.1236	1.5117
Frc consts --	0.9458	1.3275	0.9900

Supporting Information file

IR Inten --		103.1622			55.8150			230.1743		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	-0.04	-0.00	-0.04	0.04	0.00	0.00	-0.01	-0.00
2	6	-0.05	0.00	-0.00	0.02	0.06	0.00	-0.00	-0.00	0.00
3	6	0.03	-0.04	-0.00	-0.04	-0.04	-0.00	0.00	0.01	0.00
4	6	0.01	0.03	0.00	0.05	0.01	0.00	-0.01	0.00	-0.00
5	6	0.05	0.00	-0.00	0.02	-0.06	-0.00	-0.00	0.00	-0.00
6	6	0.04	0.01	0.00	0.05	-0.02	-0.00	-0.00	0.00	0.00
7	6	-0.01	0.03	0.00	0.05	-0.01	-0.00	-0.01	-0.00	0.00
8	6	0.05	-0.02	-0.00	-0.03	-0.00	-0.00	0.00	0.00	-0.00
9	6	-0.04	0.01	0.00	0.05	0.02	0.00	-0.00	-0.00	-0.00
10	6	0.04	-0.02	0.00	-0.03	0.01	0.00	0.01	-0.01	-0.00
11	6	-0.05	-0.02	-0.00	-0.03	0.00	0.00	0.00	-0.00	0.00
12	6	-0.02	0.05	-0.01	-0.04	0.08	-0.01	0.00	-0.01	0.02
13	6	-0.04	-0.02	0.00	-0.03	-0.01	-0.00	0.01	0.01	0.00
14	6	0.02	0.05	-0.01	-0.04	-0.08	0.01	0.00	0.01	-0.02
15	6	-0.04	0.02	0.04	-0.03	0.12	-0.02	0.01	-0.10	-0.06
16	6	0.04	0.02	0.04	-0.03	-0.12	0.02	0.01	0.10	0.06
17	7	0.02	-0.01	-0.06	0.08	-0.05	0.05	-0.02	0.06	0.07
18	7	-0.02	-0.01	-0.06	0.08	0.05	-0.05	-0.02	-0.06	-0.07
19	1	-0.14	0.39	0.08	-0.11	-0.41	0.01	0.12	-0.44	-0.08
20	1	-0.06	0.02	0.16	-0.13	0.40	-0.16	0.04	0.08	-0.20
21	1	0.14	0.39	0.08	-0.11	0.41	-0.01	0.12	0.44	0.08
22	1	0.06	0.02	0.16	-0.13	-0.40	0.16	0.04	-0.08	0.20
23	1	0.05	-0.35	0.17	-0.10	-0.17	-0.08	-0.08	0.38	-0.19
24	1	-0.18	-0.29	0.04	-0.13	-0.02	-0.08	0.14	0.09	0.02
25	1	0.18	-0.29	0.04	-0.13	0.02	0.08	0.14	-0.09	-0.02
26	1	-0.05	-0.35	0.17	-0.10	0.17	0.08	-0.08	-0.38	0.19

	43	44	45
	A	A	A
Frequencies --	1066.7496	1113.6200	1125.9605
Red. masses --	1.4557	3.3847	3.0776
Frc consts --	0.9760	2.4731	2.2988
IR Inten --	83.3527	68.9901	9.7793

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	-0.03	-0.00	0.03	0.04	0.00	-0.05	0.10	0.00
2	6	-0.03	-0.00	-0.00	0.05	-0.00	0.00	0.05	0.09	0.00
3	6	0.02	-0.03	-0.00	-0.03	0.04	0.00	-0.05	-0.10	-0.00
4	6	0.02	0.03	0.00	-0.03	-0.04	-0.00	0.11	-0.00	0.00
5	6	0.03	-0.00	-0.00	-0.05	-0.00	0.00	0.05	-0.09	-0.00
6	6	0.03	0.00	-0.00	-0.05	-0.00	-0.00	0.04	-0.04	-0.00
7	6	-0.02	0.03	0.00	0.03	-0.04	-0.00	0.11	0.00	-0.00
8	6	0.03	-0.02	-0.00	-0.04	0.02	0.00	-0.10	0.02	-0.00
9	6	-0.03	0.00	-0.00	0.05	-0.00	-0.00	0.04	0.04	0.00
10	6	0.02	-0.01	0.00	0.01	0.04	0.00	-0.12	0.05	0.00
11	6	-0.03	-0.02	-0.00	0.04	0.02	0.00	-0.10	-0.02	0.00
12	6	-0.03	0.02	-0.00	-0.03	-0.19	-0.01	-0.04	0.03	0.02
13	6	-0.02	-0.01	0.00	-0.01	0.04	0.00	-0.12	-0.05	-0.00

14	6	0.03	0.02	-0.00	0.03	-0.19	-0.01	-0.04	-0.03	-0.02
15	6	-0.06	-0.01	-0.03	-0.01	0.20	0.02	0.13	0.02	-0.01
16	6	0.06	-0.01	-0.03	0.01	0.20	0.02	0.13	-0.02	0.01
17	7	0.06	0.03	0.05	0.10	-0.08	-0.02	-0.06	-0.03	-0.01
18	7	-0.06	0.03	0.05	-0.10	-0.08	-0.02	-0.06	0.03	0.01
19	1	-0.09	-0.40	-0.01	-0.17	0.03	0.06	0.15	0.12	-0.03
20	1	-0.12	0.45	-0.19	-0.12	0.27	0.02	0.11	-0.36	0.07
21	1	0.09	-0.40	-0.01	0.17	0.03	0.06	0.15	-0.12	0.03
22	1	0.12	0.45	-0.19	0.12	0.27	0.02	0.11	0.36	-0.07
23	1	-0.11	-0.06	-0.11	0.00	-0.41	0.06	0.07	0.21	0.01
24	1	-0.12	-0.15	-0.01	-0.02	0.30	-0.08	0.28	0.31	0.00
25	1	0.12	-0.15	-0.01	0.02	0.30	-0.08	0.28	-0.31	-0.00
26	1	0.11	-0.06	-0.11	-0.00	-0.41	0.06	0.07	-0.21	-0.01

	46	47	48
	A	A	A
Frequencies --	1266.6625	1310.0900	1376.7968
Red. masses --	3.1247	2.1000	9.2692
Frc consts --	2.9538	2.1236	10.3522
IR Inten --	150.3820	983.8932	210.9428

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	0.08	0.00	-0.02	0.02	0.00	-0.00	0.25	0.01
2	6	0.08	-0.02	-0.00	0.04	0.04	0.00	0.16	0.11	0.00
3	6	-0.06	0.08	0.00	-0.02	-0.02	-0.00	-0.00	-0.25	-0.01
4	6	-0.11	-0.06	-0.00	-0.00	-0.01	-0.00	0.03	-0.08	-0.00
5	6	-0.08	-0.02	-0.00	0.04	-0.04	-0.00	0.16	-0.11	-0.00
6	6	-0.13	0.03	0.00	0.00	-0.01	-0.00	-0.17	-0.01	-0.00
7	6	0.11	-0.06	-0.00	-0.00	0.01	0.00	0.03	0.08	0.00
8	6	0.03	0.02	0.00	-0.04	0.02	0.00	-0.11	0.05	0.00
9	6	0.13	0.03	0.00	0.00	0.01	0.00	-0.17	0.01	0.00
10	6	0.06	-0.05	-0.00	-0.01	-0.01	0.00	-0.05	0.07	0.00
11	6	-0.03	0.02	0.00	-0.04	-0.02	-0.00	-0.11	-0.05	-0.00
12	6	0.19	0.01	-0.02	0.12	0.16	-0.01	0.26	-0.35	-0.02
13	6	-0.06	-0.05	-0.00	-0.01	0.01	-0.00	-0.05	-0.07	-0.00
14	6	-0.19	0.01	-0.02	0.12	-0.16	0.01	0.26	0.35	0.02
15	6	-0.06	0.02	0.01	-0.02	-0.02	-0.00	-0.15	-0.04	0.00
16	6	0.06	0.02	0.01	-0.02	0.02	0.00	-0.15	0.04	-0.00
17	7	-0.01	0.02	0.01	-0.04	0.03	0.01	0.06	0.02	0.00
18	7	0.01	0.02	0.01	-0.04	-0.03	-0.01	0.05	-0.02	-0.00
19	1	-0.00	-0.05	-0.00	0.05	-0.02	-0.02	-0.10	-0.03	0.03
20	1	0.02	-0.02	-0.01	0.08	-0.18	0.02	-0.07	0.25	-0.05
21	1	0.00	-0.05	-0.00	0.05	0.03	0.02	-0.10	0.03	-0.03
22	1	-0.02	-0.02	-0.01	0.08	0.18	-0.02	-0.07	-0.25	0.05
23	1	-0.03	0.02	-0.01	-0.02	0.08	0.01	-0.04	-0.09	-0.04
24	1	-0.35	-0.52	-0.05	-0.22	-0.59	0.08	-0.17	0.00	-0.04
25	1	0.35	-0.52	-0.05	-0.22	0.59	-0.08	-0.17	-0.00	0.04
26	1	0.03	0.02	-0.01	-0.02	-0.08	-0.01	-0.04	0.09	0.05

	49	50	51
	A	A	A

Supporting Information file

Frequencies --		1410.9474			1451.8536			1466.5122		
Red. masses --		2.0180			1.7018			1.8079		
Frc consts --		2.3670			2.1135			2.2908		
IR Inten --		3.1672			403.5353			3.9321		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.03	0.00	-0.01	0.00	-0.00	0.02	0.03	0.00
2	6	0.02	-0.01	-0.00	0.02	0.02	0.00	0.02	-0.01	-0.00
3	6	-0.02	0.03	0.00	-0.01	-0.00	0.00	-0.02	0.03	0.00
4	6	-0.06	-0.02	-0.00	-0.02	-0.00	-0.00	-0.06	-0.02	-0.00
5	6	-0.02	-0.01	-0.00	0.02	-0.02	-0.00	-0.02	-0.01	-0.00
6	6	-0.05	0.02	0.00	0.00	-0.00	0.00	-0.04	0.02	0.00
7	6	0.06	-0.02	-0.00	-0.02	0.00	0.00	0.06	-0.02	-0.00
8	6	0.06	-0.01	-0.00	-0.01	0.01	0.00	0.06	-0.02	-0.00
9	6	0.05	0.02	0.00	0.00	0.00	-0.00	0.04	0.02	0.00
10	6	0.05	-0.04	-0.00	0.01	-0.02	-0.00	0.06	-0.02	-0.00
11	6	-0.05	-0.01	-0.00	-0.01	-0.01	-0.00	-0.06	-0.02	-0.00
12	6	0.01	0.08	0.01	0.05	0.10	0.01	-0.11	0.02	0.00
13	6	-0.05	-0.04	-0.00	0.01	0.02	0.00	-0.06	-0.02	-0.00
14	6	-0.01	0.08	0.01	0.05	-0.10	-0.01	0.11	0.02	0.00
15	6	-0.09	-0.10	0.02	-0.08	-0.08	0.03	0.05	0.01	-0.01
16	6	0.09	-0.10	0.02	-0.08	0.08	-0.03	-0.05	0.01	-0.01
17	7	0.04	0.00	-0.03	0.03	0.04	-0.03	-0.01	-0.07	0.02
18	7	-0.04	0.00	-0.03	0.03	-0.04	0.03	0.01	-0.07	0.02
19	1	-0.10	0.04	0.03	-0.10	-0.15	-0.02	0.05	0.34	0.07
20	1	-0.04	0.08	0.06	0.08	-0.13	0.11	-0.17	0.29	-0.11
21	1	0.10	0.04	0.03	-0.10	0.15	0.02	-0.05	0.34	0.07
22	1	0.04	0.08	0.06	0.08	0.13	-0.11	0.17	0.29	-0.11
23	1	0.01	-0.16	0.03	-0.03	-0.31	0.08	0.07	0.42	-0.14
24	1	0.15	0.61	-0.08	0.08	0.52	-0.13	0.04	-0.11	0.06
25	1	-0.15	0.61	-0.08	0.08	-0.52	0.13	-0.04	-0.12	0.06
26	1	-0.01	-0.16	0.03	-0.03	0.31	-0.08	-0.07	0.42	-0.14
		52			53			54		
		A			A			A		
Frequencies --		1484.3261			1491.3786			1536.0257		
Red. masses --		1.3300			2.1895			11.2960		
Frc consts --		1.7265			2.8693			15.7026		
IR Inten --		196.0432			391.6844			6.7303		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	0.00	-0.00	0.02	0.03	0.00	-0.00	0.26	0.01
2	6	0.01	0.01	0.00	0.02	-0.01	-0.00	0.25	0.16	0.01
3	6	-0.00	-0.00	0.00	-0.02	0.03	0.00	-0.00	-0.26	-0.01
4	6	-0.01	-0.00	-0.00	-0.07	-0.02	-0.00	-0.25	-0.12	-0.00
5	6	0.01	-0.01	-0.00	-0.02	-0.01	-0.00	0.25	-0.16	-0.01
6	6	-0.00	0.00	0.00	-0.04	0.02	0.00	-0.23	0.05	0.00
7	6	-0.01	0.00	0.00	0.07	-0.02	-0.00	-0.25	0.12	0.00
8	6	-0.00	0.00	0.00	0.07	-0.02	-0.00	0.17	-0.03	0.00
9	6	-0.00	-0.00	-0.00	0.04	0.02	0.00	-0.23	-0.05	-0.00
10	6	0.01	-0.01	-0.00	0.07	-0.02	-0.00	0.22	-0.13	-0.00

11	6	-0.00	-0.00	-0.00	-0.07	-0.02	-0.00	0.17	0.03	-0.00
12	6	0.03	0.07	0.00	-0.16	0.01	0.00	-0.25	0.11	0.01
13	6	0.01	0.01	0.00	-0.07	-0.02	-0.00	0.22	0.12	0.00
14	6	0.03	-0.07	-0.00	0.16	0.01	0.00	-0.25	-0.11	-0.01
15	6	-0.03	-0.05	0.01	0.06	0.04	-0.02	0.09	0.06	-0.01
16	6	-0.03	0.05	-0.01	-0.06	0.04	-0.02	0.09	-0.06	0.01
17	7	0.01	-0.07	-0.00	-0.02	0.06	0.01	-0.02	-0.00	0.00
18	7	0.01	0.07	0.00	0.02	0.06	0.01	-0.02	0.00	-0.00
19	1	-0.03	0.39	0.10	0.05	-0.37	-0.10	0.07	-0.04	-0.03
20	1	-0.19	0.33	-0.05	0.19	-0.33	0.03	0.04	-0.10	-0.02
21	1	-0.03	-0.39	-0.09	-0.05	-0.37	-0.10	0.07	0.04	0.03
22	1	-0.19	-0.33	0.05	-0.19	-0.34	0.04	0.04	0.10	0.02
23	1	0.08	0.36	-0.14	-0.08	-0.31	0.12	0.00	-0.01	0.04
24	1	0.01	0.16	-0.05	0.07	-0.13	0.09	0.08	-0.06	0.04
25	1	0.01	-0.16	0.05	-0.06	-0.13	0.09	0.08	0.06	-0.04
26	1	0.08	-0.35	0.14	0.08	-0.31	0.13	0.00	0.01	-0.04

	55	56	57
	A	A	A
Frequencies --	1636.7833	1637.8099	1660.9397
Red. masses --	1.0467	1.0454	1.0493
Frc consts --	1.6522	1.6522	1.7055
IR Inten --	128.6661	16.2640	76.5109

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	-0.00	-0.00	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
3	6	-0.00	0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00	0.00
4	6	-0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00	-0.00	0.00
5	6	0.00	-0.00	0.00	-0.00	0.00	0.00	0.00	-0.00	-0.00
6	6	-0.00	0.00	0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00
7	6	0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00	-0.00	0.00
8	6	0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00	-0.00	-0.00
9	6	0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00	0.00	-0.00
10	6	-0.00	0.00	0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00
11	6	-0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00	-0.00	-0.00
12	6	-0.00	-0.00	0.00	-0.00	-0.00	-0.00	0.01	-0.00	0.00
13	6	0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00	0.00	-0.00
14	6	0.00	-0.00	0.00	-0.00	0.00	0.00	-0.01	-0.00	0.00
15	6	0.00	0.00	-0.01	0.00	0.00	-0.01	-0.01	-0.00	0.00
16	6	-0.00	0.00	-0.01	0.00	-0.00	0.01	0.01	-0.00	0.00
17	7	-0.01	-0.00	-0.04	-0.00	-0.00	-0.04	-0.04	-0.01	0.00
18	7	0.01	-0.00	-0.04	-0.00	0.00	0.04	0.04	-0.01	0.00
19	1	-0.06	-0.26	-0.06	-0.08	-0.26	-0.05	0.49	0.02	-0.13
20	1	-0.19	0.10	0.43	-0.19	0.10	0.45	-0.07	0.17	-0.24
21	1	0.06	-0.26	-0.06	-0.08	0.26	0.05	-0.48	0.02	-0.13
22	1	0.19	0.10	0.45	-0.18	-0.09	-0.44	0.06	0.17	-0.23
23	1	0.30	0.20	0.22	0.30	0.21	0.21	0.18	-0.15	0.32
24	1	-0.00	-0.03	0.00	-0.00	-0.03	0.01	-0.01	0.03	-0.01
25	1	0.00	-0.03	0.00	-0.00	0.03	-0.01	0.01	0.03	-0.01

26	1	-0.31	0.21	0.23	0.29	-0.21	-0.21	-0.18	-0.14	0.32

	58	59	60
	A	A	A
Frequencies --	1662.8748	1911.2074	2094.3825
Red. masses --	1.0541	11.7354	11.9369
Frc consts --	1.7173	25.2560	30.8499
IR Inten --	144.1489	1042.9688	127.0623

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	-0.16	-0.35	-0.01	-0.19	-0.31	-0.01
2	6	-0.00	-0.00	-0.00	0.23	0.27	0.01	0.24	0.33	0.01
3	6	0.00	-0.00	-0.00	-0.16	0.35	0.01	0.19	-0.31	-0.01
4	6	0.00	-0.00	0.00	-0.24	-0.03	-0.00	0.17	-0.01	0.00
5	6	-0.00	0.00	0.00	0.23	-0.27	-0.01	-0.24	0.33	0.01
6	6	-0.00	0.00	0.00	0.24	-0.02	-0.00	-0.23	-0.00	-0.00
7	6	0.00	0.00	-0.00	-0.24	0.03	0.00	-0.16	-0.01	0.00
8	6	0.00	-0.00	-0.00	-0.21	0.10	0.00	-0.17	0.09	0.00
9	6	-0.00	-0.00	-0.00	0.24	0.02	0.00	0.23	-0.00	-0.00
10	6	-0.00	0.00	-0.00	0.12	-0.07	-0.00	0.25	-0.13	-0.00
11	6	0.00	0.00	0.00	-0.21	-0.10	-0.00	0.17	0.09	0.00
12	6	0.01	0.01	0.00	-0.01	-0.16	-0.01	-0.05	0.03	0.00
13	6	-0.00	-0.00	0.00	0.12	0.07	0.00	-0.24	-0.13	-0.00
14	6	0.01	-0.01	-0.00	-0.01	0.16	0.01	0.05	0.03	0.00
15	6	-0.02	-0.00	0.00	0.03	0.03	0.01	-0.01	-0.01	-0.01
16	6	-0.02	0.01	-0.00	0.03	-0.03	-0.01	0.01	-0.01	-0.01
17	7	-0.04	-0.01	0.00	-0.00	0.00	-0.01	-0.00	0.00	0.00
18	7	-0.04	0.01	-0.00	-0.00	-0.00	0.01	0.00	0.00	0.00
19	1	0.48	0.00	-0.13	0.06	0.03	-0.01	0.01	-0.02	-0.01
20	1	-0.07	0.18	-0.21	-0.01	0.03	0.00	-0.01	0.01	0.00
21	1	0.48	-0.00	0.14	0.06	-0.03	0.01	-0.01	-0.02	-0.01
22	1	-0.07	-0.18	0.22	-0.01	-0.03	-0.00	0.01	0.01	0.00
23	1	0.19	-0.14	0.33	0.03	0.02	0.04	0.01	0.00	0.02
24	1	-0.00	0.04	-0.01	-0.04	-0.04	-0.02	0.01	-0.01	0.04
25	1	-0.00	-0.04	0.01	-0.04	0.04	0.02	-0.01	-0.01	0.04
26	1	0.19	0.14	-0.33	0.03	-0.02	-0.04	-0.01	0.00	0.01

	61	62	63
	A	A	A
Frequencies --	2171.2718	2180.5722	2220.2522
Red. masses --	11.9867	11.8206	11.9648
Frc consts --	33.2951	33.1154	34.7503
IR Inten --	4.7933	711.3139	36.5912

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	-0.18	-0.01	0.02	0.01	0.00	-0.12	-0.20	-0.01
2	6	-0.01	0.05	0.00	0.03	0.01	0.00	0.25	0.26	0.01
3	6	-0.06	0.18	0.01	-0.02	0.01	0.00	0.12	-0.20	-0.01
4	6	0.40	0.05	0.00	-0.32	-0.04	-0.00	-0.33	-0.06	-0.00
5	6	-0.01	-0.05	-0.00	-0.03	0.01	0.00	-0.25	0.26	0.01
6	6	-0.35	-0.00	-0.00	0.42	-0.02	0.00	0.17	0.01	0.00
7	6	0.40	-0.05	-0.00	0.32	-0.04	-0.00	0.33	-0.06	-0.00

8	6	-0.21	0.11	0.00	-0.35	0.15	0.00	0.24	-0.12	-0.00
9	6	-0.35	0.00	0.00	-0.42	-0.02	0.00	-0.18	0.01	0.00
10	6	0.30	-0.16	-0.01	0.23	-0.12	-0.00	-0.27	0.14	0.00
11	6	-0.21	-0.11	-0.00	0.35	0.15	0.00	-0.24	-0.12	-0.00
12	6	-0.07	0.03	0.00	-0.00	0.02	0.00	0.05	-0.03	-0.00
13	6	0.30	0.16	0.01	-0.23	-0.12	-0.00	0.27	0.14	0.00
14	6	-0.07	-0.03	-0.00	0.00	0.02	0.00	-0.05	-0.03	-0.00
15	6	0.00	0.00	-0.00	-0.03	-0.01	-0.01	0.01	0.01	0.01
16	6	0.00	-0.00	0.00	0.03	-0.01	-0.01	-0.01	0.01	0.01
17	7	-0.00	-0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00	-0.00
18	7	-0.00	0.00	0.00	0.00	0.00	0.00	-0.00	-0.00	-0.00
19	1	0.01	-0.00	-0.00	0.02	-0.03	-0.02	-0.01	0.01	0.01
20	1	-0.01	0.00	0.00	-0.01	0.02	-0.00	0.01	-0.01	-0.00
21	1	0.01	0.00	0.00	-0.02	-0.03	-0.02	0.01	0.01	0.01
22	1	-0.01	-0.00	-0.00	0.01	0.02	-0.00	-0.01	-0.01	-0.00
23	1	0.01	0.01	0.01	0.01	0.01	0.02	-0.01	-0.00	-0.01
24	1	0.01	0.01	0.01	0.00	-0.02	0.07	-0.01	0.00	-0.03
25	1	0.01	-0.01	-0.01	-0.00	-0.02	0.07	0.01	0.00	-0.03
26	1	0.01	-0.01	-0.01	-0.01	0.01	0.02	0.01	-0.00	-0.01

	64	65	66
	A	A	A
Frequencies --	2239.2316	3159.1229	3172.6197
Red. masses --	11.9717	1.0871	1.0874
Frc consts --	35.3675	6.3923	6.4485
IR Inten --	42.8938	3.4042	24.9600

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.13	-0.31	-0.01	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
2	6	0.16	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00
3	6	-0.13	0.31	0.01	0.00	-0.00	-0.00	-0.00	0.00	0.00
4	6	0.09	-0.00	-0.00	-0.00	0.00	-0.00	-0.00	-0.00	-0.00
5	6	0.16	-0.20	-0.01	-0.00	0.00	0.00	0.00	-0.00	-0.00
6	6	-0.25	0.02	0.00	0.00	-0.00	0.00	0.00	-0.00	0.00
7	6	0.09	0.00	0.00	0.00	0.00	-0.00	-0.00	0.00	0.00
8	6	0.35	-0.16	-0.01	-0.00	0.00	-0.00	-0.00	0.00	-0.00
9	6	-0.25	-0.02	-0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00
10	6	-0.28	0.15	0.00	0.00	-0.00	0.00	0.00	-0.00	0.00
11	6	0.35	0.16	0.01	0.00	0.00	-0.00	-0.00	-0.00	0.00
12	6	0.05	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	-0.28	-0.15	-0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00
14	6	0.05	-0.02	-0.00	-0.00	0.00	0.00	0.00	-0.00	-0.00
15	6	-0.01	-0.01	-0.00	-0.05	0.02	0.03	-0.05	0.02	0.03
16	6	-0.00	0.01	0.00	0.05	0.02	0.03	-0.05	-0.02	-0.03
17	7	0.00	0.00	0.00	0.00	-0.00	0.00	0.00	-0.00	-0.00
18	7	0.00	-0.00	-0.00	-0.00	-0.00	0.00	0.00	0.00	0.00
19	1	-0.02	-0.01	0.00	-0.00	0.00	-0.01	0.00	0.00	0.00
20	1	0.00	-0.01	-0.00	-0.00	0.00	-0.00	-0.00	0.00	-0.00
21	1	-0.02	0.01	-0.00	0.00	0.00	-0.01	0.00	-0.00	-0.00
22	1	0.00	0.01	0.00	0.00	0.00	0.00	-0.00	-0.00	0.00

23	1	-0.01	-0.01	-0.02	-0.01	0.00	0.01	-0.01	0.00	0.01
24	1	0.01	-0.00	0.00	0.56	-0.25	-0.36	0.55	-0.24	-0.35
25	1	0.01	0.00	-0.00	-0.55	-0.24	-0.35	0.56	0.25	0.36
26	1	-0.01	0.01	0.02	0.01	0.00	0.01	-0.01	-0.00	-0.01

	67	68	69
	A	A	A
Frequencies --	3288.4400	3289.9400	3458.2766
Red. masses --	1.0584	1.0578	1.0663
Frc consts --	6.7432	6.7459	7.5139
IR Inten --	238.0132	49.2815	62.5825

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	-0.00	-0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00
2	6	0.00	-0.00	0.00	0.00	0.00	-0.00	0.00	-0.00	-0.00
3	6	0.00	-0.00	-0.00	-0.00	0.00	-0.00	0.00	0.00	0.00
4	6	-0.00	0.00	-0.00	-0.00	-0.00	0.00	-0.00	0.00	0.00
5	6	-0.00	0.00	0.00	0.00	-0.00	0.00	-0.00	-0.00	-0.00
6	6	0.00	-0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00	-0.00
7	6	0.00	0.00	-0.00	-0.00	0.00	-0.00	0.00	0.00	0.00
8	6	-0.00	0.00	0.00	-0.00	0.00	-0.00	0.00	-0.00	0.00
9	6	-0.00	-0.00	-0.00	0.00	-0.00	0.00	-0.00	-0.00	-0.00
10	6	0.00	-0.00	-0.00	0.00	-0.00	0.00	-0.00	-0.00	-0.00
11	6	0.00	0.00	0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00
12	6	-0.00	-0.00	0.00	-0.00	0.00	-0.00	-0.00	0.00	-0.00
13	6	-0.00	-0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00	-0.00
14	6	0.00	-0.00	-0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00
15	6	-0.00	0.00	0.00	0.00	-0.00	0.00	0.00	-0.00	0.00
16	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.00	-0.00	0.00
17	7	-0.01	0.01	-0.04	0.01	-0.01	0.04	0.02	-0.02	-0.03
18	7	0.01	0.01	-0.04	0.01	0.01	-0.04	-0.02	-0.02	-0.04
19	1	0.19	-0.14	0.68	-0.18	0.13	-0.63	0.02	-0.02	0.06
20	1	-0.07	-0.04	-0.03	0.07	0.03	0.03	0.15	0.08	0.04
21	1	-0.18	-0.13	0.63	-0.19	-0.14	0.68	-0.03	-0.02	0.08
22	1	0.06	-0.03	-0.03	0.07	-0.04	-0.03	-0.20	0.11	0.05
23	1	0.05	-0.02	-0.06	-0.05	0.02	0.06	-0.41	0.18	0.34
24	1	0.01	-0.01	-0.00	0.00	0.00	-0.00	-0.01	0.01	0.00
25	1	-0.01	-0.01	-0.00	0.00	-0.00	0.00	0.01	0.01	0.01
26	1	-0.04	-0.02	-0.06	-0.05	-0.02	-0.06	0.55	0.25	0.46

	70	71	72
	A	A	A
Frequencies --	3458.6828	3569.9295	3570.2793
Red. masses --	1.0667	1.0850	1.0850
Frc consts --	7.5181	8.1467	8.1483
IR Inten --	1.4031	54.5060	166.5297

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	-0.00	-0.00	0.00	0.00	0.00	0.00	0.00	-0.00
2	6	0.00	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	0.00
3	6	-0.00	0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00	0.00
4	6	-0.00	-0.00	-0.00	0.00	0.00	0.00	0.00	-0.00	-0.00

5	6	0.00	-0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00	-0.00
6	6	0.00	-0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00	0.00
7	6	-0.00	0.00	0.00	-0.00	0.00	0.00	0.00	0.00	0.00
8	6	-0.00	0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	-0.00	-0.00	-0.00	-0.00
10	6	0.00	-0.00	0.00	-0.00	0.00	-0.00	0.00	-0.00	0.00
11	6	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	0.00	-0.00	-0.00
12	6	0.00	0.00	-0.00	0.00	-0.00	0.00	0.00	0.00	-0.00
13	6	0.00	0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00	-0.00
14	6	0.00	-0.00	0.00	-0.00	-0.00	0.00	0.00	-0.00	0.00
15	6	-0.00	0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00	0.00
16	6	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
17	7	-0.02	0.02	0.04	0.05	0.02	0.00	-0.05	-0.02	-0.01
18	7	-0.02	-0.02	-0.03	-0.05	0.02	0.01	-0.05	0.02	0.01
19	1	-0.03	0.02	-0.08	-0.00	0.01	-0.04	0.00	-0.01	0.05
20	1	-0.20	-0.11	-0.05	-0.54	-0.31	-0.15	0.59	0.34	0.16
21	1	-0.02	-0.02	0.06	0.00	0.01	-0.05	0.00	0.01	-0.04
22	1	-0.15	0.08	0.04	0.59	-0.34	-0.16	0.54	-0.31	-0.15
23	1	0.55	-0.25	-0.46	-0.13	0.07	0.12	0.14	-0.08	-0.13
24	1	0.01	-0.01	-0.01	-0.00	0.00	0.00	0.00	-0.00	-0.00
25	1	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
26	1	0.41	0.18	0.34	0.15	0.08	0.13	0.13	0.07	0.12

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 6 and mass 12.00000
Atom 2 has atomic number 6 and mass 12.00000
Atom 3 has atomic number 6 and mass 12.00000
Atom 4 has atomic number 6 and mass 12.00000
Atom 5 has atomic number 6 and mass 12.00000
Atom 6 has atomic number 6 and mass 12.00000
Atom 7 has atomic number 6 and mass 12.00000
Atom 8 has atomic number 6 and mass 12.00000
Atom 9 has atomic number 6 and mass 12.00000
Atom 10 has atomic number 6 and mass 12.00000
Atom 11 has atomic number 6 and mass 12.00000
Atom 12 has atomic number 6 and mass 12.00000
Atom 13 has atomic number 6 and mass 12.00000
Atom 14 has atomic number 6 and mass 12.00000
Atom 15 has atomic number 6 and mass 12.00000
Atom 16 has atomic number 6 and mass 12.00000
Atom 17 has atomic number 7 and mass 14.00307
Atom 18 has atomic number 7 and mass 14.00307
Atom 19 has atomic number 1 and mass 1.00783
Atom 20 has atomic number 1 and mass 1.00783
Atom 21 has atomic number 1 and mass 1.00783

Atom 22 has atomic number 1 and mass 1.00783
Atom 23 has atomic number 1 and mass 1.00783
Atom 24 has atomic number 1 and mass 1.00783
Atom 25 has atomic number 1 and mass 1.00783
Atom 26 has atomic number 1 and mass 1.00783
Molecular mass: 228.06875 amu.
Principal axes and moments of inertia in atomic units:

	1	2	3
Eigenvalues --	2998.13692	6657.61836	9621.10731
X	1.00000	-0.00000	-0.00000
Y	0.00000	0.99999	-0.00528
Z	0.00000	0.00528	0.99999

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.02889 0.01301 0.00900
Rotational constants (GHZ): 0.60195 0.27108 0.18758
Zero-point vibrational energy 482138.8 (Joules/Mol)
115.23394 (Kcal/Mol)
Warning -- explicit consideration of 33 degrees of freedom as
vibrations may cause significant error
Vibrational temperatures: 56.65 73.51 82.82 99.82 146.90
(Kelvin) 166.83 193.49 223.80 231.00 234.56
250.66 296.91 313.57 396.70 407.86
451.53 454.38 513.42 527.67 546.98
587.17 608.01 614.77 628.01 665.52
672.73 673.05 684.68 712.46 713.28
749.00 793.41 888.70 976.01 1021.25
1095.19 1126.74 1346.11 1379.40 1472.63
1481.97 1516.90 1534.81 1602.25 1620.01
1822.44 1884.93 1980.90 2030.04 2088.89
2109.98 2135.61 2145.76 2210.00 2354.97
2356.44 2389.72 2392.51 2749.80 3013.35
3123.98 3137.36 3194.45 3221.75 4545.27
4564.69 4731.33 4733.49 4975.69 4976.27
5136.33 5136.84

Zero-point correction= 0.183637 (Hartree/Particle)
Thermal correction to Energy= 0.202058
Thermal correction to Enthalpy= 0.203002
Thermal correction to Gibbs Free Energy= 0.137204
Sum of electronic and zero-point Energies= -723.230311
Sum of electronic and thermal Energies= -723.211890
Sum of electronic and thermal Enthalpies= -723.210946
Sum of electronic and thermal Free Energies= -723.276744

	E (Thermal)	CV	S

Supporting Information file

		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total		126.793	65.952	138.483
Electronic		0.000	0.000	0.000
Translational		0.889	2.981	42.176
Rotational		0.889	2.981	33.618
Vibrational		125.016	59.991	62.690
Vibration	1	0.594	1.981	5.290
Vibration	2	0.595	1.977	4.775
Vibration	3	0.596	1.974	4.539
Vibration	4	0.598	1.969	4.171
Vibration	5	0.604	1.947	3.414
Vibration	6	0.608	1.936	3.167
Vibration	7	0.613	1.919	2.881
Vibration	8	0.620	1.896	2.603
Vibration	9	0.622	1.891	2.543
Vibration	10	0.623	1.888	2.514
Vibration	11	0.627	1.874	2.390
Vibration	12	0.641	1.831	2.076
Vibration	13	0.646	1.814	1.976
Vibration	14	0.677	1.718	1.560
Vibration	15	0.682	1.704	1.513
Vibration	16	0.702	1.647	1.342
Vibration	17	0.703	1.643	1.332
Vibration	18	0.732	1.561	1.136
Vibration	19	0.740	1.541	1.093
Vibration	20	0.750	1.512	1.038
Vibration	21	0.773	1.453	0.933
Vibration	22	0.785	1.421	0.883
Vibration	23	0.789	1.411	0.868
Vibration	24	0.797	1.391	0.838
Vibration	25	0.820	1.333	0.759
Vibration	26	0.825	1.322	0.744
Vibration	27	0.825	1.322	0.744
Vibration	28	0.833	1.304	0.721
Vibration	29	0.851	1.261	0.670
Vibration	30	0.851	1.259	0.669
Vibration	31	0.876	1.204	0.609
Vibration	32	0.907	1.137	0.541
Vibration	33	0.977	0.995	0.420

		Q	Log10(Q)	Ln(Q)
Total Bot		0.777306D-63	-63.109408	-145.314782
Total V=0		0.227857D+22	21.357662	49.177834
Vib (Bot)		0.115743D-77	-77.936504	-179.455432
Vib (Bot)	1	0.525473D+01	0.720551	1.659129
Vib (Bot)	2	0.404538D+01	0.606959	1.397575
Vib (Bot)	3	0.358829D+01	0.554887	1.277675
Vib (Bot)	4	0.297295D+01	0.473187	1.089553
Vib (Bot)	5	0.200921D+01	0.303025	0.697741

Vib (Bot)	6	0.176405D+01	0.246510	0.567611
Vib (Bot)	7	0.151418D+01	0.180179	0.414876
Vib (Bot)	8	0.130147D+01	0.114434	0.263493
Vib (Bot)	9	0.125897D+01	0.100016	0.230295
Vib (Bot)	10	0.123888D+01	0.093031	0.214211
Vib (Bot)	11	0.115515D+01	0.062637	0.144226
Vib (Bot)	12	0.963868D+00	-0.015982	-0.036801
Vib (Bot)	13	0.908376D+00	-0.041734	-0.096097
Vib (Bot)	14	0.698873D+00	-0.155601	-0.358286
Vib (Bot)	15	0.676973D+00	-0.169428	-0.390123
Vib (Bot)	16	0.601187D+00	-0.220990	-0.508849
Vib (Bot)	17	0.596715D+00	-0.224233	-0.516315
Vib (Bot)	18	0.514712D+00	-0.288435	-0.664147
Vib (Bot)	19	0.497514D+00	-0.303195	-0.698132
Vib (Bot)	20	0.475534D+00	-0.322818	-0.743316
Vib (Bot)	21	0.434135D+00	-0.362375	-0.834400
Vib (Bot)	22	0.414682D+00	-0.382285	-0.880245
Vib (Bot)	23	0.408645D+00	-0.388654	-0.894909
Vib (Bot)	24	0.397155D+00	-0.401040	-0.923429
Vib (Bot)	25	0.366931D+00	-0.435415	-1.002580
Vib (Bot)	26	0.361480D+00	-0.441916	-1.017549
Vib (Bot)	27	0.361244D+00	-0.442199	-1.018201
Vib (Bot)	28	0.352687D+00	-0.452611	-1.042174
Vib (Bot)	29	0.333320D+00	-0.477138	-1.098651
Vib (Bot)	30	0.332766D+00	-0.477861	-1.100315
Vib (Bot)	31	0.309898D+00	-0.508781	-1.171511
Vib (Bot)	32	0.284189D+00	-0.546393	-1.258117
Vib (Bot)	33	0.237339D+00	-0.624631	-1.438267
Vib (V=0)		0.339286D+07	6.530566	15.037184
Vib (V=0)	1	0.577847D+01	0.761813	1.754138
Vib (V=0)	2	0.457616D+01	0.660501	1.520861
Vib (V=0)	3	0.412295D+01	0.615208	1.416570
Vib (V=0)	4	0.351470D+01	0.545888	1.256954
Vib (V=0)	5	0.257049D+01	0.410016	0.944096
Vib (V=0)	6	0.233354D+01	0.368015	0.847386
Vib (V=0)	7	0.209460D+01	0.321101	0.739363
Vib (V=0)	8	0.189421D+01	0.277428	0.638801
Vib (V=0)	9	0.185463D+01	0.268256	0.617683
Vib (V=0)	10	0.183598D+01	0.263867	0.607577
Vib (V=0)	11	0.175871D+01	0.245195	0.564583
Vib (V=0)	12	0.158584D+01	0.200259	0.461112
Vib (V=0)	13	0.153689D+01	0.186644	0.429763
Vib (V=0)	14	0.135932D+01	0.133320	0.306982
Vib (V=0)	15	0.134160D+01	0.127624	0.293864
Vib (V=0)	16	0.128194D+01	0.107867	0.248372
Vib (V=0)	17	0.127850D+01	0.106702	0.245691
Vib (V=0)	18	0.121759D+01	0.085499	0.196870
Vib (V=0)	19	0.120535D+01	0.081114	0.186771

Vib (V=0)	20	0.119002D+01	0.075556	0.173973
Vib (V=0)	21	0.116217D+01	0.065271	0.150292
Vib (V=0)	22	0.114959D+01	0.060541	0.139401
Vib (V=0)	23	0.114575D+01	0.059089	0.136058
Vib (V=0)	24	0.113854D+01	0.056348	0.129746
Vib (V=0)	25	0.112019D+01	0.049293	0.113501
Vib (V=0)	26	0.111698D+01	0.048046	0.110631
Vib (V=0)	27	0.111684D+01	0.047993	0.110508
Vib (V=0)	28	0.111187D+01	0.046055	0.106046
Vib (V=0)	29	0.110092D+01	0.041755	0.096144
Vib (V=0)	30	0.110061D+01	0.041634	0.095865
Vib (V=0)	31	0.108825D+01	0.036728	0.084570
Vib (V=0)	32	0.107512D+01	0.031457	0.072432
Vib (V=0)	33	0.105347D+01	0.022622	0.052090
Electronic		0.100000D+01	0.000000	0.000000
Translational		0.135379D+09	8.131553	18.723592
Rotational		0.496070D+07	6.695543	15.417058

title card
IR Spectrum

```
   33 33    33  33                  2222  2     1    1111  111111 111111111
      55  44       22   11                                  2211   0       9      6666   544444
33211000099777665544444444443333322221111111
      77  55       98   75                                  3287   9       1      6633   398651
71621653253861715299766632208651187107665310655 3
      00  98       08   39                                  9011   4       1      3187   614721
70764740496310881165688367380776436864316462981 9

    XX XX     XX  XX                        XXXX  X     X    XXXX  XXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXX XXXXXXXXXXXXXXXXXX
  X      X                  X  X    X   X X  XX X XXX XX X   X XXX X X   X
  X      X                  X     X   X    XX X XXX  X    X XXX X X   X
        X                  X     X      XX X XX   X    X X X  X   X
        X                  X     X      X X  X      X X   X
                          X     X      X X  X      X X
                          X     X      X X  X       X
                          X     X      X X  X       X
                          X     X         X       X
                          X     X         X       X
                          X     X         X
                          X     X         X
                          X     X         X
                          X     X         X
                               X          X
                               X          X
                               X          X
                               X          X
```

X X
X

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000013390	0.000040569	-0.000084106
2	6	0.000027862	-0.000037545	0.000097503
3	6	-0.000008332	-0.000043168	0.000083863
4	6	-0.000032400	0.000037813	-0.000114298
5	6	0.000023907	0.000041323	-0.000096853
6	6	0.000030299	-0.000026412	0.000090045
7	6	-0.000032875	-0.000039996	0.000114045
8	6	-0.000022080	0.000001980	-0.000028266
9	6	0.000030847	0.000028711	-0.000091358
10	6	0.000012443	0.000004414	0.000004260
11	6	-0.000027774	-0.000001809	0.000028345
12	6	0.000004582	0.000006411	-0.000002605
13	6	0.000022346	-0.000003162	0.000000099
14	6	-0.000005512	-0.000007922	-0.000001162
15	6	-0.000011655	-0.000011629	-0.000001613
16	6	-0.000014054	0.000005023	-0.000000826
17	7	0.000032339	0.000032423	-0.000023268
18	7	0.000033918	-0.000031826	0.000020265
19	1	-0.000010976	-0.000012545	0.000020263
20	1	-0.000001664	-0.000005961	-0.000000849
21	1	-0.000014213	0.000012307	-0.000018607
22	1	-0.000000816	0.000004726	-0.000000334
23	1	-0.000013060	-0.000009412	0.000003612
24	1	-0.000001467	0.000000379	0.000005669
25	1	0.000002823	0.000005295	-0.000000503
26	1	-0.000011098	0.000010012	-0.000003322

Cartesian Forces: Max 0.000114298 RMS 0.000036473
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Leave Link 716 at Sat Sep 26 13:47:50 2026, MaxMem= 805306368 cpu: 0.3 elap: 0.0
(Enter /home/user/gauss16/g16/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Red2BG is reusing G-inverse.
Internal Forces: Max 0.000024642 RMS 0.000010093
Search for a local minimum.
Step number 1 out of a maximum of 2
All quantities printed in internal units (Hartrees-Bohrs-Radians)

Supporting Information file

Second derivative matrix not updated -- analytic derivatives used.
ITU= 0
Eigenvalues --- 0.00031 0.00146 0.00204 0.00249 0.00279
Eigenvalues --- 0.00355 0.00485 0.00872 0.00955 0.01013
Eigenvalues --- 0.01366 0.01887 0.03020 0.03484 0.04112
Eigenvalues --- 0.04212 0.04301 0.04623 0.04844 0.05672
Eigenvalues --- 0.05734 0.06078 0.06347 0.07280 0.08675
Eigenvalues --- 0.08722 0.08770 0.08782 0.09256 0.10560
Eigenvalues --- 0.10639 0.10652 0.11143 0.11160 0.13189
Eigenvalues --- 0.13311 0.13426 0.13472 0.15280 0.15786
Eigenvalues --- 0.17697 0.18842 0.19238 0.21563 0.25025
Eigenvalues --- 0.25203 0.29114 0.31305 0.33773 0.35333
Eigenvalues --- 0.35647 0.39191 0.39259 0.39412 0.41553
Eigenvalues --- 0.43277 0.43281 0.44656 0.45391 0.45553
Eigenvalues --- 0.48157 0.49480 0.49636 0.53450 0.55754
Eigenvalues --- 0.57657 0.87949 0.89191 0.94311 0.96225
Eigenvalues --- 0.97840 0.98280
Angle between quadratic step and forces= 62.01 degrees.
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.00085964 RMS(Int)= 0.00000250
Iteration 2 RMS(Cart)= 0.00000272 RMS(Int)= 0.00000194
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000194
ITry= 1 IFail=0 DXMaxC= 3.82D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
R1	2.32364	-0.00002	0.00000	-0.00008	-0.00008	2.32356
R2	2.53365	0.00002	0.00000	0.00009	0.00009	2.53375
R3	2.53104	0.00002	0.00000	0.00015	0.00015	2.53119
R4	2.32361	-0.00002	0.00000	-0.00004	-0.00004	2.32357
R5	2.32022	-0.00002	0.00000	-0.00007	-0.00007	2.32015
R6	2.53115	0.00002	0.00000	0.00003	0.00003	2.53118
R7	2.53330	0.00001	0.00000	0.00010	0.00010	2.53339
R8	2.32017	-0.00002	0.00000	-0.00001	-0.00001	2.32016
R9	2.31935	-0.00001	0.00000	-0.00007	-0.00007	2.31929
R10	2.53340	0.00001	0.00000	-0.00002	-0.00002	2.53338
R11	2.62671	0.00000	0.00000	0.00011	0.00011	2.62683
R12	2.31929	-0.00002	0.00000	0.00001	0.00001	2.31930
R13	2.69303	-0.00000	0.00000	-0.00006	-0.00006	2.69297
R14	2.69341	0.00000	0.00000	-0.00009	-0.00009	2.69332
R15	2.62686	0.00000	0.00000	-0.00007	-0.00006	2.62680
R16	2.69315	0.00000	0.00000	0.00022	0.00022	2.69337
R17	2.81300	0.00001	0.00000	0.00005	0.00005	2.81304
R18	2.05071	-0.00000	0.00000	-0.00004	-0.00004	2.05068
R19	2.81290	0.00001	0.00000	0.00017	0.00017	2.81307
R20	2.05065	-0.00000	0.00000	0.00004	0.00004	2.05069
R21	1.94494	-0.00002	0.00000	-0.00008	-0.00008	1.94486
R22	1.91731	-0.00000	0.00000	-0.00000	-0.00000	1.91731

R23	1.92984	-0.00001	0.00000	-0.00004	-0.00004	1.92981
R24	1.94493	-0.00002	0.00000	-0.00006	-0.00006	1.94487
R25	1.91731	-0.00000	0.00000	-0.00001	-0.00001	1.91731
R26	1.92986	-0.00001	0.00000	-0.00006	-0.00006	1.92980
A1	2.55914	0.00000	0.00000	0.00105	0.00104	2.56018
A2	2.61293	-0.00000	0.00000	-0.00083	-0.00083	2.61210
A3	2.56098	-0.00000	0.00000	-0.00112	-0.00113	2.55985
A4	2.71640	-0.00002	0.00000	0.00030	0.00030	2.71670
A5	2.61129	0.00000	0.00000	0.00112	0.00111	2.61240
A6	2.84214	0.00002	0.00000	-0.00003	-0.00003	2.84211
A7	2.71753	-0.00002	0.00000	-0.00102	-0.00103	2.71650
A8	2.84141	0.00002	0.00000	0.00084	0.00083	2.84224
A9	2.08547	-0.00000	0.00000	0.00001	0.00001	2.08547
A10	2.10734	0.00001	0.00000	-0.00005	-0.00005	2.10729
A11	2.08991	-0.00001	0.00000	0.00005	0.00004	2.08995
A12	2.08553	-0.00001	0.00000	-0.00006	-0.00006	2.08547
A13	2.08996	-0.00000	0.00000	-0.00002	-0.00002	2.08994
A14	2.10722	0.00001	0.00000	0.00008	0.00008	2.10731
A15	2.05604	0.00000	0.00000	0.00018	0.00018	2.05623
A16	1.92774	0.00000	0.00000	0.00007	0.00007	1.92781
A17	2.05654	-0.00001	0.00000	-0.00039	-0.00039	2.05615
A18	1.92796	0.00001	0.00000	-0.00021	-0.00021	1.92775
A19	2.01573	-0.00000	0.00000	-0.00008	-0.00008	2.01565
A20	1.92480	-0.00001	0.00000	-0.00009	-0.00009	1.92471
A21	1.88820	-0.00001	0.00000	-0.00002	-0.00002	1.88818
A22	1.89732	0.00000	0.00000	0.00004	0.00004	1.89736
A23	1.84475	0.00001	0.00000	0.00015	0.00015	1.84490
A24	1.88780	0.00000	0.00000	0.00003	0.00003	1.88783
A25	2.01566	-0.00000	0.00000	-0.00000	-0.00000	2.01566
A26	1.92485	-0.00001	0.00000	-0.00017	-0.00017	1.92468
A27	1.88820	-0.00001	0.00000	-0.00000	-0.00000	1.88820
A28	1.89732	0.00000	0.00000	0.00004	0.00004	1.89736
A29	1.84473	0.00001	0.00000	0.00017	0.00017	1.84490
A30	1.88785	0.00000	0.00000	-0.00003	-0.00003	1.88781
A31	2.90644	-0.00000	0.00000	0.00017	0.00017	2.90661
A32	3.12658	-0.00000	0.00000	-0.00016	-0.00016	3.12642
A33	2.90691	-0.00000	0.00000	-0.00038	-0.00038	2.90653
A34	3.12630	0.00000	0.00000	0.00016	0.00016	3.12645
A35	3.98378	0.00000	0.00000	0.00026	0.00026	3.98404
A36	3.98450	0.00001	0.00000	-0.00061	-0.00061	3.98390
A37	3.14546	-0.00000	0.00000	-0.00050	-0.00050	3.14496
A38	3.13969	0.00000	0.00000	0.00047	0.00047	3.14015
A39	3.14546	-0.00000	0.00000	-0.00050	-0.00050	3.14497
A40	3.13986	-0.00000	0.00000	0.00027	0.00027	3.14013
A41	4.01575	0.00001	0.00000	-0.00025	-0.00025	4.01550
A42	4.01481	0.00001	0.00000	0.00089	0.00089	4.01570
D1	0.00964	-0.00002	0.00000	-0.00963	-0.00963	0.00001
D2	-0.00614	0.00001	0.00000	0.00979	0.00978	0.00364

D3	-0.00415	0.00002	0.00000	0.01105	0.01105	0.00690
D4	0.00966	-0.00002	0.00000	-0.00964	-0.00964	0.00002
D5	-0.00420	-0.00002	0.00000	-0.01221	-0.01221	-0.01641
D6	-0.00416	0.00001	0.00000	0.01105	0.01105	0.00689
D7	-0.00065	0.00000	0.00000	0.00291	0.00291	0.00226
D8	3.10537	0.00000	0.00000	0.00318	0.00318	3.10855
D9	-0.00413	-0.00002	0.00000	-0.01226	-0.01226	-0.01639
D10	-0.00055	0.00000	0.00000	0.00279	0.00279	0.00224
D11	3.10561	0.00000	0.00000	0.00291	0.00291	3.10852
D12	0.00710	0.00000	0.00000	0.00050	0.00050	0.00760
D13	-3.10178	-0.00000	0.00000	0.00030	0.00030	-3.10148
D14	-3.10178	0.00000	0.00000	0.00031	0.00031	-3.10147
D15	0.07253	-0.00000	0.00000	0.00011	0.00011	0.07264
D16	2.51384	0.00000	0.00000	0.00047	0.00047	2.51430
D17	-0.66089	0.00000	0.00000	0.00066	0.00066	-0.66023
D18	-0.65984	0.00000	0.00000	-0.00061	-0.00061	-0.66045
D19	2.51488	-0.00000	0.00000	-0.00081	-0.00081	2.51407
D20	-1.15340	-0.00000	0.00000	-0.00087	-0.00087	-1.15427
D21	1.00583	-0.00000	0.00000	-0.00095	-0.00095	1.00487
D22	3.06729	-0.00001	0.00000	-0.00099	-0.00099	3.06630
D23	-1.15424	0.00000	0.00000	-0.00017	-0.00017	-1.15441
D24	1.00497	-0.00000	0.00000	-0.00025	-0.00025	1.00473
D25	3.06652	-0.00001	0.00000	-0.00039	-0.00039	3.06613

Item	Value	Threshold	Converged?
Maximum Force	0.000025	0.000450	YES
RMS Force	0.000010	0.000300	YES
Maximum Displacement	0.003816	0.001800	NO
RMS Displacement	0.000860	0.001200	YES

Predicted change in Energy=-6.750637D-07

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                     ---------------------------
                     ! Non-Optimized Parameters !
                     ! (Angstroms and Degrees)  !
--------------------------                     --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.2296         -DE/DX =    0.0                 !
! R2    R(1,3)                  1.3408         -DE/DX =    0.0                 !
! R3    R(2,4)                  1.3395         -DE/DX =    0.0                 !
! R4    R(3,5)                  1.2296         -DE/DX =    0.0                 !
! R5    R(4,6)                  1.2278         -DE/DX =    0.0                 !
! R6    R(5,7)                  1.3394         -DE/DX =    0.0                 !
! R7    R(6,8)                  1.3406         -DE/DX =    0.0                 !
! R8    R(7,9)                  1.2278         -DE/DX =    0.0                 !
! R9    R(8,10)                 1.2273         -DE/DX =    0.0                 !
! R10   R(9,11)                 1.3406         -DE/DX =    0.0                 !
! R11   R(10,12)                1.3901         -DE/DX =    0.0                 !
! R12   R(11,13)                1.2273         -DE/DX =    0.0                 !
! R13   R(12,14)                1.4251         -DE/DX =    0.0                 !
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! R14   R(12,15)             1.4252       -DE/DX =    0.0              !
! R15   R(13,14)             1.39         -DE/DX =    0.0              !
! R16   R(14,16)             1.4253       -DE/DX =    0.0              !
! R17   R(15,17)             1.4886       -DE/DX =    0.0              !
! R18   R(15,24)             1.0852       -DE/DX =    0.0              !
! R19   R(16,18)             1.4886       -DE/DX =    0.0              !
! R20   R(16,25)             1.0852       -DE/DX =    0.0              !
! R21   R(17,19)             1.0292       -DE/DX =    0.0              !
! R22   R(17,20)             1.0146       -DE/DX =    0.0              !
! R23   R(17,23)             1.0212       -DE/DX =    0.0              !
! R24   R(18,21)             1.0292       -DE/DX =    0.0              !
! R25   R(18,22)             1.0146       -DE/DX =    0.0              !
! R26   R(18,26)             1.0212       -DE/DX =    0.0              !
! A1    A(2,1,3)            146.6874       -DE/DX =    0.0              !
! A2    A(1,2,4)            149.6624       -DE/DX =    0.0              !
! A3    A(1,3,5)            146.6684       -DE/DX =    0.0              !
! A4    A(2,4,6)            155.6556       -DE/DX =    0.0              !
! A5    A(3,5,7)            149.6795       -DE/DX =    0.0              !
! A6    A(4,6,8)            162.8407       -DE/DX =    0.0              !
! A7    A(5,7,9)            155.6438       -DE/DX =    0.0              !
! A8    A(7,9,11)           162.8485       -DE/DX =    0.0              !
! A9    A(10,12,14)         119.4889       -DE/DX =    0.0              !
! A10   A(10,12,15)         120.7389       -DE/DX =    0.0              !
! A11   A(14,12,15)         119.7455       -DE/DX =    0.0              !
! A12   A(12,14,13)         119.4886       -DE/DX =    0.0              !
! A13   A(12,14,16)         119.7449       -DE/DX =    0.0              !
! A14   A(13,14,16)         120.7399       -DE/DX =    0.0              !
! A15   A(12,15,24)         117.8132       -DE/DX =    0.0              !
! A16   A(17,15,24)         110.4554       -DE/DX =    0.0              !
! A17   A(14,16,25)         117.8084       -DE/DX =    0.0              !
! A18   A(18,16,25)         110.4522       -DE/DX =    0.0              !
! A19   A(15,17,19)         115.488        -DE/DX =    0.0              !
! A20   A(15,17,20)         110.2777       -DE/DX =    0.0              !
! A21   A(15,17,23)         108.1848       -DE/DX =    0.0              !
! A22   A(19,17,20)         108.7105       -DE/DX =    0.0              !
! A23   A(19,17,23)         105.705        -DE/DX =    0.0              !
! A24   A(20,17,23)         108.1646       -DE/DX =    0.0              !
! A25   A(16,18,21)         115.4886       -DE/DX =    0.0              !
! A26   A(16,18,22)         110.2761       -DE/DX =    0.0              !
! A27   A(16,18,26)         108.186        -DE/DX =    0.0              !
! A28   A(21,18,22)         108.7109       -DE/DX =    0.0              !
! A29   A(21,18,26)         105.705        -DE/DX =    0.0              !
! A30   A(22,18,26)         108.1638       -DE/DX =    0.0              !
! A31   L(6,8,10,7,-1)      166.5364       -DE/DX =    0.0              !
! A32   L(8,10,12,7,-1)     179.1305       -DE/DX =    0.0              !
! A33   L(9,11,13,4,-1)     166.5318       -DE/DX =    0.0              !
! A34   L(11,13,14,4,-1)    179.1326       -DE/DX =    0.0              !
! A35   L(12,15,17,24,-1)   228.2686       -DE/DX =    0.0              !
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 ! A36   L(14,16,18,25,-1)    228.2606        -DE/DX =    0.0              !
 ! A37   L(6,8,10,7,-2)       180.1931        -DE/DX =    0.0              !
 ! A38   L(8,10,12,7,-2)      179.9175        -DE/DX =    0.0              !
 ! A39   L(9,11,13,4,-2)      180.1935        -DE/DX =    0.0              !
 ! A40   L(11,13,14,4,-2)     179.916         -DE/DX =    0.0              !
 ! A41   L(12,15,17,24,-2)    230.0713        -DE/DX =    0.0              !
 ! A42   L(14,16,18,25,-2)    230.0825        -DE/DX =    0.0              !
 ! D1    D(3,1,2,4)           0.0007        -DE/DX =    0.0              !
 ! D2    D(2,1,3,5)           0.2087        -DE/DX =    0.0              !
 ! D3    D(1,2,4,6)           0.3953        -DE/DX =    0.0              !
 ! D4    D(1,3,5,7)           0.001         -DE/DX =    0.0              !
 ! D5    D(2,4,6,8)           -0.94         -DE/DX =    0.0              !
 ! D6    D(3,5,7,9)           0.3948        -DE/DX =    0.0              !
 ! D7    D(4,6,12,14)          0.1294        -DE/DX =    0.0              !
 ! D8    D(4,6,12,15)         178.1069        -DE/DX =    0.0              !
 ! D9    D(5,7,9,11)          -0.9391        -DE/DX =    0.0              !
 ! D10   D(7,9,14,12)          0.1283        -DE/DX =    0.0              !
 ! D11   D(7,9,14,16)         178.1053        -DE/DX =    0.0              !
 ! D12   D(10,12,14,13)        0.4353        -DE/DX =    0.0              !
 ! D13   D(10,12,14,16)      -177.7018        -DE/DX =    0.0              !
 ! D14   D(15,12,14,13)      -177.7012        -DE/DX =    0.0              !
 ! D15   D(15,12,14,16)        4.1618        -DE/DX =    0.0              !
 ! D16   D(10,12,15,24)       144.059         -DE/DX =    0.0              !
 ! D17   D(14,12,15,24)       -37.8283        -DE/DX =    0.0              !
 ! D18   D(12,14,16,25)       -37.8412        -DE/DX =    0.0              !
 ! D19   D(13,14,16,25)       144.0456        -DE/DX =    0.0              !
 ! D20   D(24,15,17,19)       -66.1347        -DE/DX =    0.0              !
 ! D21   D(24,15,17,20)        57.575         -DE/DX =    0.0              !
 ! D22   D(24,15,17,23)       175.6861        -DE/DX =    0.0              !
 ! D23   D(25,16,18,21)       -66.143         -DE/DX =    0.0              !
 ! D24   D(25,16,18,22)        57.5665        -DE/DX =    0.0              !
 ! D25   D(25,16,18,26)       175.6766        -DE/DX =    0.0              !
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 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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 0.0
 (Enter /home/user/gauss16/g16/l9999.exe)

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 Electric dipole moment (input orientation):
 (Debye = 10**-18 statcoulomb cm , SI units = C m)
                 (au)          (Debye)        (10**-30 SI)
   Tot       0.453857D+01      0.115359D+02      0.384796D+02
   x        -0.453857D+01     -0.115359D+02     -0.384796D+02
   y         0.611372D-03      0.155395D-02      0.518343D-02
   z        -0.624446D-03     -0.158718D-02     -0.529428D-02
```

Supporting Information file

Dipole polarizability, Alpha (input orientation).
(esu units = cm**3 , SI units = C**2 m**2 J**-1)
Alpha(0;0):

	(au)	(10**-24 esu)	(10**-40 SI)
iso	0.300531D+03	0.445341D+02	0.495509D+02
aniso	0.338080D+03	0.500984D+02	0.557419D+02
xx	0.496115D+03	0.735166D+02	0.817983D+02
yx	0.244670D-01	0.362564D-02	0.403406D-02
yy	0.299090D+03	0.443205D+02	0.493132D+02
zx	0.483315D-01	0.716198D-02	0.796878D-02
zy	0.112360D+02	0.166500D+01	0.185256D+01
zz	0.106388D+03	0.157651D+02	0.175411D+02

Dipole orientation:

6	0.08795385	1.26487927	-7.58465225
6	0.21880793	3.20138206	-6.30709834
6	-0.08793859	-1.26266116	-7.58385009
6	0.30219547	4.32198599	-4.03917639
6	-0.21885559	-3.20067728	-6.30865166
6	0.31499255	4.40208612	-1.72037256
6	-0.30213809	-4.32033225	-4.04014179
6	0.27462932	3.74072194	0.72473929
6	-0.31498796	-4.40201151	-1.72144712
6	0.19292222	2.63223263	2.76041332
6	-0.27459131	-3.74050525	0.72372737
6	0.10275659	1.34212279	5.04669891
6	-0.19293000	-2.63290837	2.75981783
6	-0.10232624	-1.34308313	5.04641764
6	0.28926968	2.66775096	7.38387195
6	-0.28840012	-2.66922161	7.38303981
7	-0.09215239	5.43361529	7.04115735
7	0.09306089	-5.43494164	7.04002464
1	-1.88156857	5.97128942	6.50107415
1	0.37397002	6.37276943	8.64639840
1	1.88255022	-5.97239663	6.50001017
1	-0.37313308	-6.37438613	8.64507982
1	1.08109299	6.03326948	5.63111996
1	-0.82291909	1.98144184	8.96419907
1	0.82222818	-1.98298534	8.96441083
1	-1.07998474	-6.03441226	5.62972231

Electric dipole moment (dipole orientation):
(Debye = 10**-18 statcoulomb cm , SI units = C m)

	(au)	(Debye)	(10**-30 SI)
Tot	0.453857D+01	0.115359D+02	0.384796D+02

x	0.000000D+00	0.000000D+00	0.000000D+00
y	0.000000D+00	0.000000D+00	0.000000D+00
z	0.453857D+01	0.115359D+02	0.384796D+02

Dipole polarizability, Alpha (dipole orientation).
(esu units = cm**3 , SI units = C**2 m**2 J**-1)
Alpha(0;0):

	(au)	(10**-24 esu)	(10**-40 SI)
iso	0.300531D+03	0.445341D+02	0.495509D+02
aniso	0.338080D+03	0.500984D+02	0.557419D+02
xx	0.106391D+03	0.157656D+02	0.175416D+02
yx	0.112619D+02	0.166885D+01	0.185684D+01
yy	0.299087D+03	0.443201D+02	0.493127D+02
zx	0.679615D-02	0.100709D-02	0.112053D-02
zy	-0.525543D-01	-0.778774D-02	-0.866503D-02
zz	0.496115D+03	0.735166D+02	0.817983D+02

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Geom=AllCheck Guess=TCheck SCRF=Check GenChk RwB97XD/def2TZVP Freq\\ti
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Supporting Information file

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Supporting Information file

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The archive entry for this job was punched.

ONE THORN OF EXPERIENCE IS WORTH A WHOLE WILDERNESS OF
WARNING.... LOWELL - AMONG MY BOOKS
Job cpu time: 0 days 23 hours 54 minutes 25.6 seconds.
Elapsed time: 0 days 3 hours 59 minutes 7.2 seconds.
File lengths (MBytes): RWF= 847 Int= 0 D2E= 0 Chk= 30 Scr= 1
Normal termination of Gaussian 16 at Sat Sep 26 13:47:50 2026.