*Supplementary Information for*

# Programmable Regiodivergent Light-Driven Cyclisation of Acyclic 1,5-Dienes Unlocks Rigid Bicyclic Architectures

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# 1. Computational Details

## 1.1. General Information

Density functional theory (DFT) geometry optimizations were carried out using the hybrid meta-GGA M06-2X[1] functional in conjunction with Pople's 6-31+g(d,p) double-z basis set[2-6] and Grimme's zero-damped D3 empirical dispersion[7] correction term. Single-point energy corrections were applied using the double hybrid Pr2SCAN50[8] in conjunction with Aldrich's triple-z def2-TZVPPD basis set[9,10] and D4 dispersion correction[11]. Both optimizations and single-point energy calculations included the integral equation formalism variant of the polarizable continuum model (IEF-PCM), with the SMD solvation model, accounting for an implicit description of solvation by acetonitrile .[12] The choice of level of theory was informed based on recent benchmarking studies performed against DLPNO-CCSD(T)/CBS(3,4) energetics.[13] Similarly, for triplet state calculations, wavefunction stability analyses were performed to ensure that the SCF iterations converged to the lowest energy triplet state.[13] *Gaussian16* revision C.01 was employed for all DFT geometry optimizations.[14] *ORCA* version 6.0.0 was used to compute all single-point energies,[15] with the "tightscf" convergence criteria. An "ultrafine" pruned (99,590) grid for numerical integration of the exchange-correlation functional and its derivatives was implemented for all *Gaussian16* calculations, while the *ORCA6* calculations employed the "DEFGRID2" for numerical integration. *ORCA6* additionally implements the resolution of identity (RI) approximation.[16] Open-shell singlet structures located under the Broken-Symmetry formalism have been corrected using the Yamaguchi approximate spin-projection scheme [17], as implemented in *ORCA6*.

Conformational analysis was performed using the Global Optimizer (GOAT) algorithm[18] implemented in *ORCA6* with a GFN2-xTB semiempirical tight-binding Hamiltonian[19], followed by manual conformational augmentation. Vibrational frequency calculations were performed to verify that stationary points were either minima or first-order saddle points on the potential energy surface (PES) and to calculate thermal corrections to Gibbs free energy (G). The identity of the first-order saddle points were further verified using Intrinsic Reaction Coordinate (IRC) calculations.[20] The computed thermochemistry data were corrected following Grimme's quasi-harmonic (QHA)[21] model for entropy with a frequency cut-off value of 100.0 $cm^{-1}$ using the *GoodVibes* program[22] at 298.15 K (25 °C). Additionally, 1 M standard state concentrations were applied to all individual calculations to account for reactions in solution.[23] Unless otherwise stated, the G values of all the energy profiles correspond to the Boltzmann weighted G of all the conformers found in each step,[24] calculated by *GoodVibes*. Boltzmann weighted G ($G_{av}$) were calculated with *GoodVibes* as:

$$G_{av} = \sum_i G_i p_i$$

where $G_i$ is the relative Gibbs free energy of the corresponding conformers of a certain reaction step and $p_i$ is the probability of each conformer calculated as:

$$p_i = \frac{e^{-\frac{G_i}{RT}}}{\sum_i \left(e^{-\frac{G_i}{RT}}\right)}$$

Minimum energy crossing points (MECP) were located using the *MECPro* python package[25] interface with *Gaussian16*, and Gibbs free energy was estimated using the projected frequency keyword ("freq=projected").

Molecular graphics were generated using *PyMol*.[26]

Cartesian coordinates have been compiled using *GoodVibes*.

*Example G16 optimization input command line:*

```
# M06-2X 6-31+G(d,p) emp=gd3 scrf=(smd,solvent=acetonitrile) opt freq
```

NOTE 1: For locating first-order saddle points, the "opt=(TS,calcfc,noeigen)" was used instead.
NOTE 2: For open-shell biradicals the reference wavefunction was obtained in a separate calculation employing the "guess=mix stable=opt" additional keywords.

*Example ORCA6 single point energy input command line:*

```
! Pr2SCAN50 D4 tightscf def2-tzvppd def2-tzvppd/C SMD(acetonitrile)
```

NOTE: For open-shell biradicals the following keywords were also included.

```
%SCF BrokenSym 1,1
        APMethod 3
END
```

## 1.2. Reaction Mechanism: Thermochemical Summary

A full summary of the computed reaction pathways for N–Ac substrate **2f** (**$^1$A_Ac**) is shown in Figure S1 (Figure 6 in the manuscript) and the related pathways for N–Bn substrate **1g** (**$^1$A_Bn**) is shown in Figure S2. In all cases, the initial C–C bond formation is predicted to occur irreversibly, making the 6-*endo* and 5-*exo* cyclization transition structures regiodetermining.

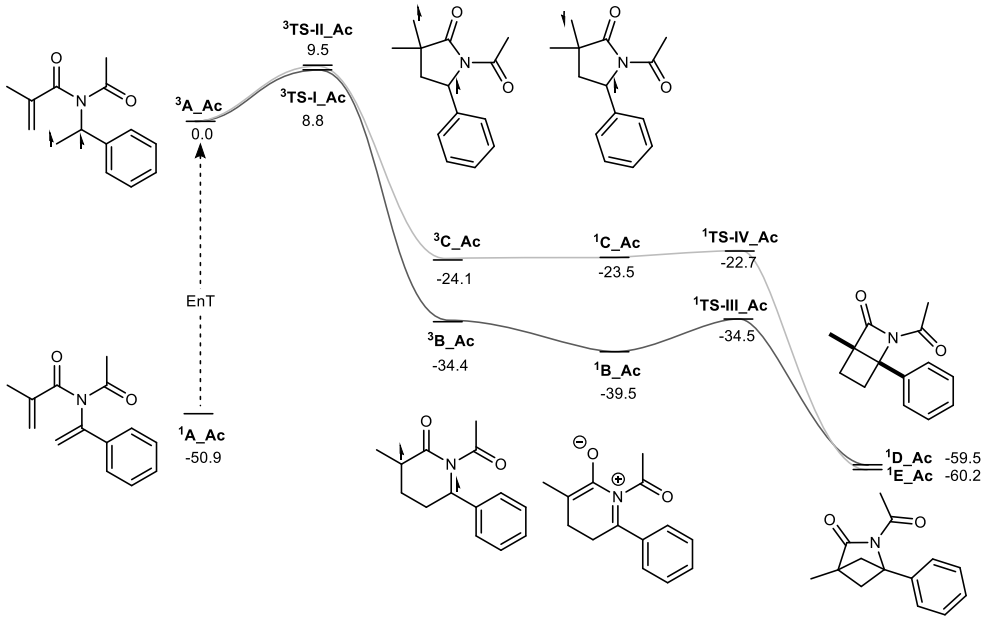



**Figure S1:** Computed potential energy surface of **$^1$A_Ac** (**2f**) cycloaddition at the Pr2SCAN50-D4/def2-TZVPPD,(SMD=MeCN)//M06-2X-D3/6-31+G(d,p),(SMD=MeCN) level of theory.

**Table S1:** Relative thermochemistry computed for **$^1$A_Ac** (**2f**) cycloaddition at the Pr2SCAN50-D4/def2-TZVPPD,(SMD=MeCN)//M06-2X-D3/6-31+G(d,p),(SMD=MeCN) level of theory.

| *Species* | *ΔE / kcal mol$^{-1}$* | *ΔZPE / kcal mol$^{-1}$* | *ΔH / kcal mol$^{-1}$* | *TΔS / kcal mol$^{-1}$* | *ΔG(298 K)_SPC / kcal mol$^{-1}$* |
|---|---|---|---|---|---|
| *$^1$A_Ac* | −54.8 | 2.9 | −52.4 | −1.5 | −50.9 |
| *$^3$A_Ac* | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| *$^3$TS-I_Ac* | 6.8 | 0.4 | 6.4 | −2.4 | 8.8 |
| *$^3$B_Ac* | −38.5 | 1.9 | −37.8 | −3.4 | −34.4 |
| *$^1$B_Ac* | −45.4 | 3.7 | −42.6 | −3.1 | −39.5 |
| *$^1$TS-III_Ac* | −39.7 | 2.5 | −38.2 | −3.7 | −34.5 |
| *$^1$D_Ac* | −67.1 | 4.5 | −63.8 | −4.3 | −59.5 |
| *$^3$TS-II_Ac* | 7.4 | 0.1 | 6.9 | −2.7 | 9.5 |
| *$^3$C_Ac* | −26.5 | 0.1 | −27.3 | −3.2 | −24.1 |
| *$^1$C_Ac* | −27.6 | 1.7 | −26.6 | −3.1 | −23.5 |
| *$^1$TS-IV_Ac* | −28.1 | 1.9 | −27.4 | −4.7 | −22.7 |
| *$^1$E_Ac* | −68.6 | 4.9 | −65.1 | −4.9 | −60.2 |

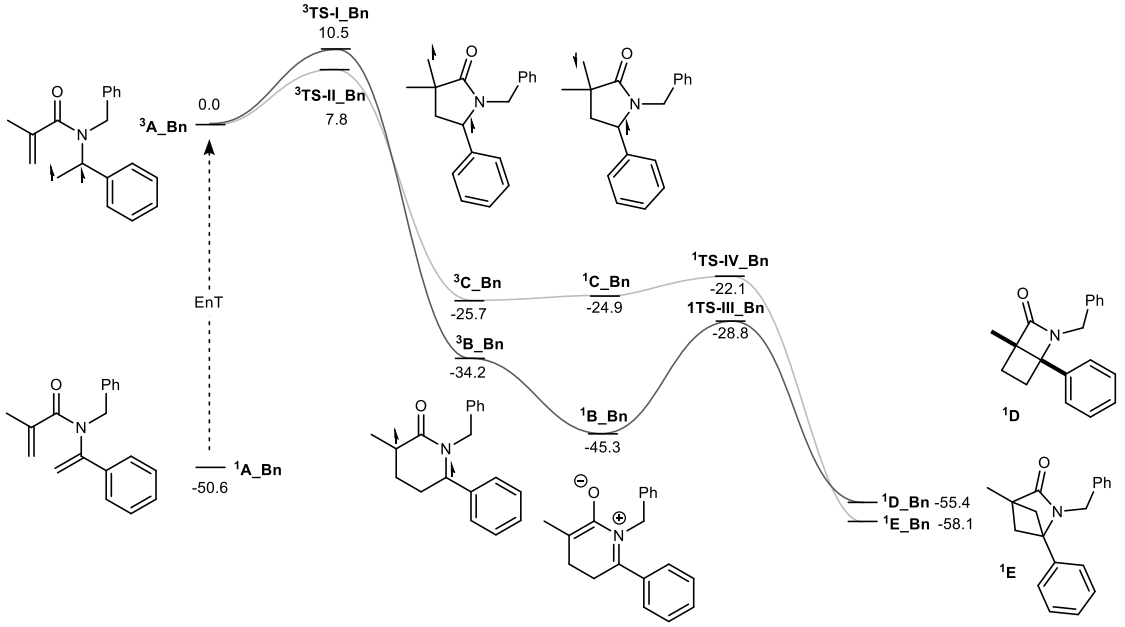



**Figure S2:** Computed potential energy surface of $^{1}$**A_Bn** (**1g**) cycloaddition at the Pr2SCAN50-D4/def2-TZVPPD,(SMD=MeCN)//M06-2X-D3/6-31+G(d,p),(SMD=MeCN) level of theory.

**Table S2:** Relative thermochemistry computed for $^{1}$**A_Bn** (**1g**) cycloaddition at the Pr2SCAN50-D4/def2-TZVPPD,(SMD=MeCN)//M06-2X-D3/6-31+G(d,p),(SMD=MeCN) level of theory.

| *Species* | *ΔE / kcal mol$^{-1}$* | *ΔZPE / kcal mol$^{-1}$* | *ΔH / kcal mol$^{-1}$* | *TΔS / kcal mol$^{-1}$* | *ΔG(298 K)_SPC / kcal mol$^{-1}$* |
|---|---|---|---|---|---|
| *$^{1}$A_Bn* | −54.3 | 2.8 | −51.9 | −1.3 | −50.6 |
| *$^{3}$A_Bn* | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| *$^{3}$TS-I_Bn* | 9.1 | 0.4 | 8.8 | −1.8 | 10.5 |
| *$^{3}$B_Bn* | −37.2 | 1.8 | −36.4 | −2.2 | −34.2 |
| *$^{1}$B_Bn* | −50.7 | 4.0 | −47.7 | −2.4 | −45.3 |
| *$^{1}$TS-III_Bn* | −32.8 | 2.2 | −31.5 | −2.8 | −28.8 |
| *$^{1}$D_Bn* | −62.0 | 4.3 | −58.8 | −3.4 | −55.4 |
| *$^{3}$TS-II_Bn* | 6.8 | 0.1 | 6.3 | −1.6 | 7.8 |
| *$^{3}$C_Bn* | −28.4 | 1.9 | −27.2 | −1.5 | −25.7 |
| *$^{1}$C_Bn* | −28.1 | 1.8 | −26.9 | −2.0 | −24.9 |
| *$^{1}$TS-IV_Bn* | −26.2 | 1.7 | −25.6 | −3.5 | −22.1 |
| *$^{1}$E_Bn* | −65.4 | 4.6 | −62.2 | −4.2 | −58.1 |

Minimum Energy Crossing Point (MECP) structures for N–Ac substrates closely resemble the corresponding triplet state minima **$^3$B** and **$^3$C** , such that minimal structural distortion is required to approach these geometries before ISC leads to the following singlet minima **$^1$B** and **$^1$C**. Computed values of ΔΔG‡ obtained from competing 6-*endo* vs. 5-*exo* TSs are highly correlated with experimental selectivities.

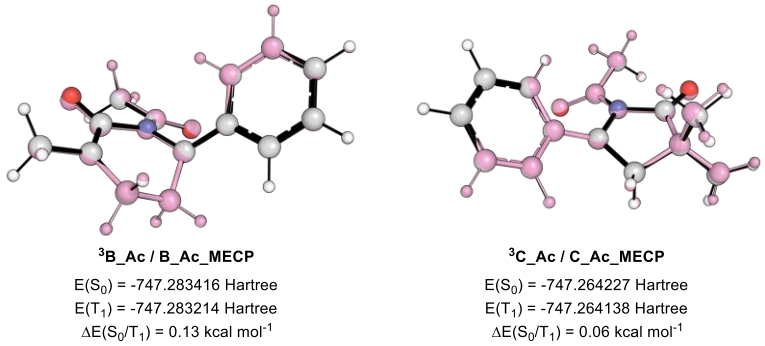
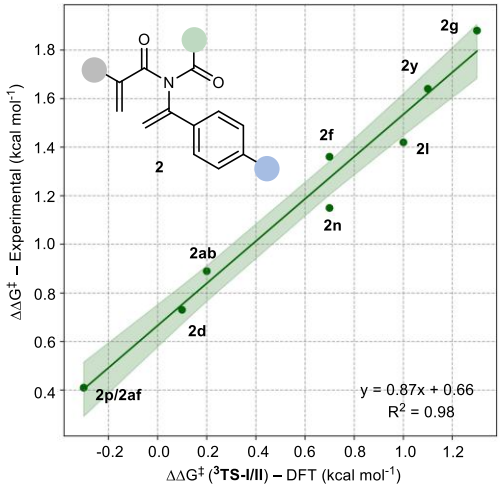



**Figure S3:** Overlay of MECP structures (grey) with their corresponding $T_1$ local minimum (pink), together with the electronic energies of the MECP computed at the Pr2SCAN50-D4/def2-TZVPPD,(SMD=MeCN)//M06-2X-D3/6-31+G(d,p),(SMD=MeCN) level of theory.




| *Substrate* | *Exp. Ratio (6:5)* | *ΔΔG‡ (exp) / kcal mol$^{-1}$* | *ΔΔG‡ (DFT)$^{(a)}$ / kcal mol$^{-1}$* |
|---|---|---|---|
| ***2g*** | 24:1 | 1.9 | 1.3 |
| ***2y*** | 16:1 | 1.6 | 1.1 |
| ***2l*** | 11:1 | 1.4 | 1.0 |
| ***2f*** | 10:1 | 1.4 | 0.7 |
| ***2n*** | 7:1 | 1.2 | 0.7 |
| ***2ab*** | 4.5:1 | 0.9 | 0.2 |
| ***2d*** | 3.4:1 | 0.7 | 0.1 |
| ***2p*** | 2:1 | 0.4 | -0.3 |
| ***2af*** | 2:1 | 0.4 | -0.3 |

**Figure S4:** Correlation plot between experimental determined ΔΔG‡ obtained from isolated **6** and **5** product ratios, and DFT computed ΔΔG‡ at the Pr2SCAN50-D4/def2-TZVPPD,(SMD=MeCN)//M06-2X-D3/6-31+G(d,p),(SMD=MeCN) level of theory. [(a)] Only the lowest energy conformer was used.

### 1.3. Dynamic vertical triplet energy analysis

Computation of dynamic vertical triplet energies (DvTE)[27] was undertaken using a total of 50 quasi-classical initiated *ab-initio* molecular dynamics trajectories (298 K, 1 fs timestep, 500 fs simulation length) using the MILO package[28] at the M06-2X/MIDI![29] basis set and employing the SMD solvation model for acetonitrile (**Figure S5**). Vertical $S_0$-$T_1$ snapshots were collected at the M06-2X/6-31G(d) (SMD=MeCN) level of theory every 8$^{th}$ frame, leading to a total of 3125 datapoints. The resulting triplet energy of 60.8 kcal/mol was determined using the previously empirically determined 0.8% population of the fitted gaussian distribution (m = 97.5, s = 7.8). Analysis of the spin density of the out of equilibrium structures with the lowest $S_0$-$T_1$ gap revealed that the spin density is localized on the styrene chromophore, consistent with Stern-Volmer quenching studies.

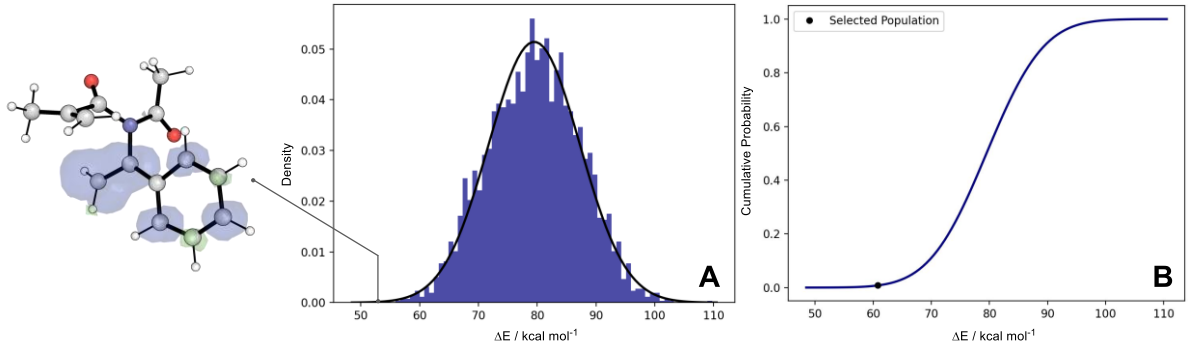



**Figure S5:** Dynamic vertical triplet energy (DvTE) analysis performed on substrate **2f** (**$^1$A_Ac**) computed at the M06-2X/6-31G(d)//M06-2X/MIDI! level of theory. (**A**) Fitted gaussian distribution together with $T_1$ spin density plot of the frame with the lowest $S_0$-$T_1$ gap. (**B**) Cumulative distribution plot of the fitted gaussian distribution with the highlighted 0.8% population.

## 1.4. Thermochemistry

**Table S3:** Compiled thermochemical data in atomic units for structures computed at the Pr2SCAN50-D4/def2-TZVPPD,(SMD=MeCN)//M06-2X-D3/6-31+G(d,p),(SMD=MeCN) level of theory. E_SPC = energy obtained in the single-point energy corrections, E = energy obtained in the geometry optimisations, ZPE = zero-point energy, H_SPC = enthalpy corrected with ESPC, T·S = temperature times entropy, G(T) = Gibbs free energy, $\nu_{imag}$ = imaginary frequencies

**Legend:**

| *Structure* | *E_SPC* | *E* | *ZPE* | *H* | *T·S* | *G(T)_SPC* | $\nu_{imag}$ |
|---|---|---|---|---|---|---|---|
| *1A_Ac_conf_1* | -747.309383 | -747.445639 | 0.251627 | -747.039863 | 0.057210 | -747.097073 | |
| *1A_Ac_conf_10* | -747.308830 | -747.445343 | 0.251608 | -747.039182 | 0.057896 | -747.097078 | |
| *1A_Ac_conf_11* | -747.309110 | -747.444933 | 0.251670 | -747.039443 | 0.057744 | -747.097187 | |
| *1A_Ac_conf_12* | -747.307724 | -747.443653 | 0.252233 | -747.037728 | 0.057154 | -747.094881 | |
| *1A_Ac_conf_13* | -747.309088 | -747.444927 | 0.251689 | -747.039418 | 0.057681 | -747.097099 | |
| *1A_Ac_conf_2* | -747.307713 | -747.443711 | 0.251532 | -747.038118 | 0.057767 | -747.095885 | |
| *1A_Ac_conf_3* | -747.310039 | -747.446079 | 0.251837 | -747.040287 | 0.057473 | -747.097760 | |
| *1A_Ac_conf_4* | -747.306773 | -747.443695 | 0.251749 | -747.037150 | 0.057254 | -747.094404 | |
| *1A_Ac_conf_5* | -747.309471 | -747.445509 | 0.251752 | -747.039731 | 0.057753 | -747.097483 | |
| *1A_Ac_conf_6* | -747.309473 | -747.445509 | 0.251752 | -747.039732 | 0.057751 | -747.097483 | |
| *1A_Ac_conf_7* | -747.308482 | -747.444523 | 0.251235 | -747.039039 | 0.058339 | -747.097377 | |
| *1A_Ac_conf_8* | -747.307684 | -747.444184 | 0.251679 | -747.038001 | 0.057742 | -747.095742 | |
| *1A_Bn_conf_1* | -864.938498 | -865.117086 | 0.322073 | -864.595938 | 0.062828 | -864.658766 | |
| *1A_Bn_conf_10* | -864.935728 | -865.114590 | 0.321996 | -864.593251 | 0.063037 | -864.656289 | |
| *1A_Bn_conf_11* | -864.934476 | -865.111966 | 0.321764 | -864.591948 | 0.063992 | -864.655940 | |
| *1A_Bn_conf_12* | -864.935815 | -865.115038 | 0.322419 | -864.593035 | 0.062464 | -864.655500 | |
| *1A_Bn_conf_15* | -864.934939 | -865.113481 | 0.322504 | -864.592168 | 0.062317 | -864.654485 | |
| *1A_Bn_conf_16* | -864.933743 | -865.111282 | 0.321699 | -864.591320 | 0.063677 | -864.654996 | |
| *1A_Bn_conf_2* | -864.938121 | -865.116456 | 0.322145 | -864.595576 | 0.062732 | -864.658308 | |
| *1A_Bn_conf_3* | -864.937994 | -865.116162 | 0.321998 | -864.595443 | 0.063328 | -864.658771 | |
| *1A_Bn_conf_4* | -864.933043 | -865.111694 | 0.321868 | -864.590609 | 0.063163 | -864.653772 | |
| *1A_Bn_conf_5* | -864.934181 | -865.111630 | 0.322030 | -864.591491 | 0.063340 | -864.654832 | |
| *1A_Bn_conf_6* | -864.936166 | -865.114182 | 0.321881 | -864.593730 | 0.063164 | -864.656894 | |
| *1A_Bn_conf_7* | -864.934461 | -865.112754 | 0.322162 | -864.591869 | 0.062809 | -864.654678 | |
| *1A_Bn_conf_8* | -864.935824 | -865.114688 | 0.321880 | -864.593472 | 0.062900 | -864.656372 | |
| *1A_Bn_conf_9* | -864.937532 | -865.116425 | 0.322212 | -864.594870 | 0.062981 | -864.657851 | |
| *1B_Ac-CS_conf_1* | -747.293936 | -747.426128 | 0.252807 | -747.023743 | 0.056424 | -747.080167 | |
| *1B_Ac-CS_conf_2* | -747.294735 | -747.426835 | 0.253240 | -747.024268 | 0.056057 | -747.080325 | |
| *1B_Ac-CS_conf_3* | -747.293389 | -747.425305 | 0.252869 | -747.023163 | 0.056355 | -747.079517 | |
| *1B_Ac-OS_conf_1* | -747.280488 | -747.410811 | 0.251813 | -747.011286 | 0.056520 | -747.067805 | |
| *1B_Ac-OS_conf_2* | -747.283915 | -747.414518 | 0.252271 | -747.014452 | 0.055985 | -747.070437 | |
| *1B_Ac-OS_conf_3* | -747.281321 | -747.412720 | 0.251834 | -747.012143 | 0.056383 | -747.068527 | |
| *1B_Ac-OS_conf_4* | -747.278773 | -747.409964 | 0.251515 | -747.009810 | 0.056679 | -747.066489 | |
| *1B_Bn_CS_conf_1* | -864.932128 | -865.106608 | 0.323810 | -864.588550 | 0.061742 | -864.650291 | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| *1B_Bn_CS_conf_2* | -864.930632 | -865.105940 | 0.323954 | -864.586994 | 0.061457 | -864.648452 | |
| *1B_Bn_CS_conf_3* | -864.932683 | -865.107515 | 0.323891 | -864.589167 | 0.061023 | -864.650190 | |
| *1B_Bn_CS_conf_4* | -864.931931 | -865.107089 | 0.323790 | -864.588397 | 0.061376 | -864.649774 | |
| *1B_Bn_CS_conf_5* | -864.931927 | -865.107089 | 0.323788 | -864.588394 | 0.061384 | -864.649778 | |
| *1B_Bn_CS_conf_6* | -864.932280 | -865.107337 | 0.324406 | -864.588370 | 0.060915 | -864.649285 | |
| *1B_Bn_OSS_conf_3* | -864.930781 | -865.107515 | 0.323891 | -864.587266 | 0.061021 | -864.648287 | |
| *1C_Ac_conf_1* | -747.265181 | -747.394196 | 0.249788 | -746.997678 | 0.056695 | -747.054373 | |
| *1C_Ac_conf_2* | -747.261906 | -747.390940 | 0.249580 | -746.994458 | 0.057196 | -747.051654 | |
| *1C_Ac_conf_3* | -747.262895 | -747.391620 | 0.249697 | -746.995473 | 0.056725 | -747.052198 | |
| *1C_Ac_conf_4* | -747.266269 | -747.394943 | 0.249835 | -746.998810 | 0.056382 | -747.055192 | |
| *1C_Bn_OSS_conf_1* | -864.893320 | -865.064764 | 0.320170 | -864.552786 | 0.062599 | -864.615384 | |
| *1C_Bn_OSS_conf_2* | -864.896415 | -865.067731 | 0.320453 | -864.555705 | 0.062162 | -864.617867 | |
| *1C_Bn_OSS_conf_3* | -864.896341 | -865.068386 | 0.320535 | -864.555582 | 0.062015 | -864.617597 | |
| *1C_Bn_OSS_conf_4* | -864.896159 | -865.067551 | 0.320549 | -864.555395 | 0.061970 | -864.617365 | |
| *1C_Bn_OSS_conf_5* | -864.893178 | -865.064630 | 0.320222 | -864.552574 | 0.062677 | -864.615251 | |
| *1C_Bn_OSS_conf_6* | -864.896124 | -865.067813 | 0.320489 | -864.555342 | 0.062317 | -864.617658 | |
| *1D_Ac_conf_1* | -747.328846 | -747.460965 | 0.254298 | -747.057712 | 0.055220 | -747.112932 | |
| *1D_Ac_conf_2* | -747.325617 | -747.458018 | 0.254233 | -747.054525 | 0.055255 | -747.109781 | |
| *1D_Bn_conf_1* | -864.950461 | -865.124266 | 0.324431 | -864.606627 | 0.060647 | -864.667274 | |
| *1D_Bn_conf_2* | -864.948995 | -865.123170 | 0.324407 | -864.605130 | 0.061107 | -864.666236 | |
| *1E_Ac_conf_1* | -747.329926 | -747.465815 | 0.254503 | -747.058465 | 0.055914 | -747.114379 | |
| *1E_Ac_conf_2* | -747.332811 | -747.468476 | 0.254245 | -747.061362 | 0.056594 | -747.117956 | |
| *1E_Bn_conf_1* | -864.955644 | -865.129882 | 0.324801 | -864.611904 | 0.059570 | -864.671473 | |
| *1E_Bn_conf_2* | -864.955282 | -865.129765 | 0.325104 | -864.611276 | 0.059479 | -864.670755 | |
| *1F_Ac_conf_1* | -747.331135 | -747.462956 | 0.254951 | -747.059777 | 0.054354 | -747.114131 | |
| *1F_Ac_conf_2* | -747.326166 | -747.458742 | 0.255186 | -747.054822 | 0.053643 | -747.108465 | |
| *1F_Bn_conf_1* | -864.955644 | -865.129882 | 0.324801 | -864.611904 | 0.059570 | -864.671473 | |
| *1F_Bn_conf_2* | -864.955282 | -865.129765 | 0.325104 | -864.611276 | 0.059479 | -864.670755 | |
| *1TS-III_Ac_conf_1* | -747.287553 | -747.416985 | 0.253079 | -747.018073 | 0.054281 | -747.072354 | -216.11 |
| *1TS-III_Ac_conf_2* | -747.281778 | -747.401930 | 0.251193 | -747.013523 | 0.055964 | -747.069487 | -623.92 |
| *1TS-III_Bn_conf_1* | -864.884564 | -865.056158 | 0.321788 | -864.543505 | 0.060801 | -864.604306 | -235.14 |
| *1TS-III_Bn_conf_2* | -864.903833 | -865.064657 | 0.321136 | -864.563002 | 0.061757 | -864.624759 | -608.10 |
| *1TS-III_Bn_conf_3* | -864.903041 | -865.063924 | 0.321150 | -864.562252 | 0.061786 | -864.624038 | -646.47 |
| *1TS-IV_Ac_conf_1* | -747.285126 | -747.404927 | 0.251079 | -747.016901 | 0.056198 | -747.073099 | -629.91 |
| *1TS-IV_Ac_conf_2* | -747.281778 | -747.401930 | 0.251193 | -747.013523 | 0.055964 | -747.069487 | -623.92 |
| *1TS-IV_Bn_conf_1* | -864.884564 | -865.056158 | 0.321788 | -864.543505 | 0.060801 | -864.604306 | -235.14 |
| *1TS-IV_Bn_conf_2* | -864.903833 | -865.064657 | 0.321136 | -864.563002 | 0.061757 | -864.624759 | -608.10 |
| *1TS-IV_Bn_conf_3* | -864.903041 | -865.063924 | 0.321150 | -864.562252 | 0.061786 | -864.624038 | -646.47 |
| *1TS-V_Ac_conf_1* | -747.266568 | -747.385165 | 0.250132 | -746.999685 | 0.054632 | -747.054317 | -570.65 |
| *1TS-V_Bn_conf_1* | -864.892512 | -865.054165 | 0.320851 | -864.552412 | 0.060025 | -864.612436 | -680.81 |
| *1TS-V_Bn_conf_2* | -864.893432 | -865.054362 | 0.320285 | -864.553662 | 0.060624 | -864.614286 | -628.57 |
| *1TS-V_Bn_conf_3* | -864.890238 | -865.051554 | 0.320025 | -864.550611 | 0.061263 | -864.611874 | -639.16 |
| *3A_Ac_conf_10* | -747.221247 | -747.353832 | 0.247140 | -746.955371 | 0.059988 | -747.015359 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| *3A_Ac_conf_11* | -747.221475 | -747.353939 | 0.247238 | -746.955526 | 0.059993 | -747.015519 |
| *3A_Ac_conf_12* | -747.221446 | -747.354064 | 0.247575 | -746.955316 | 0.059522 | -747.014838 |
| *3A_Ac_conf_13* | -747.221474 | -747.353939 | 0.247237 | -746.955525 | 0.059994 | -747.015519 |
| *3A_Ac_conf_2* | -747.222290 | -747.356181 | 0.247586 | -746.956222 | 0.059150 | -747.015372 |
| *3A_Ac_conf_3* | -747.223072 | -747.356198 | 0.247370 | -746.957106 | 0.059544 | -747.016651 |
| *3A_Ac_conf_5* | -747.221195 | -747.353947 | 0.247263 | -746.955244 | 0.059915 | -747.015159 |
| *3A_Ac_conf_6* | -747.221192 | -747.353947 | 0.247262 | -746.955242 | 0.059913 | -747.015155 |
| *3A_Ac_conf_7* | -747.221737 | -747.354297 | 0.246782 | -746.956030 | 0.060611 | -747.016641 |
| *3A_Ac_conf_8* | -747.220888 | -747.353776 | 0.246755 | -746.955174 | 0.060750 | -747.015924 |
| *3A_Ac_conf_9* | -747.221737 | -747.354297 | 0.246782 | -746.956030 | 0.060611 | -747.016641 |
| *3A_Bn_conf_1* | -864.852232 | -865.027438 | 0.317519 | -864.513456 | 0.065299 | -864.578754 |
| *3A_Bn_conf_10* | -864.846912 | -865.023439 | 0.317823 | -864.508026 | 0.064732 | -864.572758 |
| *3A_Bn_conf_11* | -864.846938 | -865.021651 | 0.317417 | -864.508093 | 0.065840 | -864.573933 |
| *3A_Bn_conf_12* | -864.850708 | -865.026878 | 0.317630 | -864.511879 | 0.065000 | -864.576879 |
| *3A_Bn_conf_13* | -864.848924 | -865.025528 | 0.317583 | -864.510097 | 0.066611 | -864.576708 |
| *3A_Bn_conf_14* | -864.848624 | -865.025313 | 0.317656 | -864.509747 | 0.065436 | -864.575183 |
| *3A_Bn_conf_15* | -864.847290 | -865.023327 | 0.317788 | -864.508418 | 0.064811 | -864.573229 |
| *3A_Bn_conf_16* | -864.847048 | -865.021653 | 0.317375 | -864.508309 | 0.065696 | -864.574005 |
| *3A_Bn_conf_2* | -864.850703 | -865.026744 | 0.317844 | -864.511760 | 0.064989 | -864.576748 |
| *3A_Bn_conf_3* | -864.850905 | -865.026750 | 0.317581 | -864.512056 | 0.065547 | -864.577602 |
| *3A_Bn_conf_4* | -864.846483 | -865.022072 | 0.317649 | -864.507668 | 0.064944 | -864.572612 |
| *3A_Bn_conf_5* | -864.847580 | -865.021662 | 0.317217 | -864.508922 | 0.065947 | -864.574869 |
| *3A_Bn_conf_6* | -864.849002 | -865.024844 | 0.317587 | -864.510263 | 0.064989 | -864.575251 |
| *3A_Bn_conf_7* | -864.846418 | -865.022301 | 0.317813 | -864.507473 | 0.064982 | -864.572455 |
| *3A_Bn_conf_8* | -864.848881 | -865.025510 | 0.317740 | -864.509996 | 0.065121 | -864.575117 |
| *3B_Ac_conf_1* | -747.279295 | -747.410690 | 0.252022 | -747.010031 | 0.057238 | -747.067269 |
| *3B_Ac_conf_2* | -747.283289 | -747.414516 | 0.252419 | -747.013758 | 0.056868 | -747.070626 |
| *3B_Ac_conf_3* | -747.281021 | -747.412818 | 0.252048 | -747.011737 | 0.057130 | -747.068867 |
| *3B_Ac_conf_4* | -747.278117 | -747.409845 | 0.251583 | -747.009115 | 0.057608 | -747.066723 |
| *3B_Ac_MECP* | -747.283214 | -747.414424 | 0.249859 | -747.016496 | 0.056385 | -747.072881 |
| *3B_Bn_conf_1* | -864.905554 | -865.078982 | 0.322246 | -864.563283 | 0.063298 | -864.626581 |
| *3B_Bn_conf_2* | -864.902908 | -865.076227 | 0.322605 | -864.560399 | 0.062897 | -864.623296 |
| *3B_Bn_conf_3* | -864.906038 | -865.079020 | 0.322130 | -864.563863 | 0.063188 | -864.627050 |
| *3B_Bn_conf_4* | -864.910871 | -865.084117 | 0.322450 | -864.568537 | 0.062957 | -864.631493 |
| *3B_Bn_conf_5* | -864.911328 | -865.084326 | 0.322500 | -864.568972 | 0.062785 | -864.631757 |
| *3B_Bn_conf_6* | -864.909935 | -865.083245 | 0.322766 | -864.567450 | 0.062488 | -864.629938 |
| *3C_Ac_conf_1* | -747.264447 | -747.393919 | 0.249736 | -746.996948 | 0.057835 | -747.054783 |
| *3C_Ac_conf_2* | -747.261162 | -747.390634 | 0.249680 | -746.993663 | 0.058072 | -747.051735 |
| *3C_Ac_conf_3* | -747.262160 | -747.391375 | 0.249718 | -746.994704 | 0.057812 | -747.052516 |
| *3C_Ac_conf_4* | -747.265354 | -747.394578 | 0.249861 | -746.997865 | 0.057426 | -747.055291 |
| *3C_Ac_MECP* | -747.264138 | -747.393643 | 0.247231 | -746.999459 | 0.057170 | -747.056629 |
| *3C_Bn_conf_1* | -864.893735 | -865.065117 | 0.320257 | -864.553153 | 0.063511 | -864.616664 |
| *3C_Bn_conf_2* | -864.896958 | -865.068139 | 0.320540 | -864.556193 | 0.063091 | -864.619285 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| *3C_Bn_conf_3* | -864.896914 | -865.068914 | 0.320661 | -864.556081 | 0.062943 | -864.619025 | |
| *3C_Bn_conf_4* | -864.896311 | -865.067641 | 0.320588 | -864.555509 | 0.063034 | -864.618543 | |
| *3C_Bn_conf_5* | -864.892988 | -865.064621 | 0.320362 | -864.552296 | 0.063541 | -864.615837 | |
| *3C_Bn_conf_6* | -864.896235 | -865.067865 | 0.320639 | -864.555404 | 0.063034 | -864.618439 | |
| *3TS-I_2ab_conf_1* | -1054.764961 | -1054.929854 | 0.365608 | -1054.373782 | 0.073989 | -1054.447772 | -458.72 |
| *3TS-I_2af_conf_1* | -707.913933 | -708.040417 | 0.220609 | -707.677338 | 0.054464 | -707.731802 | -433.29 |
| *3TS-I_2d_conf_1* | -1084.158613 | -1084.299047 | 0.252115 | -1083.885054 | 0.066498 | -1083.951552 | -452.65 |
| *3TS-I_2g_conf_1* | -861.685369 | -861.828364 | 0.279517 | -861.385524 | 0.063511 | -861.449035 | -450.21 |
| *3TS-I_2l_conf_1* | -846.420813 | -846.553931 | 0.239476 | -846.162746 | 0.060092 | -846.222838 | -454.50 |
| *3TS-I_2n_conf_1* | -1206.684692 | -1206.912860 | 0.238213 | -1206.427507 | 0.061212 | -1206.488719 | -455.86 |
| *3TS-I_2p_conf_1* | -839.408805 | -839.565257 | 0.246342 | -839.142921 | 0.062179 | -839.205100 | -451.56 |
| *3TS-I_2y_conf_1* | -1128.504015 | -1128.705302 | 0.335546 | -1128.143948 | 0.072888 | -1128.216836 | -452.32 |
| *3TS-I_Ac_conf_1* | -747.211367 | -747.342546 | 0.247672 | -746.946027 | 0.057968 | -747.003995 | -453.19 |
| *3TS-I_Ac_conf_2* | -747.209178 | -747.340486 | 0.247410 | -746.944004 | 0.058238 | -747.002242 | -461.74 |
| *3TS-I_Bn_conf_1* | -864.836325 | -865.008841 | 0.317867 | -864.498211 | 0.063299 | -864.561510 | -551.91 |
| *3TS-I_Bn_conf_2* | -864.832403 | -865.005149 | 0.318063 | -864.494224 | 0.063058 | -864.557282 | -577.29 |
| *3TS-I_Bn_conf_3* | -864.835542 | -865.008071 | 0.317935 | -864.497364 | 0.063502 | -864.560866 | -560.84 |
| *3TS-I_Bn_conf_4* | -864.837873 | -865.010101 | 0.318645 | -864.499357 | 0.062388 | -864.561745 | -149.60 |
| *3TS-II_2ab_conf_1* | -1054.764882 | -1054.927729 | 0.365511 | -1054.373873 | 0.073568 | -1054.447441 | -631.39 |
| *3TS-II_2af_conf_1* | -707.914493 | -708.039911 | 0.220485 | -707.678033 | 0.054366 | -707.732398 | -617.82 |
| *3TS-II_2d_conf_1* | -1084.158515 | -1084.297699 | 0.251894 | -1083.885257 | 0.066105 | -1083.951362 | -612.99 |
| *3TS-II_2g_conf_1* | -861.683333 | -861.825000 | 0.279090 | -861.383973 | 0.063106 | -861.447079 | -626.53 |
| *3TS-II_2l_conf_1* | -846.419443 | -846.551326 | 0.239216 | -846.161707 | 0.059594 | -846.221301 | -624.29 |
| *3TS-II_2n_conf_1* | -1206.683862 | -1206.910723 | 0.237990 | -1206.426986 | 0.060658 | -1206.487644 | -618.70 |
| *3TS-II_2p_conf_1* | -839.409554 | -839.564680 | 0.246176 | -839.143925 | 0.061610 | -839.205535 | -601.76 |
| *3TS-II_2y_conf_1* | -1128.502252 | -1128.701799 | 0.335083 | -1128.142616 | 0.072596 | -1128.215212 | -631.03 |
| *3TS-II_Ac_conf_1* | -747.210271 | -747.340148 | 0.247315 | -746.945333 | 0.057590 | -747.002923 | -623.79 |
| *3TS-II_Ac_conf_2* | -747.207359 | -747.337248 | 0.247000 | -746.942651 | 0.057808 | -747.000459 | -620.53 |
| *3TS-II_Ac_conf_3* | -747.207304 | -747.337826 | 0.247451 | -746.942337 | 0.057303 | -746.999641 | -646.14 |
| *3TS-II_Ac_conf_4* | -747.204385 | -747.334950 | 0.247145 | -746.939599 | 0.057654 | -746.997253 | -638.93 |
| *3TS-II_Bn_conf_1* | -864.840757 | -865.012827 | 0.317587 | -864.502851 | 0.063453 | -864.566303 | -595.64 |
| *3TS-II_Bn_conf_2* | -864.840473 | -865.012815 | 0.317813 | -864.502475 | 0.063104 | -864.565579 | -593.81 |
| *3TS-II_Bn_conf_4* | -864.839297 | -865.011714 | 0.318035 | -864.501161 | 0.062836 | -864.563997 | -598.37 |
| *3TS-II_Bn_conf_5* | -864.839639 | -865.012490 | 0.318091 | -864.501518 | 0.062710 | -864.564227 | -587.40 |
| *3TS-II_Bn_conf_6* | -864.837955 | -865.010652 | 0.317884 | -864.499928 | 0.063089 | -864.563016 | -616.89 |

## 1.5. XYZ Coordinates

32
1A_Ac_conf_1 Eopt -747.445639
C -0.521532 2.117739 1.770946
H -1.226253 1.470503 2.285736
H -0.005026 2.871012 2.360257
C -0.301827 2.012688 0.457531
C -1.124289 1.057910 -0.355356
O -1.612752 1.400335 -1.415529
N -1.308170 -0.241574 0.164408
C -0.225318 -0.828033 0.918514
C -0.462462 -1.419339 2.089000
H -1.459039 -1.430803 2.518797
H 0.335154 -1.925391 2.622670
C 0.644244 2.877087 -0.324349
H 1.151328 3.582280 0.337369
H 1.398251 2.259627 -0.827679
H 0.108793 3.434640 -1.098655
C 1.110689 -0.742600 0.277513
C 2.261218 -0.560722 1.056325
C 1.235903 -0.825175 -1.116204
C 3.514386 -0.482410 0.453587
H 2.166746 -0.456553 2.133941
C 2.491752 -0.749994 -1.717024
H 0.350797 -0.962090 -1.732848
C 3.633680 -0.577302 -0.934684
H 4.397866 -0.332193 1.066805
H 2.576042 -0.824499 -2.797014
H 4.610575 -0.508805 -1.403579
C -2.368042 -1.072325 -0.274138
O -2.292318 -2.278246 -0.145759
C -3.602481 -0.415379 -0.832774
H -3.785389 0.568818 -0.400804
H -3.498832 -0.300957 -1.914135
H -4.438782 -1.084152 -0.624736

32
1A_Ac_conf_10 Eopt -747.445343
C -3.170260 -2.044061 0.963224
H -3.210242 -1.851256 2.031371
H -3.906086 -2.722937 0.541095
C -2.260321 -1.453640 0.185380
C -1.237201 -0.584882 0.857796
O -0.668042 -0.935095 1.875036
N -0.846059 0.619677 0.232927
C 0.444076 1.140298 0.609277
C 0.519567 2.298034 1.268155
H -0.380102 2.822923 1.575352
H 1.479151 2.751606 1.493014
C -2.112683 -1.719279 -1.288834
H -2.914808 -2.378944 -1.627856
H -2.144367 -0.804674 -1.886210
H -1.154431 -2.212410 -1.487652
C 1.610313 0.331310 0.175896
C 2.803549 0.344519 0.910676
C 1.535647 -0.445508 -0.987714
C 3.904392 -0.391321 0.479091
H 2.862585 0.915124 1.833240
C 2.638765 -1.181759 -1.417544
H 0.614019 -0.466758 -1.563560
C 3.826608 -1.155612 -0.687040
H 4.820648 -0.378640 1.061714
H 2.568856 -1.774760 -2.324544
H 4.684320 -1.732992 -1.018627
C -1.716851 1.373516 -0.572674
O -2.915489 1.165122 -0.555418
C -1.094192 2.420268 -1.459601
H -1.739981 2.532667 -2.331590
H -1.056098 3.377874 -0.932859
H -0.081244 2.153928 -1.766840

32
1A_Ac_conf_11 Eopt -747.444933
C 3.552090 -0.239672 -0.943969
H 2.888425 -0.327041 -1.800261
H 4.614255 -0.125722 -1.143839
C 3.099635 -0.289220 0.313359
C 1.653133 -0.570643 0.563747
O 1.294027 -1.266027 1.494530
N 0.712685 -0.088289 -0.375818
C -0.442899 -0.912018 -0.642821
C -0.267388 -2.068244 -1.284391
H 0.716605 -2.356953 -1.642188
H -1.091923 -2.755705 -1.440326
C 3.968339 -0.212490 1.534435
H 3.909729 -1.142654 2.107271
H 5.007646 -0.033389 1.252554
H 3.635057 0.596691 2.193774
C -1.736709 -0.411647 -0.117393
C -1.764477 0.450142 0.986738
C -2.947917 -0.800959 -0.705335
C -2.978751 0.899392 1.503438
H -0.832923 0.763644 1.451357
C -4.160138 -0.352444 -0.186886
H -2.941115 -1.441651 -1.582507
C -4.180588 0.498150 0.920298
H -2.984012 1.562804 2.363139
H -5.090486 -0.657882 -0.656401
H -5.126457 0.851452 1.319637
C 0.727515 1.191905 -0.947502
O -0.032296 1.438438 -1.867680
C 1.607276 2.261715 -0.349956
H 1.964543 2.028554 0.653420
H 2.466253 2.438924 -1.002032
H 1.007029 3.173854 -0.320253

32
1A_Ac_conf_12 Eopt -747.443653
C 2.105578 -1.544799 1.309670
H 1.466087 -0.914318 1.921376
H 2.742549 -2.255705 1.829448
C 2.116626 -1.478035 -0.025166
C 1.153502 -0.586585 -0.745237
O 0.594704 -0.965267 -1.760373
N 0.813652 0.653702 -0.180158
C -0.476118 1.185616 -0.554499
C -0.543140 2.341183 -1.216775
H 0.358608 2.870079 -1.509719
H -1.500835 2.794418 -1.449741
C 2.960525 -2.352184 -0.907137
H 3.605088 -2.994083 -0.303483
H 2.329286 -2.978260 -1.544355
H 3.586416 -1.741927 -1.567876
C -1.654634 0.386596 -0.138063
C -2.822691 0.381864 -0.912511
C -1.620475 -0.362004 1.045081
C -3.938919 -0.341814 -0.500144
H -2.849248 0.930495 -1.849799
C -2.738261 -1.086962 1.455806
H -0.720990 -0.365584 1.654145

| | | | |
|---|---|---|---|
| C | -3.901232 | -1.078001 | 0.685732 |
| H | -4.835542 | -0.341720 | -1.112796 |
| H | -2.699504 | -1.657211 | 2.379092 |
| H | -4.770461 | -1.646337 | 1.002665 |
| C | 1.663368 | 1.443180 | 0.630466 |
| O | 1.183999 | 2.274307 | 1.375361 |
| C | 3.158067 | 1.311556 | 0.466600 |
| H | 3.535014 | 2.328231 | 0.325345 |
| H | 3.597059 | 0.911597 | 1.383390 |
| H | 3.458116 | 0.694436 | -0.379419 |

32

1A_Ac_conf_13 Eopt -747.444927

| | | | |
|---|---|---|---|
| C | 3.553055 | 0.234349 | 0.941803 |
| H | 2.890271 | 0.313060 | 1.799705 |
| H | 4.615729 | 0.120536 | 1.139425 |
| C | 3.098759 | 0.293740 | -0.314411 |
| C | 1.651251 | 0.574787 | -0.559801 |
| O | 1.289066 | 1.275588 | -1.485327 |
| N | 0.713157 | 0.084487 | 0.378132 |
| C | -0.443205 | 0.905815 | 0.652050 |
| C | -0.267223 | 2.055496 | 1.305078 |
| H | 0.716803 | 2.340052 | 1.666230 |
| H | -1.091144 | 2.742102 | 1.468340 |
| C | 3.966309 | 0.229327 | -1.537397 |
| H | 5.005262 | 0.043289 | -1.258578 |
| H | 3.630023 | -0.570041 | -2.206992 |
| H | 3.910816 | 1.167078 | -2.098128 |
| C | -1.736535 | 0.410263 | 0.121117 |
| C | -1.763610 | -0.447971 | -0.985792 |
| C | -2.948672 | 0.800434 | 0.706988 |
| C | -2.977570 | -0.893293 | -1.506886 |
| H | -0.831797 | -0.761943 | -1.449643 |
| C | -4.160505 | 0.356122 | 0.184107 |
| H | -2.943311 | 1.438874 | 1.585869 |
| C | -4.180098 | -0.491365 | -0.925626 |
| H | -2.981743 | -1.554157 | -2.368582 |
| H | -5.091368 | 0.662570 | 0.652010 |
| H | -5.125760 | -0.841647 | -1.328173 |
| C | 0.728960 | -1.199932 | 0.940369 |
| O | -0.031412 | -1.453790 | 1.858100 |
| C | 1.610975 | -2.264510 | 0.336244 |
| H | 2.474895 | -2.438327 | 0.982681 |
| H | 1.015459 | -3.179719 | 0.308386 |
| H | 1.961201 | -2.027078 | -0.668723 |

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1A_Ac_conf_2 Eopt -747.443711

| | | | |
|---|---|---|---|
| C | 0.192020 | 2.556324 | -1.003418 |
| H | 0.662492 | 2.005227 | -1.814033 |
| H | 0.597119 | 3.533770 | -0.754169 |
| C | -0.836860 | 2.052092 | -0.320624 |
| C | -1.393944 | 0.714569 | -0.727922 |
| O | -1.985745 | 0.558407 | -1.778490 |
| N | -1.206257 | -0.329414 | 0.194230 |
| C | -0.070727 | -0.252790 | 1.091274 |
| C | -0.286818 | -0.146011 | 2.402420 |
| H | -1.297666 | -0.079638 | 2.792575 |
| H | 0.536882 | -0.149800 | 3.108640 |
| C | -1.560086 | 2.759652 | 0.793346 |
| H | -2.602207 | 2.944512 | 0.509193 |
| H | -1.571358 | 2.161104 | 1.709217 |
| H | -1.079640 | 3.717957 | 1.003795 |
| C | 1.264887 | -0.353666 | 0.451802 |
| C | 2.390163 | 0.228528 | 1.052651 |
| C | 1.417359 | -1.019036 | -0.771537 |
| C | 3.641296 | 0.132013 | 0.450163 |
| H | 2.281276 | 0.780789 | 1.981888 |
| C | 2.671831 | -1.114844 | -1.373219 |
| H | 0.556542 | -1.470960 | -1.257061 |
| C | 3.787537 | -0.540549 | -0.765347 |
| H | 4.501983 | 0.595448 | 0.923132 |
| H | 2.774412 | -1.638394 | -2.318975 |
| H | 4.762916 | -0.608956 | -1.237377 |
| C | -1.909857 | -1.555318 | 0.135156 |
| O | -1.471450 | -2.523043 | 0.726753 |
| C | -3.213360 | -1.605601 | -0.613204 |
| H | -3.781159 | -2.443774 | -0.207789 |
| H | -3.778797 | -0.677741 | -0.519365 |
| H | -3.022058 | -1.778737 | -1.674638 |

32

1A_Ac_conf_3 Eopt -747.446079

| | | | |
|---|---|---|---|
| C | 1.392488 | -1.792977 | -1.492569 |
| H | 0.550479 | -1.197042 | -1.832091 |
| H | 1.525155 | -2.773739 | -1.941518 |
| C | 2.251117 | -1.346168 | -0.572958 |
| C | 2.139707 | 0.059314 | -0.060018 |
| O | 3.128566 | 0.758882 | 0.056274 |
| N | 0.857367 | 0.555164 | 0.254826 |
| C | -0.103413 | -0.303178 | 0.898545 |
| C | 0.297242 | -1.061404 | 1.923593 |
| H | 1.307732 | -0.982296 | 2.313859 |
| H | -0.362987 | -1.791675 | 2.377725 |
| C | 3.447648 | -2.110154 | -0.085334 |
| H | 4.370880 | -1.570621 | -0.316297 |
| H | 3.405914 | -2.234090 | 1.002944 |
| H | 3.485898 | -3.096935 | -0.550967 |
| C | -1.473898 | -0.309616 | 0.325066 |
| C | -2.557880 | -0.771925 | 1.085570 |
| C | -1.713832 | 0.141688 | -0.979703 |
| C | -3.839664 | -0.810774 | 0.543552 |
| H | -2.405469 | -1.085284 | 2.113882 |
| C | -2.998124 | 0.105436 | -1.520506 |
| H | -0.894522 | 0.523969 | -1.582770 |
| C | -4.065695 | -0.375601 | -0.763576 |
| H | -4.666309 | -1.170410 | 1.148966 |
| H | -3.161721 | 0.456450 | -2.534964 |
| H | -5.066787 | -0.401335 | -1.183169 |
| C | 0.594253 | 1.943526 | 0.269774 |
| O | -0.317801 | 2.366209 | 0.953997 |
| C | 1.402575 | 2.836159 | -0.631677 |
| H | 2.262279 | 3.227522 | -0.082830 |
| H | 1.767602 | 2.313978 | -1.517064 |
| H | 0.759035 | 3.668677 | -0.920211 |

32

1A_Ac_conf_4 Eopt -747.443695

| | | | |
|---|---|---|---|
| C | 0.341030 | 2.861551 | -0.644253 |
| H | 0.362102 | 2.694795 | -1.717412 |
| H | 0.932877 | 3.680782 | -0.244466 |
| C | -0.376414 | 2.075495 | 0.164590 |
| C | -1.191065 | 1.002146 | -0.500792 |
| O | -1.748737 | 1.191826 | -1.566306 |
| N | -1.283269 | -0.239877 | 0.159696 |
| C | -0.172305 | -0.680462 | 0.969067 |
| C | -0.387685 | -1.109046 | 2.212969 |
| H | -1.382751 | -1.086590 | 2.646151 |
| H | 0.423989 | -1.512947 | 2.808995 |
| C | -0.431204 | 2.260663 | 1.661283 |
| H | -1.389277 | 1.927371 | 2.070642 |
| H | 0.359888 | 1.699193 | 2.167091 |
| H | -0.299444 | 3.319462 | 1.897395 |
| C | 1.157515 | -0.652680 | 0.311676 |
| C | 2.312529 | -0.386917 | 1.058802 |
| C | 1.273484 | -0.877888 | -1.067161 |
| C | 3.560808 | -0.361061 | 0.440660 |
| H | 2.228518 | -0.178480 | 2.122063 |

C 2.523211 -0.853577 -1.682641
H 0.384699 -1.082321 -1.659443
C 3.670300 -0.593217 -0.931506
H 4.447625 -0.145142 1.028985
H 2.600057 -1.036773 -2.750162
H 4.642914 -0.565255 -1.413291
C -2.294138 -1.179849 -0.163360
O -2.131351 -2.356923 0.089885
C -3.583479 -0.673345 -0.753450
H -3.826073 0.337502 -0.425375
H -3.512025 -0.671343 -1.843256
H -4.365042 -1.371208 -0.449716
32
1A_Ac_conf_5 Eopt -747.445509
C -2.157915 1.492872 1.393119
H -1.524379 0.822118 1.967735
H -2.796870 2.172945 1.950148
C -2.162118 1.499539 0.057630
C -1.185834 0.657916 -0.704070
O -0.620038 1.091832 -1.690781
N -0.836936 -0.610086 -0.194051
C 0.441614 -1.135639 -0.587749
C 0.506754 -2.285805 -1.263757
H -0.393191 -2.801187 -1.585781
H 1.463833 -2.743535 -1.490395
C -3.004489 2.416221 -0.781496
H -3.636266 1.837171 -1.464177
H -3.644415 3.033212 -0.147532
H -2.374633 3.067593 -1.394324
C 1.624898 -0.348864 -0.158724
C 1.590948 0.390192 1.030450
C 2.795294 -0.345752 -0.929323
C 2.711839 1.105044 1.450384
H 0.688122 0.396404 1.634516
C 3.914569 0.367537 -0.507355
H 2.821573 -0.886472 -1.871178
C 3.877321 1.094434 0.684291
H 2.673191 1.669072 2.377467
H 4.813237 0.366872 -1.116935
H 4.748896 1.655062 1.008421
C -1.794465 -1.448843 0.417281
O -2.980897 -1.286415 0.212222
C -1.271289 -2.521431 1.337213
H -1.973950 -2.602698 2.168933
H -1.252811 -3.481595 0.814475
H -0.269069 -2.302208 1.708097
32
1A_Ac_conf_6 Eopt -747.445509
C 2.158026 -1.493061 -1.393102
H 1.524140 -0.822644 -1.967723
H 2.797169 -2.173024 -1.950056
C 2.162539 -1.499340 -0.057619
C 1.185924 -0.657947 0.703953
O 0.620066 -1.092047 1.690534
N 0.836850 0.610034 0.193966
C -0.441721 1.135464 0.587682
C -0.506918 2.285726 1.263542
H 0.392988 2.801237 1.585460
H -1.464043 2.743422 1.490044
C 3.005495 -2.415276 0.781695
H 3.636727 -1.835661 1.464400
H 2.376105 -3.067098 1.394533
H 3.645976 -3.031857 0.147888
C -1.625034 0.348665 0.158742
C -1.591158 -0.390526 -1.030339
C -2.795430 0.345718 0.929365
C -2.712139 -1.105284 -1.450225
H -0.688339 -0.396940 -1.634407
C -3.914785 -0.367456 0.507439
H -2.821623 0.886426 1.871226
C -3.877630 -1.094441 -0.684164
H -2.673540 -1.669422 -2.377244
H -4.813457 -0.366654 1.117013
H -4.749291 -1.654945 -1.008280
C 1.794327 1.448788 -0.417349
O 2.980805 1.286208 -0.212528
C 1.271229 2.521666 -1.336965
H 1.973484 2.602485 -2.169085
H 0.268671 2.303153 -1.707329
H 1.253762 3.481823 -0.814174
32
1A_Ac_conf_7 Eopt -747.444523
C 3.624805 0.776671 -0.421404
H 3.001312 1.617164 -0.715987
H 4.694902 0.948258 -0.341845
C 3.108294 -0.430017 -0.174555
C 1.653838 -0.669235 -0.432658
O 1.265966 -1.685224 -0.976358
N 0.748418 0.375117 -0.130043
C -0.414148 0.515166 -0.976378
C -0.249853 1.034172 -2.194919
H 0.726931 1.382691 -2.517326
H -1.074934 1.098293 -2.896287
C 3.907528 -1.638924 0.213516
H 3.805676 -2.427777 -0.537647
H 4.963421 -1.381291 0.317649
H 3.547337 -2.045736 1.164961
C -1.698960 0.019518 -0.423737
C -2.921761 0.532121 -0.880317
C -1.705115 -0.966157 0.572054
C -4.123391 0.051058 -0.367271
H -2.932621 1.322866 -1.625174
C -2.909670 -1.444830 1.085600
H -0.765791 -1.371237 0.938305
C -4.122146 -0.940231 0.616436
H -5.062743 0.460191 -0.726912
H -2.898233 -2.213628 1.852382
H -5.060185 -1.309814 1.019407
C 0.837738 1.078789 1.082144
O 1.553503 0.683118 1.983789
C -0.002966 2.321842 1.182196
H 0.289568 2.862018 2.082051
H 0.128578 2.951685 0.298408
H -1.063049 2.057684 1.254634
32
1A_Ac_conf_8 Eopt -747.444184
C -3.637935 1.820277 -0.221932
H -3.072193 2.742012 -0.322466
H -4.702223 1.850121 -0.438226
C -3.044574 0.679843 0.138213
C -1.586884 0.740937 0.490120
O -1.119377 1.655718 1.141450
N -0.768647 -0.360274 0.145496
C 0.414037 -0.574892 0.953113
C 0.268898 -1.186403 2.129748
H -0.706462 -1.543777 2.445750
H 1.107684 -1.323420 2.803802
C -3.768909 -0.624198 0.337434
H -3.605292 -1.000619 1.353329
H -4.841549 -0.476080 0.192778
H -3.431763 -1.394418 -0.360756
C 1.691883 -0.059379 0.401772
C 2.920594 -0.587069 0.825553
C 1.688565 0.956623 -0.563162

| | | | |
|---|---|---|---|
| C | 4.116403 | -0.091180 | 0.313596 |
| H | 2.942265 | -1.401546 | 1.543793 |
| C | 2.887510 | 1.450003 | -1.076242 |
| H | 0.747403 | 1.373669 | -0.909705 |
| C | 4.105102 | 0.931283 | -0.637597 |
| H | 5.059180 | -0.512728 | 0.649116 |
| H | 2.866969 | 2.241958 | -1.818868 |
| H | 5.038628 | 1.313087 | -1.039617 |
| C | -0.925356 | -1.058019 | -1.063003 |
| O | -1.687295 | -0.658185 | -1.924173 |
| C | -0.106422 | -2.310722 | -1.211264 |
| H | 0.959192 | -2.068250 | -1.272724 |
| H | -0.252556 | -2.970221 | -0.351631 |
| H | -0.412851 | -2.810748 | -2.129348 |

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1A_Bn_conf_1 Eopt -865.117086

| | | | |
|---|---|---|---|
| C | -3.037001 | -1.899656 | 0.400487 |
| H | -2.696104 | -2.168362 | 1.396640 |
| H | -4.109721 | -1.828304 | 0.238014 |
| C | -2.180908 | -1.674119 | -0.599654 |
| C | -0.707044 | -1.904600 | -0.395282 |
| O | -0.091045 | -2.621231 | -1.183242 |
| N | -0.108502 | -1.355460 | 0.708865 |
| C | -0.663404 | -0.235098 | 1.410088 |
| C | -0.680982 | -0.219368 | 2.747325 |
| H | -0.365897 | -1.081588 | 3.326896 |
| H | -0.991015 | 0.669519 | 3.285789 |
| C | -2.590867 | -1.325391 | -2.001304 |
| H | -2.236470 | -2.086238 | -2.703437 |
| H | -3.677835 | -1.248494 | -2.075991 |
| H | -2.147452 | -0.369694 | -2.304936 |
| C | -1.103753 | 0.926697 | 0.588646 |
| C | -0.437776 | 1.262641 | -0.597891 |
| C | -2.186276 | 1.713721 | 1.004484 |
| C | -0.830078 | 2.378676 | -1.336825 |
| H | 0.396676 | 0.656933 | -0.943032 |
| C | -2.580890 | 2.823806 | 0.261942 |
| H | -2.734964 | 1.438343 | 1.901118 |
| C | -1.901498 | 3.162879 | -0.910354 |
| H | -0.297133 | 2.631042 | -2.248904 |
| H | -3.427881 | 3.417982 | 0.591900 |
| H | -2.211629 | 4.026551 | -1.490783 |
| C | 1.286824 | -1.736295 | 1.006340 |
| H | 1.395057 | -1.795837 | 2.090530 |
| H | 1.446554 | -2.727442 | 0.581829 |
| C | 2.264897 | -0.739820 | 0.427849 |
| C | 2.707825 | 0.343982 | 1.192977 |
| C | 2.678984 | -0.848137 | -0.905204 |
| C | 3.537083 | 1.316186 | 0.630825 |
| H | 2.397317 | 0.427370 | 2.232004 |
| C | 3.511056 | 0.119615 | -1.467047 |
| H | 2.331163 | -1.688269 | -1.500496 |
| C | 3.936645 | 1.207517 | -0.701469 |
| H | 3.871645 | 2.155623 | 1.233391 |
| H | 3.826577 | 0.026526 | -2.502248 |
| H | 4.581971 | 1.962995 | -1.139984 |

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1A_Bn_conf_10 Eopt -865.114590

| | | | |
|---|---|---|---|
| C | -4.532624 | 0.283151 | 0.481826 |
| H | -4.928976 | 0.766946 | -0.406694 |
| H | -5.240981 | -0.160543 | 1.176576 |
| C | -3.219674 | 0.224378 | 0.712533 |
| C | -2.298011 | 0.928353 | -0.255018 |
| O | -2.498189 | 2.103740 | -0.557376 |
| N | -1.197764 | 0.252189 | -0.718265 |
| C | -1.070190 | -1.171216 | -0.700981 |
| C | -2.043352 | -1.956608 | -1.174487 |
| H | -2.944380 | -1.535211 | -1.608509 |
| H | -1.958706 | -3.036715 | -1.109478 |
| C | -2.615375 | -0.395098 | 1.943974 |
| H | -1.961512 | 0.322879 | 2.452459 |
| H | -3.406629 | -0.695538 | 2.635170 |
| H | -2.011969 | -1.276742 | 1.707713 |
| C | 0.216660 | -1.695560 | -0.169073 |
| C | 0.806028 | -1.121757 | 0.966016 |
| C | 0.856693 | -2.770771 | -0.797417 |
| C | 2.005307 | -1.620617 | 1.468369 |
| H | 0.321642 | -0.279971 | 1.452503 |
| C | 2.059641 | -3.267782 | -0.296586 |
| H | 0.419510 | -3.203586 | -1.693217 |
| C | 2.637347 | -2.693701 | 0.836318 |
| H | 2.449143 | -1.167715 | 2.350196 |
| H | 2.550834 | -4.095650 | -0.799075 |
| H | 3.577845 | -3.076054 | 1.221626 |
| C | -0.232568 | 0.976561 | -1.565257 |
| H | 0.106148 | 0.291355 | -2.346334 |
| H | -0.779853 | 1.792811 | -2.042911 |
| C | 0.958834 | 1.516432 | -0.804027 |
| C | 2.255916 | 1.218063 | -1.226496 |
| C | 0.779038 | 2.302817 | 0.339687 |
| C | 3.361082 | 1.686241 | -0.512723 |
| H | 2.401850 | 0.598115 | -2.108373 |
| C | 1.879807 | 2.766674 | 1.057315 |
| H | -0.227703 | 2.537786 | 0.677594 |
| C | 3.175204 | 2.457118 | 0.634283 |
| H | 4.364372 | 1.438009 | -0.846738 |
| H | 1.728163 | 3.369367 | 1.948178 |
| H | 4.032498 | 2.815146 | 1.196626 |

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1A_Bn_conf_11 Eopt -865.111966

| | | | |
|---|---|---|---|
| C | -2.641115 | -3.106037 | -0.094287 |
| H | -3.139218 | -2.601896 | 0.730171 |
| H | -3.245329 | -3.743372 | -0.735287 |
| C | -1.334449 | -2.958760 | -0.314605 |
| C | -0.495260 | -2.136881 | 0.633887 |
| O | -0.050848 | -2.650891 | 1.657656 |
| N | -0.220104 | -0.847938 | 0.269937 |
| C | 0.650999 | -0.041265 | 1.076140 |
| C | 0.260894 | 0.367215 | 2.285356 |
| H | -0.721230 | 0.105461 | 2.666317 |
| H | 0.924464 | 0.940220 | 2.925296 |
| C | -0.567122 | -3.633514 | -1.418332 |
| H | 0.221436 | -4.269301 | -1.000067 |
| H | -1.231212 | -4.250743 | -2.028100 |
| H | -0.077931 | -2.896135 | -2.065999 |
| C | 1.965310 | 0.286571 | 0.464810 |
| C | 2.578880 | -0.618503 | -0.412190 |
| C | 2.613126 | 1.494533 | 0.756781 |
| C | 3.825698 | -0.332869 | -0.965259 |
| H | 2.078369 | -1.552903 | -0.655732 |
| C | 3.859761 | 1.778857 | 0.203187 |
| H | 2.129941 | 2.220230 | 1.405363 |
| C | 4.471177 | 0.865586 | -0.657625 |
| H | 4.292308 | -1.046611 | -1.637643 |
| H | 4.348651 | 2.720549 | 0.434541 |
| H | 5.440041 | 1.090850 | -1.093084 |
| C | -0.706235 | -0.215179 | -0.963346 |
| H | 0.150363 | 0.049281 | -1.593534 |
| H | -1.311987 | -0.942329 | -1.505467 |
| C | -1.524201 | 1.021868 | -0.664531 |
| C | -1.108689 | 2.276106 | -1.113225 |
| C | -2.700538 | 0.918584 | 0.086404 |
| C | -1.861330 | 3.417073 | -0.822526 |
| H | -0.189651 | 2.360542 | -1.689063 |

C -3.452221 2.053983 0.379310
H -3.021121 -0.057392 0.445854
C -3.033076 3.307665 -0.075839
H -1.527601 4.388635 -1.175005
H -4.364525 1.964091 0.961760
H -3.617917 4.193314 0.154212
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1A_Bn_conf_12 Eopt -865.115038
C -2.535396 -1.311110 -2.001649
H -1.798787 -1.195830 -2.792046
H -3.580900 -1.154737 -2.254649
C -2.169495 -1.621742 -0.755400
C -0.702413 -1.881825 -0.510136
O -0.057048 -2.584469 -1.286619
N -0.135717 -1.370571 0.630704
C -0.697249 -0.264859 1.348017
C -0.766645 -0.297523 2.683708
H -0.485177 -1.185155 3.241939
H -1.085531 0.575207 3.243088
C -3.152892 -1.808028 0.372256
H -4.154917 -1.956794 -0.037626
H -2.889418 -2.679057 0.981426
H -3.186328 -0.941416 1.039346
C -1.096163 0.930111 0.553417
C -2.182153 1.715838 0.960191
C -0.391502 1.293341 -0.603375
C -2.547601 2.848832 0.235308
H -2.756182 1.425543 1.836196
C -0.754518 2.428780 -1.323910
H 0.445465 0.687050 -0.941342
C -1.834419 3.209877 -0.908459
H -3.397840 3.442356 0.557818
H -0.194927 2.700323 -2.214162
H -2.122418 4.089288 -1.476596
C 1.246650 -1.771741 0.961606
H 1.319600 -1.855904 2.047151
H 1.410977 -2.754226 0.519369
C 2.251736 -0.771333 0.439003
C 2.711630 -0.853043 -0.880805
C 2.675186 0.291725 1.243320
C 3.569061 0.120972 -1.391393
H 2.379089 -1.677070 -1.506492
C 3.529495 1.270463 0.732361
H 2.329138 0.354286 2.272540
C 3.974537 1.188638 -0.587358
H 3.920048 0.048550 -2.416775
H 3.848132 2.093884 1.364914
H 4.639278 1.949199 -0.986306
40
1A_Bn_conf_15 Eopt -865.113481
C -0.668764 2.732949 -0.726575
H 0.075125 2.489115 -1.481445
H -1.246575 3.643185 -0.866534
C -0.861930 1.957590 0.342916
C 0.049014 0.781465 0.579612
O 0.694203 0.713181 1.620954
N 0.150719 -0.174574 -0.406496
C 1.187680 -1.148251 -0.288657
C 0.941546 -2.459979 -0.397560
H -0.066100 -2.850281 -0.501855
H 1.761061 -3.169968 -0.418144
C -1.854228 2.243979 1.433080
H -2.394323 3.170734 1.226490
H -2.578740 1.424770 1.519164
H -1.346135 2.333357 2.398456
C 2.569531 -0.609021 -0.151276
C 3.538716 -1.306964 0.579231
C 2.929357 0.586499 -0.786373
C 4.844915 -0.827454 0.659698
H 3.263696 -2.218089 1.103213
C 4.235600 1.065108 -0.705908
H 2.183755 1.139842 -1.351534
C 5.199165 0.359177 0.016043
H 5.584291 -1.376565 1.235315
H 4.500819 1.990236 -1.209263
H 6.215943 0.734425 0.082672
C -0.944687 -0.371774 -1.370736
H -0.987790 0.470032 -2.065586
H -0.689135 -1.257953 -1.954430
C -2.293958 -0.551474 -0.705659
C -2.426670 -1.279201 0.482046
C -3.430103 0.029202 -1.275485
C -3.676561 -1.434130 1.081206
H -1.547593 -1.714994 0.952115
C -4.681638 -0.123767 -0.677724
H -3.329979 0.617388 -2.184962
C -4.808240 -0.856780 0.502938
H -3.764496 -1.999893 2.004120
H -5.554763 0.339081 -1.128365
H -5.780188 -0.970906 0.973522
40
1A_Bn_conf_16 Eopt -865.111282
C -3.051665 -1.646067 -1.672363
H -2.089316 -2.094130 -1.910219
H -3.853449 -1.764383 -2.397051
C -3.250974 -0.980952 -0.532715
C -2.176653 -0.958858 0.526704
O -2.425485 -1.460667 1.620197
N -0.956714 -0.416584 0.212446
C 0.153599 -0.562168 1.107663
C 0.091544 -0.128785 2.368994
H -0.796805 0.365575 2.746182
H 0.919195 -0.292193 3.052016
C -4.550959 -0.343337 -0.134294
H -5.301635 -0.475368 -0.916707
H -4.922488 -0.782348 0.796712
H -4.412669 0.729666 0.044094
C 1.353026 -1.218710 0.523004
C 1.208437 -2.241330 -0.424162
C 2.642120 -0.827469 0.908742
C 2.329191 -2.874297 -0.958600
H 0.211508 -2.543846 -0.736485
C 3.762166 -1.461325 0.374610
H 2.765332 -0.009226 1.613265
C 3.609508 -2.487061 -0.559967
H 2.202225 -3.669489 -1.687204
H 4.755502 -1.144537 0.678439
H 4.483040 -2.975391 -0.981372
C -0.690150 0.362359 -1.011275
H -0.058965 -0.216067 -1.694799
H -1.642731 0.545070 -1.506138
C -0.023850 1.680532 -0.685942
C -0.697083 2.632973 0.087690
C 1.265991 1.958428 -1.139853
C -0.088537 3.845823 0.400775
H -1.700740 2.415519 0.448880
C 1.878586 3.175767 -0.830506
H 1.795037 1.216325 -1.734187
C 1.203225 4.119615 -0.058882
H -0.619054 4.579109 1.001160
H 2.883162 3.381338 -1.188492
H 1.678602 5.064965 0.185471
40
1A_Bn_conf_2 Eopt -865.116456

| | | | |
|---|---|---|---|
| C | -0.850696 | 1.586651 | 1.870278 |
| H | -0.177451 | 0.824331 | 2.253418 |
| H | -1.458057 | 2.127689 | 2.591756 |
| C | -0.936154 | 1.864137 | 0.566557 |
| C | 0.004357 | 1.210484 | -0.408076 |
| O | 0.636042 | 1.907655 | -1.199342 |
| N | 0.194585 | -0.149406 | -0.354521 |
| C | -0.680046 | -1.047190 | 0.327540 |
| C | -0.184561 | -2.055813 | 1.055316 |
| H | 0.883086 | -2.160697 | 1.224772 |
| H | -0.842873 | -2.812907 | 1.466808 |
| C | -1.828962 | 2.922195 | -0.014541 |
| H | -2.496849 | 2.490424 | -0.769008 |
| H | -2.434269 | 3.385239 | 0.767771 |
| H | -1.233918 | 3.694737 | -0.510921 |
| C | -2.136841 | -0.884272 | 0.068208 |
| C | -2.589623 | -0.451256 | -1.184641 |
| C | -3.075010 | -1.188362 | 1.062900 |
| C | -3.955786 | -0.342515 | -1.442860 |
| H | -1.872323 | -0.207541 | -1.964571 |
| C | -4.438895 | -1.074712 | 0.805123 |
| H | -2.731612 | -1.490610 | 2.048632 |
| C | -4.884449 | -0.652643 | -0.449619 |
| H | -4.292692 | -0.013020 | -2.421291 |
| H | -5.155050 | -1.303683 | 1.588659 |
| H | -5.947909 | -0.559863 | -0.648249 |
| C | 1.310946 | -0.688331 | -1.131729 |
| H | 1.132617 | -1.758988 | -1.255117 |
| H | 1.295919 | -0.227263 | -2.123767 |
| C | 2.671761 | -0.462270 | -0.499544 |
| C | 2.821235 | -0.023426 | 0.817376 |
| C | 3.816705 | -0.721276 | -1.261738 |
| C | 4.093916 | 0.153092 | 1.365567 |
| H | 1.940717 | 0.186666 | 1.419987 |
| C | 5.087223 | -0.550316 | -0.715638 |
| H | 3.708965 | -1.056292 | -2.291199 |
| C | 5.230208 | -0.111333 | 0.602766 |
| H | 4.193613 | 0.498315 | 2.390600 |
| H | 5.966131 | -0.755241 | -1.320065 |
| H | 6.219560 | 0.026247 | 1.028712 |

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1A_Bn_conf_3 Eopt -865.116162

| | | | |
|---|---|---|---|
| C | -1.693198 | 3.234333 | 0.119298 |
| H | -2.261820 | 2.498465 | -0.443082 |
| H | -2.248681 | 4.026468 | 0.615013 |
| C | -0.362542 | 3.181319 | 0.202238 |
| C | 0.410515 | 2.163940 | -0.596802 |
| O | 1.294265 | 2.550998 | -1.359802 |
| N | 0.061006 | 0.840543 | -0.503763 |
| C | -0.606436 | 0.279104 | 0.628607 |
| C | -0.172786 | 0.535035 | 1.868166 |
| H | 0.707861 | 1.148786 | 2.034831 |
| H | -0.711322 | 0.169239 | 2.736132 |
| C | 0.479868 | 4.174753 | 0.949230 |
| H | -0.148886 | 4.920885 | 1.440129 |
| H | 1.085937 | 3.668762 | 1.710142 |
| H | 1.170566 | 4.681028 | 0.268101 |
| C | -1.761512 | -0.606313 | 0.326481 |
| C | -2.548719 | -0.388916 | -0.812707 |
| C | -2.082568 | -1.672829 | 1.177624 |
| C | -3.650390 | -1.200365 | -1.077845 |
| H | -2.295386 | 0.420865 | -1.492045 |
| C | -3.184948 | -2.482320 | 0.912800 |
| H | -1.455308 | -1.880416 | 2.039958 |
| C | -3.974841 | -2.246962 | -0.213832 |
| H | -4.253835 | -1.015047 | -1.961409 |
| H | -3.419191 | -3.306414 | 1.579992 |
| H | -4.830494 | -2.881905 | -0.423027 |
| C | 0.700134 | -0.123764 | -1.413080 |
| H | -0.065085 | -0.814462 | -1.777855 |
| H | 1.085869 | 0.444831 | -2.260431 |
| C | 1.805878 | -0.899074 | -0.731364 |
| C | 1.749488 | -2.291661 | -0.649593 |
| C | 2.886926 | -0.224709 | -0.149945 |
| C | 2.763423 | -3.006775 | -0.006892 |
| H | 0.905205 | -2.818730 | -1.088561 |
| C | 3.896733 | -0.935027 | 0.495447 |
| H | 2.930567 | 0.860789 | -0.204700 |
| C | 3.838055 | -2.329720 | 0.566933 |
| H | 2.707716 | -4.089963 | 0.049874 |
| H | 4.731135 | -0.402593 | 0.942687 |
| H | 4.625519 | -2.882650 | 1.070432 |

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1A_Bn_conf_4 Eopt -865.111694

| | | | |
|---|---|---|---|
| C | 1.240640 | 2.594794 | -1.331540 |
| H | 0.225461 | 2.568982 | -1.721027 |
| H | 2.003445 | 3.064122 | -1.948204 |
| C | 1.546917 | 2.081256 | -0.138984 |
| C | 0.452677 | 1.552959 | 0.757271 |
| O | 0.183472 | 2.167212 | 1.786085 |
| N | -0.202081 | 0.415288 | 0.361759 |
| C | -1.321888 | -0.081853 | 1.103975 |
| C | -1.227910 | -0.340787 | 2.411207 |
| H | -0.290769 | -0.207951 | 2.940280 |
| H | -2.097810 | -0.655120 | 2.978720 |
| C | 2.919987 | 2.102472 | 0.471121 |
| H | 3.641082 | 2.542786 | -0.221845 |
| H | 2.915289 | 2.685209 | 1.398318 |
| H | 3.247798 | 1.086679 | 0.724389 |
| C | -2.572695 | -0.247944 | 0.316271 |
| C | -2.831274 | 0.589000 | -0.777992 |
| C | -3.512447 | -1.231672 | 0.653981 |
| C | -4.015537 | 0.462450 | -1.502244 |
| H | -2.104269 | 1.348255 | -1.054944 |
| C | -4.695701 | -1.356714 | -0.070511 |
| H | -3.308640 | -1.911614 | 1.476464 |
| C | -4.952738 | -0.509180 | -1.149881 |
| H | -4.205255 | 1.123863 | -2.342397 |
| H | -5.412662 | -2.125964 | 0.200613 |
| H | -5.873067 | -0.611422 | -1.716951 |
| C | 0.260780 | -0.400422 | -0.778330 |
| H | -0.442210 | -1.233233 | -0.862529 |
| H | 0.208631 | 0.165207 | -1.711206 |
| C | 1.660275 | -0.939370 | -0.569780 |
| C | 2.626001 | -0.807538 | -1.569104 |
| C | 2.003532 | -1.567049 | 0.632905 |
| C | 3.920453 | -1.291967 | -1.371571 |
| H | 2.367822 | -0.305136 | -2.498714 |
| C | 3.295264 | -2.050467 | 0.833559 |
| H | 1.257029 | -1.667694 | 1.417908 |
| C | 4.258808 | -1.911272 | -0.168355 |
| H | 4.665492 | -1.175654 | -2.153316 |
| H | 3.551380 | -2.534073 | 1.771780 |
| H | 5.267184 | -2.282137 | -0.010330 |

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1A_Bn_conf_5 Eopt -865.111630

| | | | |
|---|---|---|---|
| C | -3.236032 | 0.878495 | 1.751300 |
| H | -2.369191 | 0.848880 | 2.407274 |
| H | -4.051263 | 1.544894 | 2.022448 |
| C | -3.305756 | 0.123550 | 0.654442 |
| C | -2.192215 | -0.845845 | 0.343583 |
| O | -2.159217 | -1.948004 | 0.892065 |
| N | -1.262963 | -0.471539 | -0.577451 |
| C | -0.242003 | -1.421012 | -0.952436 |

| | | | |
|---|---|---|---|
| C | -0.455099 | -2.174621 | -2.034023 |
| H | -1.378568 | -2.072002 | -2.596138 |
| H | 0.265970 | -2.910795 | -2.373167 |
| C | -4.475013 | 0.087218 | -0.290840 |
| H | -5.247128 | 0.793189 | 0.023938 |
| H | -4.165192 | 0.333833 | -1.313156 |
| H | -4.907875 | -0.919142 | -0.319812 |
| C | 0.988788 | -1.452768 | -0.118043 |
| C | 0.990235 | -0.915013 | 1.175707 |
| C | 2.182165 | -1.994029 | -0.620294 |
| C | 2.149954 | -0.923614 | 1.949707 |
| H | 0.081937 | -0.480695 | 1.581702 |
| C | 3.339120 | -2.005175 | 0.154058 |
| H | 2.217680 | -2.385018 | -1.632684 |
| C | 3.329145 | -1.469153 | 1.443444 |
| H | 2.129511 | -0.499600 | 2.949396 |
| H | 4.254601 | -2.420571 | -0.256625 |
| H | 4.234039 | -1.470215 | 2.043573 |
| C | -1.206997 | 0.845012 | -1.233926 |
| H | -1.217179 | 0.682362 | -2.316714 |
| H | -2.102780 | 1.402465 | -0.959032 |
| C | 0.029476 | 1.617343 | -0.828964 |
| C | 1.199901 | 1.535944 | -1.586953 |
| C | 0.031756 | 2.364600 | 0.353014 |
| C | 2.366620 | 2.170604 | -1.157450 |
| H | 1.200910 | 0.957830 | -2.508824 |
| C | 1.192945 | 3.005556 | 0.782145 |
| H | -0.879684 | 2.432571 | 0.943299 |
| C | 2.365740 | 2.902262 | 0.030518 |
| H | 3.274343 | 2.092421 | -1.748731 |
| H | 1.184921 | 3.582950 | 1.702031 |
| H | 3.273042 | 3.395323 | 0.366917 |

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1A_Bn_conf_6 Eopt -865.114182

| | | | |
|---|---|---|---|
| C | -2.701290 | 0.233902 | 1.926722 |
| H | -1.638966 | 0.249339 | 2.155358 |
| H | -3.382287 | 0.622238 | 2.679887 |
| C | -3.166219 | -0.245665 | 0.771768 |
| C | -2.230970 | -0.909338 | -0.205784 |
| O | -2.433902 | -2.081109 | -0.523037 |
| N | -1.140883 | -0.218880 | -0.665896 |
| C | -1.041639 | 1.208272 | -0.656269 |
| C | -2.038600 | 1.965428 | -1.126095 |
| H | -2.934024 | 1.515676 | -1.544809 |
| H | -1.986495 | 3.047774 | -1.069349 |
| C | -4.621240 | -0.315346 | 0.407606 |
| H | -4.923766 | -1.353299 | 0.237919 |
| H | -5.237509 | 0.110244 | 1.202663 |
| H | -4.812710 | 0.235793 | -0.520597 |
| C | 0.236654 | 1.764853 | -0.140356 |
| C | 0.802251 | 2.904779 | -0.727667 |
| C | 0.893474 | 1.163497 | 0.941691 |
| C | 1.990516 | 3.439564 | -0.233448 |
| H | 0.317920 | 3.360688 | -1.586844 |
| C | 2.080137 | 1.699755 | 1.437259 |
| H | 0.474561 | 0.269258 | 1.392830 |
| C | 2.632898 | 2.839155 | 0.850655 |
| H | 2.421305 | 4.318495 | -0.703673 |
| H | 2.574734 | 1.223638 | 2.278849 |
| H | 3.562314 | 3.252457 | 1.230755 |
| C | -0.183471 | -0.930008 | -1.532656 |
| H | -0.743970 | -1.714522 | -2.048367 |
| H | 0.176562 | -0.221535 | -2.282415 |
| C | 0.991523 | -1.528839 | -0.790012 |
| C | 0.796368 | -2.326326 | 0.343676 |
| C | 2.293762 | -1.280443 | -1.229174 |
| C | 1.887686 | -2.853780 | 1.031536 |
| H | -0.213158 | -2.523465 | 0.696088 |
| C | 3.388734 | -1.812898 | -0.545584 |
| H | 2.452397 | -0.650991 | -2.102010 |
| C | 3.188170 | -2.597362 | 0.589595 |
| H | 1.724021 | -3.465229 | 1.914255 |
| H | 4.396149 | -1.604490 | -0.894024 |
| H | 4.037854 | -3.006241 | 1.128272 |

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1A_Bn_conf_7 Eopt -865.112754

| | | | |
|---|---|---|---|
| C | 1.601290 | 2.673153 | 1.128363 |
| H | 2.003055 | 1.992362 | 1.874627 |
| H | 2.107253 | 3.625125 | 0.987969 |
| C | 0.526530 | 2.358352 | 0.404888 |
| C | -0.199745 | 1.061568 | 0.659223 |
| O | -0.915413 | 0.921744 | 1.643851 |
| N | -0.067043 | 0.078354 | -0.297329 |
| C | -0.922505 | -1.060389 | -0.244641 |
| C | -0.444971 | -2.301262 | -0.406657 |
| H | 0.617777 | -2.503693 | -0.489791 |
| H | -1.126915 | -3.140375 | -0.489642 |
| C | -0.109382 | 3.255190 | -0.623813 |
| H | 0.467573 | 4.175963 | -0.737305 |
| H | -0.182483 | 2.761789 | -1.599479 |
| H | -1.129379 | 3.515329 | -0.317691 |
| C | -2.382560 | -0.781534 | -0.146947 |
| C | -3.231418 | -1.668936 | 0.524534 |
| C | -2.933461 | 0.347209 | -0.767079 |
| C | -4.605803 | -1.439426 | 0.564424 |
| H | -2.811122 | -2.532092 | 1.033189 |
| C | -4.307138 | 0.575834 | -0.727246 |
| H | -2.283447 | 1.045712 | -1.288265 |
| C | -5.149081 | -0.317126 | -0.061990 |
| H | -5.251269 | -2.133502 | 1.094614 |
| H | -4.720625 | 1.452353 | -1.217391 |
| H | -6.219177 | -0.136122 | -0.027083 |
| C | 1.082522 | 0.073951 | -1.202446 |
| H | 0.826723 | -0.572591 | -2.046079 |
| H | 1.220960 | 1.081500 | -1.604523 |
| C | 2.387383 | -0.386286 | -0.576577 |
| C | 2.475067 | -0.831954 | 0.743450 |
| C | 3.547023 | -0.350493 | -1.359758 |
| C | 3.702968 | -1.235189 | 1.274068 |
| H | 1.584244 | -0.871139 | 1.366146 |
| C | 4.772019 | -0.753740 | -0.833001 |
| H | 3.486589 | -0.000482 | -2.388148 |
| C | 4.853950 | -1.197639 | 0.489085 |
| H | 3.755339 | -1.579357 | 2.302837 |
| H | 5.663334 | -0.719742 | -1.452709 |
| H | 5.808048 | -1.511167 | 0.901940 |

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1A_Bn_conf_8 Eopt -865.114688

| | | | |
|---|---|---|---|
| C | 1.909284 | 2.630235 | -0.361927 |
| H | 2.021309 | 2.661310 | -1.442463 |
| H | 2.594405 | 3.225744 | 0.236031 |
| C | 0.974603 | 1.874687 | 0.217803 |
| C | 0.008849 | 1.124070 | -0.666333 |
| O | -0.646141 | 1.718518 | -1.518186 |
| N | -0.185448 | -0.222541 | -0.448186 |
| C | 0.673697 | -1.027990 | 0.352246 |
| C | 0.178532 | -1.961935 | 1.175013 |
| H | -0.889849 | -2.085227 | 1.325257 |
| H | 0.847508 | -2.643563 | 1.688743 |
| C | 0.742305 | 1.824869 | 1.704910 |
| H | 0.793088 | 0.806972 | 2.103189 |
| H | 1.486475 | 2.437508 | 2.219767 |
| H | -0.254335 | 2.215101 | 1.942661 |
| C | 2.136603 | -0.856679 | 0.138125 |

| | | | |
|---|---|---|---|
| C | 3.020949 | -0.880733 | 1.221434 |
| C | 2.643086 | -0.686814 | -1.157395 |
| C | 4.392121 | -0.731691 | 1.014118 |
| H | 2.630010 | -0.990477 | 2.229632 |
| C | 4.012176 | -0.546382 | -1.364087 |
| H | 1.959533 | -0.659152 | -2.002712 |
| C | 4.890636 | -0.561752 | -0.277697 |
| H | 5.068861 | -0.737510 | 1.863383 |
| H | 4.394861 | -0.418928 | -2.372336 |
| H | 5.957575 | -0.439221 | -0.438373 |
| C | -1.337877 | -0.835871 | -1.108427 |
| H | -1.356072 | -0.504674 | -2.150234 |
| H | -1.176716 | -1.916450 | -1.101176 |
| C | -2.668520 | -0.506423 | -0.457404 |
| C | -2.756887 | 0.059497 | 0.816149 |
| C | -3.847493 | -0.799745 | -1.152028 |
| C | -4.002887 | 0.325031 | 1.388757 |
| H | -1.849522 | 0.298068 | 1.366851 |
| C | -5.091817 | -0.539742 | -0.580945 |
| H | -3.787283 | -1.231899 | -2.148551 |
| C | -5.173607 | 0.024956 | 0.693947 |
| H | -4.055008 | 0.767258 | 2.379457 |
| H | -5.997840 | -0.772588 | -1.132953 |
| H | -6.142247 | 0.231841 | 1.139063 |

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1A_Bn_conf_9 Eopt -865.116425

| | | | |
|---|---|---|---|
| C | 0.116407 | 4.117416 | 0.944200 |
| H | -0.961382 | 4.254806 | 0.949736 |
| H | 0.721094 | 4.821623 | 1.509602 |
| C | 0.682528 | 3.111462 | 0.274035 |
| C | -0.220323 | 2.216819 | -0.541429 |
| O | -1.063337 | 2.702713 | -1.292619 |
| N | -0.012951 | 0.860054 | -0.477631 |
| C | 0.595558 | 0.212228 | 0.640388 |
| C | 0.196323 | 0.489096 | 1.887375 |
| H | -0.620383 | 1.180323 | 2.070733 |
| H | 0.699658 | 0.052667 | 2.744026 |
| C | 2.169707 | 2.892379 | 0.198736 |
| H | 2.473386 | 1.953547 | 0.671440 |
| H | 2.499392 | 2.854724 | -0.845510 |
| H | 2.691549 | 3.711991 | 0.698701 |
| C | 1.658384 | -0.775421 | 0.314337 |
| C | 2.468947 | -0.595689 | -0.815023 |
| C | 1.870477 | -1.894712 | 1.130391 |
| C | 3.487029 | -1.500959 | -1.106839 |
| H | 2.300563 | 0.261341 | -1.462333 |
| C | 2.890325 | -2.798448 | 0.838881 |
| H | 1.222918 | -2.066777 | 1.985686 |
| C | 3.703558 | -2.603305 | -0.278620 |
| H | 4.110818 | -1.345158 | -1.981912 |
| H | 3.041511 | -3.662857 | 1.478473 |
| H | 4.494464 | -3.311077 | -0.507774 |
| C | -0.753088 | -0.015937 | -1.399956 |
| H | -1.069749 | 0.601818 | -2.241306 |
| H | -0.067018 | -0.783394 | -1.768925 |
| C | -1.939896 | -0.670989 | -0.729113 |
| C | -2.978596 | 0.112280 | -0.210059 |
| C | -1.999012 | -2.059008 | -0.588834 |
| C | -4.060307 | -0.486665 | 0.432035 |
| H | -2.931840 | 1.194142 | -0.312250 |
| C | -3.084645 | -2.662251 | 0.051331 |
| H | -1.189196 | -2.670531 | -0.981037 |
| C | -4.116346 | -1.877070 | 0.563160 |
| H | -4.861688 | 0.129534 | 0.829448 |
| H | -3.118928 | -3.742934 | 0.154114 |
| H | -4.959985 | -2.343228 | 1.063485 |

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1B_Ac-CS_conf_1 Eopt -747.426128

| | | | |
|---|---|---|---|
| C | 2.000641 | -1.980800 | -0.544408 |
| H | 1.846444 | -2.020609 | -1.635258 |
| H | 2.512420 | -2.910048 | -0.272676 |
| C | 2.846885 | -0.797935 | -0.144716 |
| C | 2.280786 | 0.402509 | 0.152796 |
| O | 2.729075 | 1.529041 | 0.502185 |
| N | 0.758992 | 0.418648 | 0.007972 |
| C | -0.010493 | -0.623974 | 0.013589 |
| C | 0.650995 | -1.960035 | 0.163888 |
| H | 0.793652 | -2.108424 | 1.246516 |
| H | -0.021947 | -2.739194 | -0.197809 |
| C | 4.340088 | -0.943094 | -0.173131 |
| H | 4.685728 | -1.275229 | -1.162635 |
| H | 4.830609 | 0.006472 | 0.055505 |
| H | 4.692682 | -1.692219 | 0.548904 |
| C | -1.481671 | -0.517780 | -0.063598 |
| C | -2.243852 | -1.275068 | 0.838775 |
| C | -2.120437 | 0.292959 | -1.011367 |
| C | -3.631384 | -1.180647 | 0.822472 |
| H | -1.750608 | -1.916307 | 1.563508 |
| C | -3.511914 | 0.361451 | -1.036222 |
| H | -1.539188 | 0.836710 | -1.748272 |
| C | -4.266761 | -0.362210 | -0.114020 |
| H | -4.217154 | -1.750099 | 1.536967 |
| H | -4.003648 | 0.978988 | -1.781020 |
| H | -5.350408 | -0.298384 | -0.131092 |
| C | 0.244983 | 1.815884 | -0.007530 |
| O | 0.264135 | 2.415044 | -1.043456 |
| C | -0.222888 | 2.300063 | 1.321290 |
| H | -1.035714 | 1.661852 | 1.683600 |
| H | 0.610642 | 2.223239 | 2.025514 |
| H | -0.561995 | 3.332102 | 1.235715 |

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1B_Ac-CS_conf_2 Eopt -747.426835

| | | | |
|---|---|---|---|
| C | 1.899630 | -1.985794 | -0.660589 |
| H | 1.704024 | -1.927538 | -1.743845 |
| H | 2.394247 | -2.947658 | -0.489141 |
| C | 2.791851 | -0.863579 | -0.190766 |
| C | 2.262722 | 0.305676 | 0.259269 |
| O | 2.748493 | 1.376410 | 0.724647 |
| N | 0.748497 | 0.382615 | 0.158961 |
| C | -0.052476 | -0.634372 | 0.081390 |
| C | 0.578900 | -1.993047 | 0.103387 |
| H | 0.764507 | -2.225447 | 1.164473 |
| H | -0.125622 | -2.727854 | -0.288487 |
| C | 4.278907 | -1.040916 | -0.278851 |
| H | 4.583909 | -1.305852 | -1.301151 |
| H | 4.800210 | -0.122724 | 0.003658 |
| H | 4.635117 | -1.850067 | 0.373390 |
| C | -1.517662 | -0.486222 | -0.020203 |
| C | -2.331875 | -1.299907 | 0.779123 |
| C | -2.096751 | 0.410312 | -0.927113 |
| C | -3.716217 | -1.177403 | 0.704730 |
| H | -1.882979 | -2.007087 | 1.470707 |
| C | -3.482692 | 0.509168 | -1.013215 |
| H | -1.471103 | 1.000310 | -1.591151 |
| C | -4.292561 | -0.274407 | -0.190478 |
| H | -4.345110 | -1.792000 | 1.340904 |
| H | -3.928506 | 1.194952 | -1.726568 |
| H | -5.373005 | -0.189558 | -0.254511 |
| C | 0.288297 | 1.786625 | 0.315559 |
| O | -0.366792 | 2.062409 | 1.280196 |
| C | 0.673605 | 2.716690 | -0.789008 |
| H | 1.151506 | 3.595301 | -0.351682 |
| H | 1.343318 | 2.243423 | -1.505934 |
| H | -0.245662 | 3.036000 | -1.291542 |

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1B_Ac-CS_conf_3 Eopt -747.425305

| | | | |
|---|---|---|---|
| C | -1.938059 | -2.048416 | -0.128858 |
| H | -1.773847 | -2.257405 | -1.199112 |
| H | -2.436670 | -2.933164 | 0.281719 |
| C | -2.810611 | -0.833964 | 0.063510 |
| C | -2.278175 | 0.410246 | 0.201375 |
| O | -2.763762 | 1.569861 | 0.311636 |
| N | -0.751478 | 0.446701 | 0.141408 |
| C | 0.038865 | -0.569449 | 0.280471 |
| C | -0.597240 | -1.891543 | 0.576243 |
| H | 0.103227 | -2.693302 | 0.336222 |
| H | -0.739717 | -1.899573 | 1.669122 |
| C | -4.297927 | -1.006227 | -0.038313 |
| H | -4.689858 | -1.654630 | 0.756991 |
| H | -4.809385 | -0.042447 | 0.024779 |
| H | -4.576004 | -1.477845 | -0.992013 |
| C | 1.510681 | -0.461445 | 0.173692 |
| C | 2.169949 | -1.330322 | -0.708931 |
| C | 2.250310 | 0.438698 | 0.952510 |
| C | 3.553424 | -1.266053 | -0.841800 |
| H | 1.597282 | -2.037336 | -1.302568 |
| C | 3.637919 | 0.475070 | 0.833578 |
| H | 1.747582 | 1.083400 | 1.664513 |
| C | 4.288725 | -0.365712 | -0.068833 |
| H | 4.057105 | -1.924932 | -1.541885 |
| H | 4.209142 | 1.161751 | 1.450162 |
| H | 5.369557 | -0.326627 | -0.163881 |
| C | -0.281250 | 1.810773 | -0.211778 |
| O | 0.110098 | 2.541805 | 0.650608 |
| C | -0.337477 | 2.074577 | -1.677294 |
| H | 0.437949 | 1.467319 | -2.160291 |
| H | -1.306726 | 1.765634 | -2.075846 |
| H | -0.154782 | 3.131523 | -1.869146 |

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1B_Ac-OS_conf_1 Eopt -747.410811

| | | | |
|---|---|---|---|
| C | 1.439994 | -2.007768 | 0.943212 |
| H | 0.823300 | -2.828066 | 0.545840 |
| H | 2.184864 | -2.477575 | 1.598893 |
| C | 2.132144 | -1.370885 | -0.218017 |
| C | 1.888200 | -0.007692 | -0.646733 |
| O | 2.489571 | 0.519382 | -1.576832 |
| N | 0.877341 | 0.699589 | 0.082932 |
| C | -0.095448 | -0.132593 | 0.722317 |
| C | 0.525562 | -1.043002 | 1.724719 |
| H | 1.127280 | -0.444181 | 2.419200 |
| H | -0.203399 | -1.606958 | 2.306292 |
| C | 3.151331 | -2.170709 | -0.947615 |
| H | 2.826195 | -3.212566 | -1.037136 |
| H | 3.354498 | -1.759340 | -1.937377 |
| H | 4.094294 | -2.178214 | -0.382528 |
| C | -1.415165 | -0.217991 | 0.183234 |
| C | -2.401140 | -1.048422 | 0.776926 |
| C | -1.787641 | 0.531882 | -0.963817 |
| C | -3.682270 | -1.120665 | 0.247226 |
| H | -2.160051 | -1.633088 | 1.658275 |
| C | -3.071310 | 0.448830 | -1.483368 |
| H | -1.052544 | 1.170611 | -1.444428 |
| C | -4.029972 | -0.375803 | -0.884389 |
| H | -4.418591 | -1.763666 | 0.720441 |
| H | -3.328815 | 1.029009 | -2.364681 |
| H | -5.033500 | -0.436720 | -1.293470 |
| C | 0.998467 | 2.056825 | 0.392894 |
| O | 1.918702 | 2.742880 | -0.014477 |
| C | -0.082226 | 2.608500 | 1.291242 |
| H | -1.054151 | 2.582565 | 0.789614 |
| H | -0.163309 | 2.020321 | 2.210482 |
| H | 0.173194 | 3.639598 | 1.533540 |

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1B_Ac-OS_conf_2 Eopt -747.414518

| | | | |
|---|---|---|---|
| C | 1.363759 | -2.210129 | 0.667946 |
| H | 0.741731 | -2.920811 | 0.102854 |
| H | 2.061926 | -2.817856 | 1.258472 |
| C | 2.132538 | -1.395709 | -0.318789 |
| C | 1.936963 | 0.029193 | -0.501156 |
| O | 2.652294 | 0.704064 | -1.239164 |
| N | 0.858684 | 0.615593 | 0.224208 |
| C | -0.135121 | -0.289729 | 0.717595 |
| C | 0.452273 | -1.359620 | 1.571508 |
| H | 1.051214 | -0.893229 | 2.363127 |
| H | -0.300309 | -1.990427 | 2.043500 |
| C | 3.199384 | -2.062878 | -1.110629 |
| H | 2.916208 | -3.095441 | -1.337333 |
| H | 3.413964 | -1.524680 | -2.035386 |
| H | 4.129015 | -2.105229 | -0.524804 |
| C | -1.458279 | -0.243613 | 0.184638 |
| C | -2.473712 | -1.114785 | 0.657501 |
| C | -1.805281 | 0.674199 | -0.841419 |
| C | -3.757683 | -1.064771 | 0.131084 |
| H | -2.256206 | -1.826490 | 1.446511 |
| C | -3.090787 | 0.711302 | -1.361086 |
| H | -1.050417 | 1.348001 | -1.234465 |
| C | -4.079623 | -0.154431 | -0.880245 |
| H | -4.516110 | -1.741542 | 0.513784 |
| H | -3.326822 | 1.419832 | -2.149743 |
| H | -5.085081 | -0.119748 | -1.287740 |
| C | 0.793031 | 1.956754 | 0.620021 |
| O | -0.144389 | 2.322875 | 1.313027 |
| C | 1.878036 | 2.908619 | 0.197093 |
| H | 2.869420 | 2.513496 | 0.426154 |
| H | 1.835540 | 3.079219 | -0.880488 |
| H | 1.708902 | 3.843840 | 0.730827 |

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1B Ac-OS conf 3 Eopt -747.412720

| | | | |
|---|---|---|---|
| C | -1.986398 | -1.732475 | -0.983543 |
| H | -2.319958 | -1.140172 | -1.848872 |
| H | -2.403126 | -2.735616 | -1.097030 |
| C | -2.509436 | -1.081499 | 0.254132 |
| C | -1.937614 | 0.186461 | 0.620465 |
| O | -2.359133 | 0.925210 | 1.506303 |
| N | -0.785505 | 0.549051 | -0.166167 |
| C | 0.128498 | -0.509019 | -0.428645 |
| C | -0.452064 | -1.783807 | -0.968719 |
| H | -0.074584 | -1.980252 | -1.982092 |
| H | -0.121508 | -2.624028 | -0.345556 |
| C | -3.631493 | -1.662429 | 1.028527 |
| H | -3.375647 | -2.678869 | 1.353157 |
| H | -3.881142 | -1.054283 | 1.898854 |
| H | -4.519510 | -1.754471 | 0.389241 |
| C | 1.502420 | -0.376693 | -0.056079 |
| C | 2.437907 | -1.375418 | -0.426924 |
| C | 1.975590 | 0.720215 | 0.707505 |
| C | 3.774305 | -1.272014 | -0.060588 |
| H | 2.112032 | -2.228149 | -1.014533 |
| C | 3.310659 | 0.808029 | 1.074030 |
| H | 1.282015 | 1.492994 | 1.023817 |
| C | 4.223031 | -0.182296 | 0.690999 |
| H | 4.471927 | -2.047601 | -0.363206 |
| H | 3.646595 | 1.654636 | 1.665916 |
| H | 5.267434 | -0.105501 | 0.976892 |
| C | -0.621820 | 1.804858 | -0.750142 |
| O | 0.325223 | 2.016818 | -1.492275 |
| C | -1.651046 | 2.862338 | -0.448522 |
| H | -2.669347 | 2.481036 | -0.552080 |

H -1.532390 3.219357 0.577174
H -1.488194 3.683837 -1.145721
32
1B_Ac-OS_conf_4 Eopt -747.409964
C 2.061969 -1.500218 1.104326
H 2.384561 -0.789288 1.880001
H 2.516295 -2.464828 1.341515
C 2.550224 -0.999172 -0.216936
C 1.915978 0.177025 -0.746550
O 2.240096 0.769387 -1.769390
N 0.788918 0.617396 0.050937
C -0.095503 -0.427933 0.430869
C 0.528721 -1.606471 1.123114
H 0.169687 -1.680478 2.159726
H 0.219839 -2.530775 0.619827
C 3.680104 -1.645069 -0.926048
H 3.444033 -2.697741 -1.127511
H 3.911116 -1.139271 -1.864451
H 4.572945 -1.643540 -0.287208
C -1.470154 -0.380684 0.042671
C -2.382714 -1.350684 0.530409
C -1.966393 0.610964 -0.841573
C -3.719906 -1.319460 0.156512
H -2.035993 -2.122069 1.211211
C -3.303679 0.627402 -1.211523
H -1.286061 1.354843 -1.246319
C -4.192370 -0.332876 -0.714839
H -4.401177 -2.069778 0.547126
H -3.658577 1.391952 -1.896519
H -5.237997 -0.313590 -1.005507
C 0.787538 1.894992 0.600320
O 1.652458 2.707641 0.311295
C -0.311886 2.202656 1.586071
H -1.254670 2.383065 1.060930
H -0.467359 1.376163 2.284721
H -0.031074 3.104510 2.129719
40
1B_Bn_CS_conf_1 Eopt -865.106608
C -0.194997 2.722366 1.171997
H -0.415269 2.125559 2.073608
H -0.126323 3.764364 1.503094
C -1.267367 2.588082 0.122544
C -1.210028 1.602801 -0.816862
O -1.943896 1.304369 -1.795465
N -0.035472 0.627068 -0.633393
C 1.069343 0.954894 -0.042871
C 1.152481 2.304400 0.602877
H 1.943718 2.285289 1.355938
H 1.471769 3.003571 -0.186223
C -2.423420 3.545323 0.145168
H -2.108335 4.580614 -0.047790
H -3.169611 3.273437 -0.605908
H -2.915482 3.547820 1.128307
C 2.265514 0.080009 -0.016862
C 2.865560 -0.227252 1.210080
C 2.839910 -0.376204 -1.210865
C 4.010723 -1.019997 1.243063
H 2.425981 0.137153 2.134605
C 3.999314 -1.145805 -1.172046
H 2.385426 -0.116341 -2.163298
C 4.580139 -1.475639 0.053747
H 4.461785 -1.273640 2.197174
H 4.448039 -1.488332 -2.099085
H 5.479607 -2.083088 0.080975
C -0.320928 -0.718553 -1.158357
H -0.607509 -0.615834 -2.204212
H 0.580552 -1.324005 -1.086011
C -1.439023 -1.363299 -0.366907
C -2.393226 -2.140485 -1.027850
C -1.503396 -1.238462 1.023764
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H -0.767600 -0.634265 1.550939
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1B_Bn_CS_conf_2 Eopt -865.105940
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O 2.167644 2.112405 0.735876
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C 1.959870 -1.578157 -1.015140
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H 1.837831 -1.116872 -2.009258
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H 4.693180 1.910018 0.263474
H 5.461585 0.335987 0.546566
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H -1.591372 -0.324619 -1.225066
C -2.779501 -3.286376 -0.045568
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H -3.693796 -3.870880 -0.011201
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H -0.534478 -0.143212 1.805821
C -1.012983 1.555393 0.582829
C -2.315832 1.636617 1.083074
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C -3.273173 2.421864 0.441542
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C -1.637988 3.047466 -1.217853
H 0.335424 2.219119 -0.958453
C -2.937421 3.126560 -0.715362
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1B_Bn_CS_conf_3 Eopt -865.107515
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C -2.680918 -0.257397 -0.746509
O -2.994953 -0.876533 -1.798613
N -1.186809 0.105305 -0.676126
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C -1.676430 1.803102 0.957133
H -1.101170 2.283089 1.752477
H -2.119327 2.604548 0.344216
C -4.844170 -0.266928 0.470402

H -5.505806 0.610425 0.495341
H -5.151485 -0.898800 -0.366658
H -5.027789 -0.821558 1.401847
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C 1.449237 1.355529 1.208784
C 1.284546 1.959027 -1.135222
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H 0.691399 2.067531 -2.038884
C 3.391814 2.174153 0.029410
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H 3.083308 2.715066 -2.034948
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C 2.066175 -1.480550 -1.011088
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1B_Bn_CS_conf_4 Eopt -865.107089
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C -2.572162 -0.701645 -0.385250
O -2.610242 -1.900080 -0.772903
N -1.180425 -0.056514 -0.543231
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H -1.695506 1.072438 2.017258
H -1.454621 2.654969 1.258749
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H -5.620253 0.346046 -0.328974
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H -5.304221 -0.337246 1.262713
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H 0.464923 2.169435 -1.986779
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1B_Bn_CS_conf_5 Eopt -865.107089
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C 3.521855 -0.133050 0.121524
C 2.571899 0.701212 -0.385315
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C 0.806594 -0.982534 0.130404
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H 1.695201 -1.072106 2.017348
H 1.454173 -2.654929 1.259382
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H -3.307845 -1.794476 2.070076
H -2.794212 -3.018381 -2.021576
H -4.227276 -2.808119 -0.004366
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H -4.238274 1.840373 -0.618084
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1B_Bn_CS_conf_6 Eopt -865.107337
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C 1.196610 1.854109 -0.700676
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H 1.855172 -2.582765 -2.153037
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H 0.691838 2.066598 -2.039315
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H 3.083906 2.713356 -2.035167
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H 0.187536 -0.155042 -2.265867
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C 2.615552 -2.788151 0.946528
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H 3.351164 -3.291205 1.566972
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1C_Ac_conf_1 Eopt -747.394196
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H 3.432077 -1.908885 -1.567974
H 3.926837 -2.536886 0.121798
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C 2.123289 0.103085 0.160432
O 3.123355 0.719347 0.446907
N 0.861760 0.670690 -0.133706
C -0.062759 -0.341270 -0.486735
C 0.722617 -1.566788 -0.830343
H 0.182295 -2.492935 -0.624214
H 1.023845 -1.558870 -1.887154
C 1.709991 -1.935444 1.488045
H 2.556670 -1.709233 2.142907
H 0.808440 -1.477769 1.908994
H 1.568117 -3.019739 1.459615
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H -4.320481 -2.031257 -0.851265
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1C_Ac_conf_2 Eopt -747.390940
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H 3.549758 -1.586997 -1.673842
H 4.149805 -2.241004 -0.029306
C 2.121374 -1.293535 0.017938
C 2.156884 0.235211 0.207286
O 3.115411 0.906457 0.500818
N 0.849751 0.722599 -0.040301
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H 0.376378 -2.445181 -0.684912
H 1.128128 -1.399216 -1.916391
C 1.923351 -1.906699 1.416038
H 2.770215 -1.659764 2.063174
H 1.004717 -1.539234 1.885484
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H -1.415756 1.313962 1.254373
C -4.163901 -0.506361 0.426051
H -4.176720 -2.193051 -0.920077
H -3.816327 1.183507 1.721479
H -5.225734 -0.562634 0.643669
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O 1.186167 2.925184 0.471550
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H -0.078179 3.444833 -1.686033
H -0.488077 1.737394 -2.045002
H -1.391664 2.642928 -0.813225
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1C_Ac_conf_3 Eopt -747.391620
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H 0.884943 -1.957683 1.847184

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H 3.587169 -1.288355 -1.503187
H 4.253147 -1.572690 0.120027
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H -3.854773 1.199680 1.679973
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O 1.167538 2.941733 0.426138
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H -1.408177 2.614124 -0.857152

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1C_Ac_conf_4 Eopt -747.394943

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C 2.106492 0.124727 0.195802
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H 1.032168 -1.587866 -1.820876
C 3.254510 -2.021114 -0.443188
H 3.125131 -3.103555 -0.535588
H 3.479854 -1.608689 -1.431186
H 4.102224 -1.827267 0.219730
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C -2.318709 -1.313968 -0.681018
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H -1.433634 1.470790 1.093053
C -4.241295 -0.313797 0.395174
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H -3.838810 1.455289 1.562506
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H 1.096023 4.032718 0.053003

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1C_Bn_OSS_conf_1 Eopt -865.064764

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C 0.719854 1.662054 -0.715686
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H -0.433979 1.507883 1.940240
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H -1.871587 -1.125615 -1.940626
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H -3.801786 -2.628942 -1.928008
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1C_Bn_OSS_conf_2 Eopt -865.067731

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H 4.832380 0.687678 -1.075837
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C 2.358274 -0.858000 -0.538757
O 2.813626 -1.902629 -0.974054
N 1.058817 -0.421255 -0.726987
C 0.790491 0.744879 -0.003077
C 1.956894 0.992919 0.913061
H 2.193351 2.055294 1.013333
H 1.742376 0.597370 1.917945
C 4.044807 -0.467964 1.286463
H 4.534532 0.296851 1.897045
H 3.484922 -1.137856 1.946595
H 4.815131 -1.048420 0.771157
C -0.370375 1.561238 -0.076999
C -0.579348 2.525842 0.951237
C -1.338342 1.511162 -1.118714
C -1.684837 3.362587 0.942779
H 0.130833 2.595874 1.769220
C -2.438985 2.357112 -1.113164
H -1.215366 0.832815 -1.952944
C -2.631064 3.287162 -0.086057
H -1.814373 4.079279 1.748902
H -3.154186 2.295145 -1.928746
H -3.496012 3.942699 -0.090221

C 0.093793 -1.300648 -1.380506
H -0.273433 -0.858255 -2.308864
H 0.662131 -2.193399 -1.656676
C -1.055406 -1.683413 -0.472487
C -2.337486 -1.842635 -1.003099
C -0.847487 -1.913531 0.890900
C -3.398829 -2.233113 -0.185587
H -2.506206 -1.651539 -2.060551
C -1.908196 -2.296742 1.711094
H 0.147045 -1.787493 1.314756
C -3.187112 -2.458073 1.174818
H -4.391606 -2.351058 -0.609856
H -1.735756 -2.468864 2.769492
H -4.013425 -2.753583 1.814373
40
1C_Bn_OSS_conf_3 Eopt -865.068386
C -1.215219 -2.566462 1.752756
H -1.245618 -1.711007 2.419115
H -0.716315 -3.473440 2.077967
C -1.642418 -2.434454 0.321290
C -0.365568 -2.174597 -0.486415
O 0.447934 -2.999711 -0.869252
N -0.250492 -0.813783 -0.687850
C -1.370647 -0.114377 -0.234737
C -2.431137 -1.131020 0.092911
H -3.023010 -0.850562 0.967804
H -3.118963 -1.254564 -0.756985
C -2.349937 -3.696257 -0.168848
H -3.282584 -3.835237 0.386405
H -2.584268 -3.620363 -1.235275
H -1.717135 -4.574107 -0.010935
C -1.518920 1.292828 -0.110888
C -2.832098 1.816346 0.074438
C -0.447565 2.231233 -0.125406
C -3.052914 3.177727 0.215487
H -3.679906 1.138244 0.087801
C -0.686992 3.590640 0.018940
H 0.578797 1.895218 -0.207996
C -1.985807 4.083409 0.185349
H -4.068922 3.539563 0.346413
H 0.156045 4.276035 0.013229
H -2.161974 5.148523 0.296229
C 0.898597 -0.298967 -1.413801
H 1.164317 -1.057985 -2.156115
H 0.596019 0.599672 -1.956404
C 2.106798 -0.020405 -0.538734
C 3.236070 0.560440 -1.126947
C 2.129909 -0.325567 0.823147
C 4.370932 0.830639 -0.365494
H 3.221319 0.803517 -2.187224
C 3.267979 -0.056056 1.587298
H 1.258073 -0.771050 1.297460
C 4.390320 0.522039 0.996917
H 5.239667 1.283678 -0.834188
H 3.272418 -0.297973 2.646078
H 5.273709 0.733185 1.592008
40
1C_Bn_OSS_conf_4 Eopt -865.067551
C 4.004260 -0.559892 1.344159
H 3.574607 -0.975881 2.249571
H 5.032871 -0.797579 1.096902
C 3.123598 0.091284 0.336114
C 2.346852 -0.946665 -0.487158
O 2.781868 -1.993891 -0.938152
N 1.056965 -0.483443 -0.673930
C 0.815104 0.696532 0.032981
C 1.979321 0.919066 0.957255
H 2.244539 1.975364 1.051841
H 1.742100 0.537466 1.962180
C 3.943246 0.930012 -0.661082
H 4.660501 0.297495 -1.192696
H 3.290558 1.414953 -1.394783
H 4.493515 1.704583 -0.118455
C -0.317937 1.549109 -0.064788
C -0.510182 2.528558 0.952409
C -1.271795 1.521226 -1.120138
C -1.587503 3.400811 0.920721
H 0.189350 2.581046 1.780855
C -2.344062 2.402616 -1.137953
H -1.159903 0.830644 -1.945905
C -2.520156 3.347738 -0.121746
H -1.705569 4.128008 1.719177
H -3.049070 2.356870 -1.963428
H -3.362962 4.031149 -0.144193
C 0.077138 -1.333537 -1.344991
H -0.250928 -0.885832 -2.285551
H 0.620213 -2.247950 -1.600420
C -1.106344 -1.666897 -0.462185
C -2.381328 -1.778333 -1.021052
C -0.938397 -1.898893 0.906411
C -3.475632 -2.121564 -0.226037
H -2.518832 -1.585632 -2.082733
C -2.031814 -2.234671 1.704127
H 0.050589 -1.810958 1.352098
C -3.303864 -2.347046 1.139906
H -4.462484 -2.201965 -0.672308
H -1.890168 -2.408027 2.766891
H -4.155652 -2.605254 1.761966
40
1C_Bn_OSS_conf_5 Eopt -865.064630
C 0.724792 3.555426 0.954424
H 1.246531 3.171525 1.825173
H 0.995814 4.533359 0.572384
C -0.148896 2.653464 0.157865
C 0.680084 1.660948 -0.678567
O 1.708537 1.888460 -1.294047
N 0.052434 0.433117 -0.642239
C -1.060943 0.437793 0.201161
C -0.996337 1.689053 1.027924
H -1.984260 2.098321 1.254510
H -0.474334 1.499235 1.977643
C -1.033623 3.446635 -0.819122
H -0.413875 4.013302 -1.520721
H -1.687062 2.778116 -1.389865
H -1.658247 4.148780 -0.258669
C -2.156546 -0.468614 0.123950
C -3.061559 -0.549058 1.216471
C -2.429746 -1.271783 -1.015825
C -4.153469 -1.403701 1.178988
H -2.881570 0.056216 2.100563
C -3.528001 -2.121932 -1.038357
H -1.808822 -1.187954 -1.901952
C -4.394877 -2.204582 0.056181
H -4.823425 -1.450237 2.032899
H -3.720483 -2.715463 -1.927727
H -5.249888 -2.872676 0.030864
C 0.745232 -0.741392 -1.165248
H 0.066911 -1.592738 -1.099341
H 0.982785 -0.577262 -2.219653
C 2.011019 -1.056544 -0.389499
C 3.089048 -1.649734 -1.050983
C 2.106844 -0.811249 0.983415
C 4.245325 -1.998210 -0.352131
H 3.024256 -1.834098 -2.120814

C 3.263826 -1.154834 1.682920
H 1.278728 -0.344182 1.512203
C 4.336234 -1.751112 1.017962
H 5.077301 -2.454972 -0.880183
H 3.326542 -0.955724 2.748795
H 5.237321 -2.016490 1.562764
40
1C_Bn_OSS_conf_6 Eopt -865.067813
C -2.244183 -3.737945 -0.255469
H -2.790027 -3.709081 -1.192654
H -2.025373 -4.700671 0.192866
C -1.586307 -2.506743 0.259451
C -0.292693 -2.189504 -0.504047
O 0.570050 -2.976725 -0.858978
N -0.226026 -0.825039 -0.701171
C -1.374553 -0.166413 -0.262964
C -2.408000 -1.218745 0.031821
H -3.023371 -0.970133 0.900502
H -3.076165 -1.347253 -0.832630
C -1.196694 -2.659696 1.740937
H -0.487939 -3.483707 1.867569
H -0.739323 -1.740243 2.121996
H -2.092482 -2.872778 2.332097
C -1.567577 1.234037 -0.122509
C -2.898345 1.714126 0.054224
C -0.526141 2.205599 -0.114995
C -3.163183 3.066076 0.209600
H -3.724682 1.010025 0.049578
C -0.809583 3.554999 0.042793
H 0.511085 1.903349 -0.192219
C -2.124780 4.004856 0.201801
H -4.191318 3.394376 0.334093
H 0.011567 4.266401 0.053347
H -2.335284 5.062521 0.323542
C 0.910259 -0.267780 -1.417862
H 1.202408 -1.012339 -2.164827
H 0.578025 0.624119 -1.954471
C 2.107898 0.045359 -0.540656
C 3.234376 0.625773 -1.134619
C 2.123518 -0.224444 0.828411
C 4.359424 0.929462 -0.371263
H 3.225785 0.840942 -2.200982
C 3.251775 0.078313 1.594656
H 1.252838 -0.668240 1.305091
C 4.371660 0.655322 0.998615
H 5.226483 1.381013 -0.844471
H 3.250519 -0.136929 2.659193
H 5.247822 0.891798 1.594863
32
1D_Ac_conf_1 Eopt -747.460965
C -1.225819 2.194039 1.086553
H -0.742123 3.158548 1.257524
H -2.302059 2.302269 1.238677
C -0.805066 1.597426 -0.289377
C -1.828218 0.586529 -0.774292
O -2.812319 0.606902 -1.473501
N -1.223537 -0.456650 -0.061748
C -0.138634 0.384839 0.476561
C -0.532680 1.024113 1.830084
H -1.172174 0.384860 2.442552
H 0.327999 1.338809 2.422005
C -0.099219 2.461257 -1.299951
H -0.792487 3.205633 -1.705448
H 0.733540 2.991379 -0.827426
H 0.291990 1.862826 -2.129083
C 1.258518 -0.061929 0.178844
C 2.336448 0.714099 0.626723
C 1.519772 -1.195690 -0.598224
C 3.646342 0.357762 0.311311
H 2.153719 1.607598 1.218062
C 2.831609 -1.554795 -0.909262
H 0.697393 -1.805386 -0.960051
C 3.899052 -0.780782 -0.455505
H 4.469710 0.971277 0.664927
H 3.017086 -2.442473 -1.506813
H 4.919784 -1.060880 -0.697762
C -1.674810 -1.689968 0.393502
O -1.042112 -2.279364 1.252061
C -2.933440 -2.200555 -0.243842
H -3.752572 -1.496925 -0.069263
H -2.797348 -2.285745 -1.325606
H -3.175386 -3.173589 0.182725
32
1D_Ac_conf_2 Eopt -747.458018
C 1.716490 -1.774131 1.370329
H 1.516436 -2.803577 1.674643
H 2.776204 -1.556624 1.521634
C 1.192243 -1.487323 -0.069174
C 1.989240 -0.360749 -0.702637
O 2.947770 -0.282049 -1.430439
N 1.190337 0.616714 -0.095990
C 0.267515 -0.358739 0.536826
C 0.717486 -0.748049 1.961602
H 1.134658 0.071455 2.551255
H -0.074732 -1.235711 2.531392
C 0.715448 -2.631557 -0.923239
H 1.560540 -3.279247 -1.179171
H -0.018765 -3.229394 -0.373975
H 0.256517 -2.279316 -1.851711
C -1.174570 -0.187957 0.156223
C -2.194348 -0.217314 1.110248
C -1.510076 0.009543 -1.191292
C -3.527783 -0.055103 0.726433
H -1.955846 -0.353871 2.160525
C -2.839064 0.166447 -1.574734
H -0.723659 0.050230 -1.941648
C -3.853994 0.133960 -0.614751
H -4.309042 -0.073961 1.480467
H -3.083596 0.317444 -2.621924
H -4.890570 0.259781 -0.912589
C 1.309749 1.995080 0.031368
O 2.204953 2.601113 -0.529436
C 0.246321 2.649896 0.869343
H -0.689261 2.678693 0.299981
H 0.061232 2.092328 1.791644
H 0.557798 3.668241 1.101135
40
1D_Bn_conf_1 Eopt -865.124266
C -3.566933 -0.206148 -0.817403
H -4.271167 -1.030112 -0.680181
H -4.117735 0.682497 -1.135533
C -2.667646 -0.003479 0.437404
C -2.119449 1.420342 0.451483
O -2.483423 2.492994 0.906845
N -1.054489 1.083661 -0.324682
C -1.409618 -0.338068 -0.456035
C -2.333567 -0.599445 -1.669193
H -2.116017 0.019082 -2.543886
H -2.362303 -1.647815 -1.970690
C -3.034222 -0.687332 1.727843
H -3.969153 -0.268890 2.116557
H -3.186146 -1.758738 1.560745
H -2.259364 -0.559459 2.489638
C -0.315786 -1.292033 -0.067782

| | | | |
|---|---|---|---|
| C | 0.093291 | -2.325656 | -0.912954 |
| C | 0.346773 | -1.117256 | 1.156736 |
| C | 1.149729 | -3.165699 | -0.549171 |
| H | -0.396177 | -2.471585 | -1.871217 |
| C | 1.394889 | -1.955756 | 1.523471 |
| H | 0.050090 | -0.302690 | 1.813561 |
| C | 1.802718 | -2.983835 | 0.667464 |
| H | 1.462355 | -3.958089 | -1.222903 |
| H | 1.900975 | -1.803606 | 2.472565 |
| H | 2.625911 | -3.633687 | 0.949144 |
| C | -0.106440 | 1.885682 | -1.074486 |
| H | -0.375604 | 2.932870 | -0.904856 |
| H | -0.223464 | 1.666002 | -2.142629 |
| C | 1.316636 | 1.616197 | -0.634452 |
| C | 2.151206 | 0.788432 | -1.388272 |
| C | 1.783383 | 2.135513 | 0.577479 |
| C | 3.431390 | 0.468489 | -0.931362 |
| H | 1.790722 | 0.380285 | -2.330020 |
| C | 3.062045 | 1.821977 | 1.035179 |
| H | 1.133441 | 2.777475 | 1.169087 |
| C | 3.887718 | 0.982840 | 0.282526 |
| H | 4.068724 | -0.183955 | -1.521375 |
| H | 3.414883 | 2.228956 | 1.978388 |
| H | 4.882133 | 0.733280 | 0.640767 |

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1D_Bn_conf_2 Eopt -865.123170

| | | | |
|---|---|---|---|
| C | -0.011872 | 2.049426 | 1.832213 |
| H | 0.488869 | 2.364354 | 2.750719 |
| H | -0.909992 | 2.656497 | 1.690893 |
| C | 0.949447 | 2.031617 | 0.607983 |
| C | 0.154594 | 2.210680 | -0.682404 |
| O | -0.190785 | 3.156959 | -1.372480 |
| N | -0.101693 | 0.879855 | -0.777907 |
| C | 0.643358 | 0.491285 | 0.429005 |
| C | -0.205198 | 0.516335 | 1.725344 |
| H | -1.226831 | 0.142667 | 1.626912 |
| H | 0.288698 | -0.003270 | 2.548190 |
| C | 2.328053 | 2.623055 | 0.730492 |
| H | 2.260204 | 3.711293 | 0.836107 |
| H | 2.834733 | 2.226162 | 1.616360 |
| H | 2.939845 | 2.401241 | -0.149696 |
| C | 1.694421 | -0.553232 | 0.183741 |
| C | 1.901544 | -1.621466 | 1.061639 |
| C | 2.496582 | -0.458931 | -0.963988 |
| C | 2.894309 | -2.570329 | 0.804846 |
| H | 1.283977 | -1.727040 | 1.948159 |
| C | 3.490141 | -1.400517 | -1.217783 |
| H | 2.332974 | 0.356887 | -1.664267 |
| C | 3.693449 | -2.461300 | -0.331254 |
| H | 3.038054 | -3.395901 | 1.495679 |
| H | 4.103643 | -1.310255 | -2.109399 |
| H | 4.465820 | -3.198404 | -0.529357 |
| C | -0.955503 | 0.105673 | -1.657438 |
| H | -0.363259 | -0.693969 | -2.117158 |
| H | -1.289251 | 0.786038 | -2.446780 |
| C | -2.131022 | -0.477507 | -0.905663 |
| C | -2.131670 | -1.818217 | -0.516905 |
| C | -3.194735 | 0.347460 | -0.523385 |
| C | -3.179239 | -2.330637 | 0.252361 |
| H | -1.304267 | -2.460807 | -0.810124 |
| C | -4.241672 | -0.160787 | 0.242511 |
| H | -3.192945 | 1.394134 | -0.821279 |
| C | -4.233571 | -1.502290 | 0.635074 |
| H | -3.168918 | -3.374101 | 0.553340 |
| H | -5.063625 | 0.486408 | 0.534348 |
| H | -5.048086 | -1.898501 | 1.234213 |

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1E_Ac_conf_1 Eopt -747.465815

| | | | |
|---|---|---|---|
| C | 0.881445 | 2.400065 | 0.560213 |
| H | 0.828334 | 2.280165 | 1.653222 |
| H | 1.158363 | 3.441878 | 0.372845 |
| C | 1.950299 | 1.480244 | 0.029973 |
| C | 1.542284 | 0.274287 | -0.384343 |
| O | 2.432601 | -0.650375 | -0.925616 |
| N | 0.238359 | -0.220598 | -0.316204 |
| C | -0.726750 | 0.612700 | -0.137757 |
| C | -0.472879 | 2.103035 | -0.078752 |
| H | -0.487968 | 2.474959 | -1.114300 |
| H | -1.270260 | 2.614475 | 0.461796 |
| C | 3.379601 | 1.913169 | 0.103284 |
| H | 3.625940 | 2.197387 | 1.134190 |
| H | 4.069294 | 1.130287 | -0.218470 |
| H | 3.542889 | 2.800525 | -0.518900 |
| C | -2.109519 | 0.078390 | -0.051306 |
| C | -3.217798 | 0.909121 | -0.265059 |
| C | -2.322275 | -1.280763 | 0.227355 |
| C | -4.510784 | 0.388524 | -0.213228 |
| H | -3.080626 | 1.962287 | -0.489999 |
| C | -3.612770 | -1.794990 | 0.291517 |
| H | -1.465789 | -1.924730 | 0.400406 |
| C | -4.712395 | -0.961747 | 0.068556 |
| H | -5.359838 | 1.041291 | -0.391833 |
| H | -3.763474 | -2.846371 | 0.517572 |
| H | -5.719894 | -1.363983 | 0.117207 |
| C | 2.948616 | -1.633965 | -0.141631 |
| O | 3.642509 | -2.467715 | -0.673279 |
| C | 2.641146 | -1.588331 | 1.327641 |
| H | 3.038594 | -0.665406 | 1.761719 |
| H | 1.560854 | -1.602240 | 1.495576 |
| H | 3.104876 | -2.450069 | 1.804785 |

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1E_Ac_conf_2 Eopt -747.468476

| | | | |
|---|---|---|---|
| C | 0.787269 | 2.470520 | 0.519146 |
| H | 0.716210 | 2.405564 | 1.615527 |
| H | 1.043185 | 3.507949 | 0.283156 |
| C | 1.886925 | 1.550731 | 0.055047 |
| C | 1.514505 | 0.319016 | -0.311338 |
| O | 2.440058 | -0.608380 | -0.790488 |
| N | 0.223513 | -0.205626 | -0.244649 |
| C | -0.763980 | 0.611291 | -0.123829 |
| C | -0.547860 | 2.109173 | -0.127350 |
| H | -0.554745 | 2.433931 | -1.178841 |
| H | -1.367080 | 2.623713 | 0.376653 |
| C | 3.304101 | 2.022772 | 0.128706 |
| H | 3.520788 | 2.381963 | 1.142349 |
| H | 4.018532 | 1.236319 | -0.123069 |
| H | 3.462116 | 2.869113 | -0.549674 |
| C | -2.136112 | 0.048194 | -0.045081 |
| C | -3.257932 | 0.838979 | -0.328622 |
| C | -2.324390 | -1.299851 | 0.297774 |
| C | -4.539324 | 0.289840 | -0.281966 |
| H | -3.140326 | 1.882316 | -0.604669 |
| C | -3.603717 | -1.842179 | 0.355928 |
| H | -1.457632 | -1.912124 | 0.525619 |
| C | -4.716610 | -1.048990 | 0.063692 |
| H | -5.398619 | 0.911521 | -0.514565 |
| H | -3.735341 | -2.884133 | 0.632144 |
| H | -5.715377 | -1.472924 | 0.108265 |
| C | 2.926724 | -1.510452 | 0.099795 |
| O | 2.644470 | -1.488919 | 1.274151 |
| C | 3.837300 | -2.490413 | -0.572909 |
| H | 3.271952 | -3.054057 | -1.320266 |
| H | 4.636590 | -1.953860 | -1.090759 |
| H | 4.257545 | -3.169306 | 0.167421 |

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1E_Bn_conf_1 Eopt -865.129882

| | | | |
|---|---|---|---|
| C | 2.514868 | 1.167582 | -0.668133 |
| C | 3.212889 | 0.129467 | 0.279848 |
| C | 2.202674 | 0.608351 | 1.364098 |
| C | 1.268708 | 0.720558 | 0.139931 |
| H | 2.824927 | 2.193568 | -0.452090 |
| H | 2.519226 | 0.963683 | -1.743639 |
| H | 2.478475 | 1.586153 | 1.766835 |
| H | 1.917678 | -0.094412 | 2.151955 |
| N | 1.174051 | -0.731191 | -0.234376 |
| C | 2.493251 | -1.120092 | -0.225712 |
| O | 2.960662 | -2.185936 | -0.595980 |
| C | -0.041013 | 1.441719 | 0.150588 |
| C | -0.445536 | 2.190539 | -0.956201 |
| C | -0.893901 | 1.329575 | 1.254738 |
| C | -1.697523 | 2.809236 | -0.969329 |
| H | 0.217987 | 2.284816 | -1.812736 |
| C | -2.144826 | 1.942447 | 1.241882 |
| H | -0.579539 | 0.748502 | 2.118713 |
| C | -2.550333 | 2.680660 | 0.126403 |
| H | -2.005667 | 3.387432 | -1.835470 |
| H | -2.804608 | 1.844314 | 2.099088 |
| H | -3.526287 | 3.156969 | 0.115556 |
| C | 4.699463 | 0.043941 | 0.486257 |
| H | 4.942552 | -0.706514 | 1.245530 |
| H | 5.203839 | -0.237106 | -0.443839 |
| H | 5.094318 | 1.009193 | 0.816204 |
| C | 0.215531 | -1.245792 | -1.197030 |
| H | 0.145219 | -0.572259 | -2.062611 |
| H | 0.619840 | -2.200645 | -1.549903 |
| C | -1.159886 | -1.450772 | -0.597719 |
| C | -2.294768 | -0.948070 | -1.236494 |
| C | -1.307781 | -2.137602 | 0.612048 |
| C | -3.561001 | -1.118232 | -0.671488 |
| H | -2.185566 | -0.404118 | -2.172284 |
| C | -2.568998 | -2.309133 | 1.178802 |
| H | -0.424863 | -2.522450 | 1.117647 |
| C | -3.700595 | -1.794561 | 0.540001 |
| H | -4.434622 | -0.710760 | -1.172384 |
| H | -2.670908 | -2.839556 | 2.121300 |
| H | -4.682995 | -1.919912 | 0.985653 |

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1E_Bn_conf_2 Eopt -865.129765

| | | | |
|---|---|---|---|
| C | -1.810214 | -0.254736 | -1.425196 |
| C | -3.036537 | -0.217229 | -0.455242 |
| C | -2.449835 | -1.530389 | 0.154046 |
| C | -1.112494 | -0.809746 | -0.159467 |
| H | -1.935251 | -1.007831 | -2.208166 |
| H | -1.441585 | 0.692755 | -1.828489 |
| H | -2.625628 | -2.394268 | -0.492323 |
| H | -2.662418 | -1.753788 | 1.203312 |
| N | -1.234003 | 0.365001 | 0.764509 |
| C | -2.505668 | 0.797502 | 0.568260 |
| O | -3.073106 | 1.758596 | 1.074946 |
| C | 0.226325 | -1.474126 | -0.153603 |
| C | 1.081848 | -1.353477 | -1.251781 |
| C | 0.646814 | -2.191382 | 0.971498 |
| C | 2.352547 | -1.928393 | -1.220303 |
| H | 0.757503 | -0.795642 | -2.127177 |
| C | 1.916906 | -2.765551 | 1.004611 |
| H | -0.020576 | -2.291239 | 1.824750 |
| C | 2.773859 | -2.630033 | -0.089819 |
| H | 3.014658 | -1.823548 | -2.074808 |
| H | 2.238553 | -3.316817 | 1.883325 |
| H | 3.764727 | -3.073679 | -0.062776 |
| C | -4.461516 | -0.061740 | -0.908977 |
| H | -5.149892 | -0.142919 | -0.061519 |
| H | -4.614275 | 0.915469 | -1.378451 |
| H | -4.716304 | -0.838076 | -1.636380 |
| C | -0.204442 | 0.986758 | 1.565931 |
| H | 0.147719 | 0.295774 | 2.340435 |
| H | -0.689488 | 1.830560 | 2.069035 |
| C | 0.975906 | 1.464089 | 0.742690 |
| C | 2.278037 | 1.112068 | 1.103742 |
| C | 0.772636 | 2.240353 | -0.402972 |
| C | 3.364347 | 1.519560 | 0.326774 |
| H | 2.441004 | 0.498840 | 1.987533 |
| C | 1.854260 | 2.646757 | -1.182650 |
| H | -0.240262 | 2.514942 | -0.690581 |
| C | 3.154205 | 2.282778 | -0.821698 |
| H | 4.371598 | 1.229713 | 0.612281 |
| H | 1.684231 | 3.245015 | -2.073203 |
| H | 3.996654 | 2.592581 | -1.432990 |

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1F_Ac_conf_1 Eopt -747.462956

| | | | |
|---|---|---|---|
| C | -0.883989 | -1.378539 | -1.064165 |
| C | -1.997271 | -1.354843 | 0.035988 |
| C | -0.829624 | -1.443914 | 1.062170 |
| C | -0.103328 | -0.576981 | 0.003668 |
| H | -0.487896 | -2.387322 | -1.202922 |
| H | -1.087661 | -0.886028 | -2.019003 |
| H | -0.413477 | -2.452712 | 1.109974 |
| H | -0.974578 | -1.013785 | 2.056866 |
| N | -0.947564 | 0.670425 | 0.081016 |
| C | -2.253259 | 0.139859 | 0.099469 |
| O | -3.305350 | 0.737629 | 0.140409 |
| C | 1.383977 | -0.422169 | 0.025334 |
| C | 2.144033 | -0.718378 | -1.106032 |
| C | 2.025629 | -0.040487 | 1.208009 |
| C | 3.535495 | -0.611012 | -1.065708 |
| H | 1.648235 | -1.027023 | -2.023086 |
| C | 3.413106 | 0.069629 | 1.248856 |
| H | 1.433582 | 0.180239 | 2.093421 |
| C | 4.171749 | -0.213074 | 0.109553 |
| H | 4.120419 | -0.839509 | -1.951799 |
| H | 3.905053 | 0.372355 | 2.168603 |
| H | 5.254004 | -0.129428 | 0.141978 |
| C | -3.200860 | -2.255016 | 0.039149 |
| H | -3.790878 | -2.108843 | 0.949365 |
| H | -3.842750 | -2.046481 | -0.822514 |
| H | -2.887583 | -3.301590 | -0.006830 |
| C | -0.565363 | 1.976096 | -0.192746 |
| O | 0.582146 | 2.247650 | -0.505802 |
| C | -1.634973 | 3.029574 | -0.069712 |
| H | -2.384703 | 2.897333 | -0.854268 |
| H | -2.150153 | 2.960961 | 0.890359 |
| H | -1.154965 | 4.002156 | -0.177096 |

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1F_Ac_conf_2 Eopt -747.458742

| | | | |
|---|---|---|---|
| C | -0.992806 | -1.219126 | -1.131706 |
| C | -2.091439 | -1.246042 | -0.014234 |
| C | -0.920357 | -1.478816 | 0.979671 |
| C | -0.167601 | -0.552148 | -0.007041 |
| H | -0.648994 | -2.228429 | -1.370616 |
| H | -1.184690 | -0.630897 | -2.033721 |
| H | -0.543534 | -2.502666 | 0.928452 |
| H | -1.031333 | -1.133976 | 2.011391 |
| N | -0.945238 | 0.723118 | 0.207390 |
| C | -2.280120 | 0.246411 | 0.202844 |
| O | -3.303649 | 0.878506 | 0.305933 |
| C | 1.324460 | -0.471717 | 0.049623 |
| C | 2.104591 | -0.833501 | -1.048896 |
| C | 1.946308 | -0.070635 | 1.237661 |

C 3.497231 -0.776077 -0.970090
H 1.623371 -1.149207 -1.971336
C 3.335466 -0.009678 1.315674
H 1.337775 0.204845 2.096225
C 4.114013 -0.359786 0.209331
H 4.098201 -1.053969 -1.830797
H 3.811903 0.308988 2.238017
H 5.197157 -0.312297 0.269941
C -3.334659 -2.088574 -0.075076
H -3.906110 -2.002184 0.854443
H -3.977056 -1.771747 -0.902682
H -3.070667 -3.139320 -0.223370
C -0.620290 2.034516 -0.144949
O -1.371498 2.947354 0.150803
C 0.653780 2.275787 -0.914425
H 1.526631 2.180340 -0.262794
H 0.763483 1.564426 -1.736480
H 0.610239 3.293688 -1.302615
40
1F_Bn_conf_1 Eopt -865.129882
C 2.514868 1.167582 -0.668133
C 3.212889 0.129467 0.279848
C 2.202674 0.608351 1.364098
C 1.268708 0.720558 0.139931
H 2.824927 2.193568 -0.452090
H 2.519226 0.963683 -1.743639
H 2.478475 1.586153 1.766835
H 1.917678 -0.094412 2.151955
N 1.174051 -0.731191 -0.234376
C 2.493251 -1.120092 -0.225712
O 2.960662 -2.185936 -0.595980
C -0.041013 1.441719 0.150588
C -0.445536 2.190539 -0.956201
C -0.893901 1.329575 1.254738
C -1.697523 2.809236 -0.969329
H 0.217987 2.284816 -1.812736
C -2.144826 1.942447 1.241882
H -0.579539 0.748502 2.118713
C -2.550333 2.680660 0.126403
H -2.005667 3.387432 -1.835470
H -2.804608 1.844314 2.099088
H -3.526287 3.156969 0.115556
C 4.699463 0.043941 0.486257
H 4.942552 -0.706514 1.245530
H 5.203839 -0.237106 -0.443839
H 5.094318 1.009193 0.816204
C 0.215531 -1.245792 -1.197030
H 0.145219 -0.572259 -2.062611
H 0.619840 -2.200645 -1.549903
C -1.159886 -1.450772 -0.597719
C -2.294768 -0.948070 -1.236494
C -1.307781 -2.137602 0.612048
C -3.561001 -1.118232 -0.671488
H -2.185566 -0.404118 -2.172284
C -2.568998 -2.309133 1.178802
H -0.424863 -2.522450 1.117647
C -3.700595 -1.794561 0.540001
H -4.434622 -0.710760 -1.172384
H -2.670908 -2.839556 2.121300
H -4.682995 -1.919912 0.985653
40
1F_Bn_conf_2 Eopt -865.129765
C -1.810214 -0.254736 -1.425196
C -3.036537 -0.217229 -0.455242
C -2.449835 -1.530389 0.154046
C -1.112494 -0.809746 -0.159467
H -1.935251 -1.007831 -2.208166
H -1.441585 0.692755 -1.828489
H -2.625628 -2.394268 -0.492323
H -2.662418 -1.753788 1.203312
N -1.234003 0.365001 0.764509
C -2.505668 0.797502 0.568260
O -3.073106 1.758596 1.074946
C 0.226325 -1.474126 -0.153603
C 1.081848 -1.353477 -1.251781
C 0.646814 -2.191382 0.971498
C 2.352547 -1.928393 -1.220303
H 0.757503 -0.795642 -2.127177
C 1.916906 -2.765551 1.004611
H -0.020576 -2.291239 1.824750
C 2.773859 -2.630033 -0.089819
H 3.014658 -1.823548 -2.074808
H 2.238553 -3.316817 1.883325
H 3.764727 -3.073679 -0.062776
C -4.461516 -0.061740 -0.908977
H -5.149892 -0.142919 -0.061519
H -4.614275 0.915469 -1.378451
H -4.716304 -0.838076 -1.636380
C -0.204442 0.986758 1.565931
H 0.147719 0.295774 2.340435
H -0.689488 1.830560 2.069035
C 0.975906 1.464089 0.742690
C 2.278037 1.112068 1.103742
C 0.772636 2.240353 -0.402972
C 3.364347 1.519560 0.326774
H 2.441004 0.498840 1.987533
C 1.854260 2.646757 -1.182650
H -0.240262 2.514942 -0.690581
C 3.154205 2.282778 -0.821698
H 4.371598 1.229713 0.612281
H 1.684231 3.245015 -2.073203
H 3.996654 2.592581 -1.432990
32
1TS-III Ac conf 1 Eopt -747.416985
C 1.978576 -2.108824 -0.442615
H 1.941913 -2.246143 -1.534049
H 2.451904 -3.007823 -0.035020
C 2.812304 -0.890860 -0.104373
C 2.153813 0.272479 0.027909
O 2.461902 1.533950 0.221244
N 0.729350 0.321409 -0.089462
C -0.085728 -0.679239 -0.058436
C 0.555754 -2.031706 0.118624
H 0.572165 -2.198461 1.207658
H -0.082805 -2.801230 -0.318494
C 4.305314 -0.994505 -0.085891
H 4.679521 -1.390904 -1.039356
H 4.768962 -0.018972 0.082441
H 4.648717 -1.679094 0.699586
C -1.546080 -0.510192 -0.084506
C -2.347869 -1.464741 0.561003
C -2.148266 0.574780 -0.740547
C -3.731074 -1.316068 0.576967
H -1.891857 -2.310291 1.066495
C -3.533579 0.705973 -0.734677
H -1.536632 1.296003 -1.272223
C -4.325657 -0.232433 -0.071335
H -4.344591 -2.048810 1.091325
H -3.995032 1.540017 -1.253761
H -5.405960 -0.123641 -0.066459
C 0.635343 1.891795 0.037880
O 0.382965 2.529427 -0.962909
C 0.256533 2.288888 1.437966
H -0.835881 2.256447 1.516492

H 0.697564 1.628586 2.184803
H 0.591328 3.315348 1.602304
32
1TS-III_Ac_conf_2 Eopt -747.401930
C 1.880696 -1.545192 1.320475
H 1.894351 -2.591902 1.632316
H 2.826238 -1.099525 1.657371
C 1.789227 -1.483763 -0.193135
C 1.710306 -0.192440 -0.847017
O 2.039771 0.077679 -1.992338
N 0.998773 0.692710 0.017492
C 0.061715 -0.161125 0.676206
C 0.638511 -0.836081 1.887089
H 0.875440 -0.095130 2.662409
H -0.052837 -1.562323 2.314004
C 2.129772 -2.684780 -0.998819
H 3.179863 -2.964872 -0.826141
H 1.523194 -3.540938 -0.683527
H 1.992203 -2.509056 -2.067449
C -1.306979 -0.174095 0.225624
C -2.292680 -0.933685 0.896840
C -1.698087 0.573763 -0.910736
C -3.607512 -0.940550 0.447775
H -2.030488 -1.519537 1.770933
C -3.012381 0.549574 -1.357572
H -0.961245 1.172317 -1.438086
C -3.976008 -0.204746 -0.681603
H -4.350357 -1.526717 0.980333
H -3.289942 1.127073 -2.234208
H -5.004011 -0.216621 -1.030030
C 1.231037 2.033958 0.242177
O 2.149397 2.623891 -0.306099
C 0.260682 2.705130 1.180109
H -0.683946 2.883227 0.654398
H 0.046572 2.085684 2.055367
H 0.680423 3.660986 1.492876
40
1TS-III_Bn_conf_1 Eopt -865.056158
C -0.534181 2.652310 -1.287713
H -1.027632 3.555030 -1.654466
H 0.510984 2.687933 -1.629141
C -0.597407 2.586312 0.220840
C -0.079232 1.453380 0.854252
O 0.034867 1.175267 2.057938
N 0.221253 0.373220 -0.168031
C -1.070976 0.413031 -0.668224
C -1.255403 1.402894 -1.786747
H -0.847728 0.978545 -2.717205
H -2.315571 1.617396 -1.936090
C -1.008805 3.775978 1.022560
H -0.276269 4.590100 0.919545
H -1.969580 4.172220 0.673268
H -1.088499 3.526825 2.083520
C -2.096871 -0.564279 -0.314791
C -3.101650 -0.893179 -1.244194
C -2.113941 -1.167756 0.957845
C -4.077119 -1.828969 -0.918685
H -3.106609 -0.433803 -2.227693
C -3.115018 -2.073740 1.287805
H -1.368919 -0.892265 1.696804
C -4.090154 -2.416148 0.348295
H -4.834451 -2.093224 -1.649896
H -3.132821 -2.517079 2.278426
H -4.861660 -3.135871 0.604604
C 0.841781 -0.851360 0.331761
H 0.686628 -0.950371 1.411785
H 0.378440 -1.712014 -0.158262
C 2.332944 -0.851638 0.062637
C 3.015868 -2.071708 0.007501
C 3.057190 0.335350 -0.079643
C 4.396231 -2.106735 -0.185539
H 2.459323 -3.000480 0.112772
C 4.439472 0.302427 -0.273479
H 2.540121 1.290529 -0.045613
C 5.113751 -0.917314 -0.326676
H 4.910505 -3.062355 -0.232236
H 4.988700 1.233135 -0.383641
H 6.188451 -0.942057 -0.480612
40
1TS-III_Bn_conf_2 Eopt -865.064657
C -0.285609 2.080701 1.749004
H 0.168519 2.475853 2.661789
H -1.333851 2.414102 1.740446
C 0.465116 2.622899 0.545262
C -0.092172 2.180285 -0.761255
O -0.515216 2.907995 -1.654856
N -0.064809 0.818840 -0.773977
C 0.617207 0.334481 0.390175
C -0.125807 0.549726 1.688197
H -1.080269 0.006116 1.695647
H 0.462650 0.202312 2.538126
C 1.200457 3.914870 0.630711
H 0.495559 4.741206 0.814454
H 1.904409 3.906067 1.468900
H 1.742629 4.138621 -0.291606
C 1.743703 -0.544538 0.194070
C 2.265613 -1.332173 1.247016
C 2.367161 -0.640738 -1.074152
C 3.354860 -2.170227 1.036751
H 1.811844 -1.294994 2.231772
C 3.459911 -1.474439 -1.271403
H 1.991497 -0.040196 -1.897286
C 3.961594 -2.247790 -0.219542
H 3.733148 -2.769014 1.860198
H 3.924275 -1.524367 -2.252002
H 4.812966 -2.902413 -0.377865
C -0.863334 -0.028205 -1.655699
H -1.289281 0.635195 -2.413286
H -0.211720 -0.753641 -2.154362
C -1.944589 -0.746733 -0.880489
C -1.766794 -2.072061 -0.478142
C -3.097030 -0.059486 -0.482827
C -2.723822 -2.703711 0.319562
H -0.870936 -2.608291 -0.784409
C -4.055179 -0.687481 0.310278
H -3.235392 0.975053 -0.790973
C -3.867430 -2.011480 0.716797
H -2.574281 -3.733399 0.631021
H -4.947322 -0.146768 0.612641
H -4.612184 -2.500681 1.337597
40
1TS-III_Bn_conf_3 Eopt -865.063924
C -3.383877 0.041656 1.006767
H -3.910008 0.992098 0.867486
H -4.087142 -0.644596 1.501611
C -2.985649 -0.453036 -0.371941
C -1.937282 -1.495627 -0.463267
O -2.038725 -2.567285 -1.055102
N -0.826985 -1.054532 0.208128
C -1.076275 0.278558 0.664139
C -2.082648 0.318257 1.784964
H -1.854426 -0.469499 2.511822
H -2.121671 1.267100 2.319744
C -3.960155 -0.308925 -1.489627

H -4.891886 -0.846829 -1.254468
H -4.232725 0.742954 -1.629914
H -3.567774 -0.706523 -2.428501
C -0.308531 1.379910 0.146600
C -0.423788 2.678501 0.696166
C 0.576046 1.200402 -0.945660
C 0.319332 3.736819 0.183736
H -1.093005 2.858239 1.530874
C 1.308701 2.264011 -1.452088
H 0.677803 0.213568 -1.385328
C 1.190631 3.540775 -0.890191
H 0.217362 4.723032 0.627220
H 1.981167 2.098535 -2.289149
H 1.770334 4.369467 -1.284727
C 0.119876 -1.949578 0.876831
H -0.038125 -1.890252 1.961425
H -0.124236 -2.960909 0.540452
C 1.551740 -1.605852 0.541159
C 2.113902 -2.037323 -0.664794
C 2.304644 -0.793352 1.391743
C 3.403069 -1.647491 -1.023548
H 1.529109 -2.669094 -1.330378
C 3.595981 -0.399145 1.035796
H 1.870877 -0.456067 2.330947
C 4.145171 -0.822060 -0.174703
H 3.829431 -1.985045 -1.963772
H 4.169915 0.239358 1.701086
H 5.148351 -0.514541 -0.454994

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1TS-IV_Ac_conf_1 Eopt -747.404927

C 1.555326 -1.919046 1.186671
H 1.247246 -2.962928 1.290348
H 2.560636 -1.842791 1.623356
C 1.591063 -1.597797 -0.296234
C 1.723677 -0.227126 -0.755350
O 2.250810 0.157924 -1.790350
N 1.000792 0.612993 0.129859
C -0.012220 -0.219047 0.697674
C 0.501331 -1.017286 1.856502
H 0.929517 -0.338776 2.604503
H -0.275590 -1.608001 2.340793
C 1.890932 -2.697746 -1.252541
H 2.877800 -3.130356 -1.028536
H 1.162668 -3.508829 -1.142309
H 1.895608 -2.348644 -2.286787
C -1.365980 -0.093486 0.229953
C -2.403174 -0.883387 0.776528
C -1.689581 0.819041 -0.801652
C -3.704657 -0.763670 0.305488
H -2.187343 -1.594653 1.566646
C -2.992400 0.924751 -1.269461
H -0.910266 1.442779 -1.229118
C -4.007956 0.136223 -0.719929
H -4.488235 -1.378399 0.738109
H -3.220814 1.629918 -2.062923
H -5.026341 0.224467 -1.085415
C 1.237034 1.914580 0.521942
O 0.499097 2.444664 1.341872
C 2.405228 2.613964 -0.115722
H 3.302184 1.990802 -0.089368
H 2.179065 2.826697 -1.163863
H 2.577321 3.547255 0.420170

32

1TS-IV_Ac_conf_2 Eopt -747.401930

C 1.880696 -1.545192 1.320475
H 1.894351 -2.591902 1.632316
H 2.826238 -1.099525 1.657371
C 1.789227 -1.483763 -0.193135
C 1.710306 -0.192440 -0.847017
O 2.039771 0.077679 -1.992338
N 0.998773 0.692710 0.017492
C 0.061715 -0.161125 0.676206
C 0.638511 -0.836081 1.887089
H 0.875440 -0.095130 2.662409
H -0.052837 -1.562323 2.314004
C 2.129772 -2.684780 -0.998819
H 3.179863 -2.964872 -0.826141
H 1.523194 -3.540938 -0.683527
H 1.992203 -2.509056 -2.067449
C -1.306979 -0.174095 0.225624
C -2.292680 -0.933685 0.896840
C -1.698087 0.573763 -0.910736
C -3.607512 -0.940550 0.447775
H -2.030488 -1.519537 1.770933
C -3.012381 0.549574 -1.357572
H -0.961245 1.172317 -1.438086
C -3.976008 -0.204746 -0.681603
H -4.350357 -1.526717 0.980333
H -3.289942 1.127073 -2.234208
H -5.004011 -0.216621 -1.030030
C 1.231037 2.033958 0.242177
O 2.149397 2.623891 -0.306099
C 0.260682 2.705130 1.180109
H -0.683946 2.883227 0.654398
H 0.046572 2.085684 2.055367
H 0.680423 3.660986 1.492876

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1TS-IV_Bn_conf_1 Eopt -865.056158

C -0.534181 2.652310 -1.287713
H -1.027632 3.555030 -1.654466
H 0.510984 2.687933 -1.629141
C -0.597407 2.586312 0.220840
C -0.079232 1.453380 0.854252
O 0.034867 1.175267 2.057938
N 0.221253 0.373220 -0.168031
C -1.070976 0.413031 -0.668224
C -1.255403 1.402894 -1.786747
H -0.847728 0.978545 -2.717205
H -2.315571 1.617396 -1.936090
C -1.008805 3.775978 1.022560
H -0.276269 4.590100 0.919545
H -1.969580 4.172220 0.673268
H -1.088499 3.526825 2.083520
C -2.096871 -0.564279 -0.314791
C -3.101650 -0.893179 -1.244194
C -2.113941 -1.167756 0.957845
C -4.077119 -1.828969 -0.918685
H -3.106609 -0.433803 -2.227693
C -3.115018 -2.073740 1.287805
H -1.368919 -0.892265 1.696804
C -4.090154 -2.416148 0.348295
H -4.834451 -2.093224 -1.649896
H -3.132821 -2.517079 2.278426
H -4.861660 -3.135871 0.604604
C 0.841781 -0.851360 0.331761
H 0.686628 -0.950371 1.411785
H 0.378440 -1.712014 -0.158262
C 2.332944 -0.851638 0.062637
C 3.015868 -2.071708 0.007501
C 3.057190 0.335350 -0.079643
C 4.396231 -2.106735 -0.185539
H 2.459323 -3.000480 0.112772
C 4.439472 0.302427 -0.273479
H 2.540121 1.290529 -0.045613

C 5.113751 -0.917314 -0.326676
H 4.910505 -3.062355 -0.232236
H 4.988700 1.233135 -0.383641
H 6.188451 -0.942057 -0.480612
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1TS-IV_Bn_conf_2 Eopt -865.064657
C -0.285609 2.080701 1.749004
H 0.168519 2.475853 2.661789
H -1.333851 2.414102 1.740446
C 0.465116 2.622899 0.545262
C -0.092172 2.180285 -0.761255
O -0.515216 2.907995 -1.654856
N -0.064809 0.818840 -0.773977
C 0.617207 0.334481 0.390175
C -0.125807 0.549726 1.688197
H -1.080269 0.006116 1.695647
H 0.462650 0.202312 2.538126
C 1.200457 3.914870 0.630711
H 0.495559 4.741206 0.814454
H 1.904409 3.906067 1.468900
H 1.742629 4.138621 -0.291606
C 1.743703 -0.544538 0.194070
C 2.265613 -1.332173 1.247016
C 2.367161 -0.640738 -1.074152
C 3.354860 -2.170227 1.036751
H 1.811844 -1.294994 2.231772
C 3.459911 -1.474439 -1.271403
H 1.991497 -0.040196 -1.897286
C 3.961594 -2.247790 -0.219542
H 3.733148 -2.769014 1.860198
H 3.924275 -1.524367 -2.252002
H 4.812966 -2.902413 -0.377865
C -0.863334 -0.028205 -1.655699
H -1.289281 0.635195 -2.413286
H -0.211720 -0.753641 -2.154362
C -1.944589 -0.746733 -0.880489
C -1.766794 -2.072061 -0.478142
C -3.097030 -0.059486 -0.482827
C -2.723822 -2.703711 0.319562
H -0.870936 -2.608291 -0.784409
C -4.055179 -0.687481 0.310278
H -3.235392 0.975053 -0.790973
C -3.867430 -2.011480 0.716797
H -2.574281 -3.733399 0.631021
H -4.947322 -0.146768 0.612641
H -4.612184 -2.500681 1.337597
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1TS-IV_Bn_conf_3 Eopt -865.063924
C -3.383877 0.041656 1.006767
H -3.910008 0.992098 0.867486
H -4.087142 -0.644596 1.501611
C -2.985649 -0.453036 -0.371941
C -1.937282 -1.495627 -0.463267
O -2.038725 -2.567285 -1.055102
N -0.826985 -1.054532 0.208128
C -1.076275 0.278558 0.664139
C -2.082648 0.318257 1.784964
H -1.854426 -0.469499 2.511822
H -2.121671 1.267100 2.319744
C -3.960155 -0.308925 -1.489627
H -4.891886 -0.846829 -1.254468
H -4.232725 0.742954 -1.629914
H -3.567774 -0.706523 -2.428501
C -0.308531 1.379910 0.146600
C -0.423788 2.678501 0.696166
C 0.576046 1.200402 -0.945660
C 0.319332 3.736819 0.183736
H -1.093005 2.858239 1.530874
C 1.308701 2.264011 -1.452088
H 0.677803 0.213568 -1.385328
C 1.190631 3.540775 -0.890191
H 0.217362 4.723032 0.627220
H 1.981167 2.098535 -2.289149
H 1.770334 4.369467 -1.284727
C 0.119876 -1.949578 0.876831
H -0.038125 -1.890252 1.961425
H -0.124236 -2.960909 0.540452
C 1.551740 -1.605852 0.541159
C 2.113902 -2.037323 -0.664794
C 2.304644 -0.793352 1.391743
C 3.403069 -1.647491 -1.023548
H 1.529109 -2.669094 -1.330378
C 3.595981 -0.399145 1.035796
H 1.870877 -0.456067 2.330947
C 4.145171 -0.822060 -0.174703
H 3.829431 -1.985045 -1.963772
H 4.169915 0.239358 1.701086
H 5.148351 -0.514541 -0.454994
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1TS-V_Ac_conf_1 Eopt -747.385165
C 1.131880 -1.720848 1.377455
H 0.480595 -2.589799 1.381672
H 1.460056 -1.325873 2.335906
C 1.913294 -1.431731 0.116261
C 2.171909 0.074153 0.157253
O 3.223456 0.646274 0.313983
N 0.904404 0.675330 -0.044922
C -0.019187 -0.389084 -0.298311
C 0.784229 -1.493328 -0.933998
H 0.282881 -2.462429 -0.919956
H 1.115214 -1.251573 -1.953270
C 3.178147 -2.243935 -0.098337
H 2.928210 -3.307054 -0.154990
H 3.679217 -1.949814 -1.026197
H 3.873094 -2.094368 0.733446
C -1.437121 -0.290895 -0.112360
C -2.291860 -1.217369 -0.749687
C -2.014015 0.669546 0.750858
C -3.666156 -1.176798 -0.537506
H -1.873685 -1.960564 -1.422062
C -3.384943 0.696322 0.960517
H -1.376307 1.378383 1.269994
C -4.222731 -0.222586 0.316595
H -4.306222 -1.893389 -1.043876
H -3.807914 1.436442 1.633581
H -5.295160 -0.194170 0.482490
C 0.685941 2.023869 -0.374378
O -0.321116 2.347659 -0.977037
C 1.727195 3.015222 0.062893
H 1.298135 4.011427 -0.045562
H 2.038540 2.840320 1.094217
H 2.614313 2.928448 -0.570044
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1TS-V_Bn_conf_1 Eopt -865.054165
C 1.029471 1.917470 1.687164
H 1.926199 1.840262 2.297845
H 0.078949 1.964743 2.215739
C 1.183622 2.582803 0.330316
C -0.054930 2.173380 -0.471735
O -0.996153 2.858189 -0.837163
N 0.091645 0.824009 -0.702941
C 1.350167 0.418856 -0.197834
C 2.229370 1.645764 -0.294601
H 3.130439 1.587145 0.318736

H 2.492166 1.893901 -1.334071
C 1.432990 4.080323 0.341553
H 2.351633 4.302769 0.892318
H 1.532647 4.468281 -0.677563
H 0.602822 4.601405 0.828388
C 1.790415 -0.949860 -0.095077
C 3.172321 -1.234573 -0.182507
C 0.905316 -2.028689 0.134693
C 3.642695 -2.536652 -0.054854
H 3.875963 -0.427537 -0.362272
C 1.385666 -3.326107 0.261573
H -0.158417 -1.847122 0.247262
C 2.754888 -3.592286 0.165942
H 4.708781 -2.729196 -0.132341
H 0.685959 -4.136382 0.444533
H 3.123966 -4.608176 0.266430
C -0.920581 0.055803 -1.402461
H -0.445435 -0.830586 -1.831559
H -1.270114 0.672292 -2.237471
C -2.114391 -0.340280 -0.552860
C -3.225856 -0.910753 -1.183512
C -2.135935 -0.163431 0.831660
C -4.339149 -1.299364 -0.441481
H -3.216735 -1.047920 -2.262682
C -3.252869 -0.548946 1.576788
H -1.275568 0.272813 1.333653
C -4.356413 -1.118229 0.943715
H -5.195180 -1.740569 -0.943697
H -3.256161 -0.403575 2.653136
H -5.224994 -1.417487 1.522623

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1TS-V_Bn_conf_2 Eopt -865.054362

C 3.133015 1.375650 -0.609204
H 3.336330 2.341864 -0.153869
H 3.394813 1.252969 -1.658090
C 3.074265 0.173994 0.317318
C 2.408183 -0.937363 -0.500206
O 2.897951 -1.973523 -0.919691
N 1.109666 -0.518802 -0.684491
C 0.911604 0.665123 0.068221
C 1.895908 0.591192 1.213289
H 2.076409 1.554924 1.694140
H 1.615203 -0.162053 1.965962
C 4.384587 -0.243606 0.959844
H 4.786408 0.579625 1.557892
H 4.241684 -1.112378 1.610788
H 5.119813 -0.505445 0.192658
C -0.264983 1.491764 -0.014088
C -0.696380 2.193298 1.133919
C -0.992611 1.666455 -1.213476
C -1.816124 3.016727 1.086710
H -0.155765 2.074413 2.068438
C -2.108930 2.492368 -1.250663
H -0.661830 1.178878 -2.124569
C -2.532296 3.170320 -0.102853
H -2.134223 3.538215 1.984779
H -2.649383 2.616087 -2.184700
H -3.405760 3.813947 -0.137789
C 0.115643 -1.321204 -1.380419
H 0.637389 -2.242241 -1.660245
H -0.206741 -0.838557 -2.307171
C -1.082832 -1.642540 -0.512007
C -2.369151 -1.615076 -1.054501
C -0.917727 -1.983381 0.834321
C -3.477552 -1.930313 -0.266485
H -2.503991 -1.335509 -2.097044
C -2.023437 -2.292402 1.625221
H 0.080845 -1.998755 1.266386
C -3.307347 -2.267278 1.076290
H -4.473156 -1.901967 -0.699581
H -1.883330 -2.551766 2.670587
H -4.169004 -2.504816 1.693006

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1TS-V_Bn_conf_3 Eopt -865.051554

C -1.495011 2.929649 -0.460175
H -2.397624 3.217020 0.073487
H -1.420114 3.216448 -1.506996
C -0.244268 2.698592 0.367537
C 0.717806 1.927553 -0.544126
O 1.783900 2.288515 -1.014731
N 0.128798 0.698717 -0.735951
C -1.008730 0.620414 0.105358
C -0.732166 1.546930 1.267430
H -1.628132 1.822058 1.828174
H 0.039119 1.155467 1.948975
C 0.377870 3.927493 1.005479
H -0.342034 4.406050 1.675970
H 1.269569 3.659750 1.581786
H 0.668869 4.650499 0.237071
C -2.006894 -0.412296 0.016527
C -2.685618 -0.825244 1.184274
C -2.374867 -1.000901 -1.215258
C -3.677928 -1.797746 1.122404
H -2.419095 -0.385189 2.141209
C -3.367664 -1.971377 -1.265816
H -1.909156 -0.661422 -2.135970
C -4.022988 -2.380331 -0.099612
H -4.182546 -2.105761 2.033559
H -3.642394 -2.404777 -2.223071
H -4.798496 -3.138576 -0.145622
C 0.834616 -0.385054 -1.409893
H 1.261787 0.012684 -2.333902
H 0.111591 -1.156899 -1.677972
C 1.929610 -0.982908 -0.548261
C 3.223422 -1.129158 -1.052244
C 1.653431 -1.413291 0.754917
C 4.229379 -1.699883 -0.269658
H 3.445415 -0.788820 -2.060898
C 2.656500 -1.979537 1.539475
H 0.648209 -1.305115 1.158406
C 3.948387 -2.125100 1.028103
H 5.232596 -1.804540 -0.672470
H 2.430121 -2.309476 2.549209
H 4.730211 -2.565371 1.639800

32

3A_Ac_conf_10 Eopt -747.353832

C -3.661986 -1.399325 1.004559
H -3.751511 -0.977373 2.001443
H -4.488548 -1.996401 0.629061
C -2.581968 -1.178843 0.251841
C -1.457460 -0.400715 0.869460
O -1.038433 -0.656332 1.984101
N -0.797660 0.585125 0.101654
C 0.501093 0.988203 0.583713
C 0.544423 2.106176 1.524566
H 0.394649 1.930157 2.586527
H 0.658711 3.130646 1.181113
C -2.363529 -1.777578 -1.111471
H -3.258325 -2.319990 -1.425812
H -2.134171 -1.020717 -1.865276
H -1.525540 -2.483398 -1.081475
C 1.635824 0.205260 0.207523
C 2.916399 0.509626 0.734084
C 1.525922 -0.877779 -0.700227

C 4.027131 -0.239216 0.371281
H 3.021712 1.336860 1.430853
C 2.645199 -1.618447 -1.054866
H 0.557361 -1.125145 -1.125083
C 3.901575 -1.307429 -0.523704
H 4.999127 0.008027 0.787833
H 2.540712 -2.444237 -1.752475
H 4.773219 -1.890174 -0.804661
C -1.430702 1.338396 -0.903453
O -2.626787 1.252296 -1.105703
C -0.527725 2.245722 -1.693915
H -1.095953 2.646635 -2.532753
H -0.181050 3.074597 -1.068611
H 0.349806 1.702621 -2.055796
32
3A_Ac_conf_11 Eopt -747.353939
C 3.485742 -0.183511 -1.063638
H 2.757100 -0.222673 -1.869956
H 4.529422 -0.055871 -1.338579
C 3.131843 -0.316010 0.219023
C 1.707724 -0.627451 0.547127
O 1.415221 -1.473306 1.372806
N 0.692746 -0.011468 -0.216823
C -0.454745 -0.814674 -0.505802
C -0.206354 -2.078858 -1.200314
H -0.000528 -2.993204 -0.651684
H -0.199925 -2.113517 -2.286694
C 4.088140 -0.319635 1.374853
H 4.052820 -1.279570 1.898466
H 5.107743 -0.140901 1.028055
H 3.818749 0.457029 2.099387
C -1.750728 -0.372961 -0.092420
C -1.933203 0.767376 0.729029
C -2.902517 -1.096982 -0.489917
C -3.204805 1.161607 1.121178
H -1.071060 1.330587 1.075539
C -4.169449 -0.691284 -0.093071
H -2.786646 -1.977531 -1.115968
C -4.332138 0.440473 0.712394
H -3.320762 2.035655 1.755280
H -5.037894 -1.260105 -0.412066
H -5.324104 0.754699 1.021545
C 0.769232 1.292027 -0.753742
O 0.047396 1.601967 -1.682007
C 1.660142 2.303395 -0.076485
H 2.074748 1.963710 0.872606
H 2.473966 2.582267 -0.750056
H 1.042920 3.189340 0.096195
32
3A_Ac_conf_12 Eopt -747.354064
C 2.232099 -1.495674 1.333424
H 1.569136 -0.895407 1.951620
H 2.912775 -2.171816 1.843991
C 2.214353 -1.432938 -0.002065
C 1.200921 -0.583869 -0.701799
O 0.670393 -0.956075 -1.731909
N 0.788687 0.620161 -0.083718
C -0.518859 1.116647 -0.392920
C -0.598475 2.404455 -1.084733
H -0.690022 3.337314 -0.538662
H -0.551054 2.439095 -2.170456
C 3.082045 -2.266720 -0.899507
H 3.766988 -2.876798 -0.307480
H 2.469624 -2.922835 -1.524792
H 3.666118 -1.628560 -1.571955
C -1.668489 0.323554 -0.081430
C -2.948754 0.735084 -0.531549
C -1.587497 -0.867030 0.683240
C -4.081646 -0.010587 -0.236171
H -3.038919 1.645395 -1.117715
C -2.727753 -1.603399 0.973364
H -0.629087 -1.203274 1.066414
C -3.982099 -1.185544 0.516084
H -5.050606 0.324877 -0.594124
H -2.640473 -2.509814 1.565250
H -4.869965 -1.765977 0.746381
C 1.648240 1.499903 0.611846
O 1.154551 2.380897 1.290819
C 3.140495 1.407449 0.414670
H 3.492530 2.431228 0.266110
H 3.607819 1.014867 1.321013
H 3.437288 0.794020 -0.435566
32
3A_Ac_conf_13 Eopt -747.353939
C 3.485276 -0.183189 -1.064498
H 2.756263 -0.222277 -1.870484
H 4.528823 -0.055405 -1.339918
C 3.132050 -0.315918 0.218324
C 1.708157 -0.627280 0.547192
O 1.416122 -1.473156 1.373046
N 0.692613 -0.011291 -0.216160
C -0.454637 -0.814762 -0.504971
C -0.205992 -2.078959 -1.199391
H -0.000432 -2.993359 -0.650797
H -0.198554 -2.113368 -2.285781
C 4.088934 -0.319707 1.373651
H 5.108289 -0.140496 1.026349
H 3.819702 0.456544 2.098691
H 4.054214 -1.279882 1.896866
C -1.750762 -0.373037 -0.092260
C -1.933692 0.767468 0.728893
C -2.902336 -1.097396 -0.489827
C -3.205475 1.161569 1.120555
H -1.071687 1.330848 1.075483
C -4.169432 -0.691790 -0.093506
H -2.786042 -1.978150 -1.115531
C -4.332565 0.440170 0.711611
H -3.321728 2.035732 1.754454
H -5.037688 -1.260842 -0.412620
H -5.324686 0.754279 1.020380
C 0.768937 1.292268 -0.753144
O 0.047129 1.602126 -1.681431
C 1.659703 2.303555 -0.075676
H 2.473512 2.582689 -0.749171
H 1.042364 3.189374 0.097243
H 2.074350 1.963630 0.873319
32
3A_Ac_conf_2 Eopt -747.356181
C -0.056162 3.083132 0.085413
H -0.125836 3.264751 -0.983282
H 0.457658 3.820995 0.695686
C -0.573366 1.979201 0.633344
C -1.305786 1.054091 -0.295002
O -1.940753 1.462060 -1.249839
N -1.234118 -0.328524 -0.013220
C -0.086773 -0.872750 0.641836
C -0.306926 -1.670622 1.849650
H -0.322104 -1.197582 2.828110
H -0.427541 -2.746937 1.791177
C -0.493925 1.670532 2.107394
H -1.371498 1.111704 2.446802
H 0.395730 1.080536 2.352524
H -0.438724 2.605624 2.670123
C 1.213641 -0.623942 0.094115

| | | | |
|---|---|---|---|
| C | 2.368915 | -0.940128 | 0.852898 |
| C | 1.399001 | -0.078640 | -1.202289 |
| C | 3.639338 | -0.708387 | 0.343920 |
| H | 2.252150 | -1.361810 | 1.847530 |
| C | 2.674930 | 0.141757 | -1.702018 |
| H | 0.538602 | 0.147452 | -1.825787 |
| C | 3.803644 | -0.165155 | -0.934617 |
| H | 4.509565 | -0.952372 | 0.946079 |
| H | 2.792702 | 0.551373 | -2.700872 |
| H | 4.798760 | 0.011861 | -1.330368 |
| C | -2.233103 | -1.238320 | -0.430133 |
| O | -1.978714 | -2.428593 | -0.418352 |
| C | -3.591536 | -0.714610 | -0.806077 |
| H | -4.303154 | -1.524546 | -0.641122 |
| H | -3.873155 | 0.164649 | -0.225652 |
| H | -3.599949 | -0.440717 | -1.863492 |

32

3A_Ac_conf_3 Eopt -747.356198

| | | | |
|---|---|---|---|
| C | 1.226513 | -1.802249 | -1.479683 |
| H | 0.391400 | -1.170363 | -1.769999 |
| H | 1.287580 | -2.789357 | -1.930302 |
| C | 2.166005 | -1.387189 | -0.624264 |
| C | 2.136052 | 0.015283 | -0.099487 |
| O | 3.159303 | 0.657884 | 0.042634 |
| N | 0.871792 | 0.559232 | 0.217435 |
| C | -0.117761 | -0.299474 | 0.795694 |
| C | 0.310088 | -1.152559 | 1.906834 |
| H | 0.253682 | -0.787515 | 2.929402 |
| H | 0.652634 | -2.169969 | 1.739628 |
| C | 3.362208 | -2.196172 | -0.214946 |
| H | 4.286301 | -1.709010 | -0.540284 |
| H | 3.409254 | -2.286626 | 0.876287 |
| H | 3.314556 | -3.195704 | -0.651545 |
| C | -1.456389 | -0.271845 | 0.290014 |
| C | -2.473753 | -1.005796 | 0.948037 |
| C | -1.806466 | 0.448885 | -0.878664 |
| C | -3.776055 | -1.005987 | 0.465653 |
| H | -2.227877 | -1.571184 | 1.842924 |
| C | -3.110344 | 0.437030 | -1.354124 |
| H | -1.044716 | 1.002595 | -1.420882 |
| C | -4.105901 | -0.284686 | -0.685919 |
| H | -4.540390 | -1.572719 | 0.989259 |
| H | -3.355246 | 0.992372 | -2.254815 |
| H | -5.124294 | -0.288083 | -1.061576 |
| C | 0.690368 | 1.962272 | 0.325290 |
| O | -0.195241 | 2.398268 | 1.033973 |
| C | 1.554600 | 2.858939 | -0.519069 |
| H | 2.422960 | 3.179053 | 0.061510 |
| H | 1.908239 | 2.367927 | -1.426125 |
| H | 0.955889 | 3.736031 | -0.770582 |

32

3A_Ac_conf_5 Eopt -747.353947

| | | | |
|---|---|---|---|
| C | -2.273984 | 1.475974 | 1.385895 |
| H | -1.592826 | 0.874998 | 1.983467 |
| H | -2.959952 | 2.130639 | 1.916788 |
| C | -2.276854 | 1.429335 | 0.050791 |
| C | -1.247923 | 0.622588 | -0.677326 |
| O | -0.726345 | 1.034546 | -1.695176 |
| N | -0.807637 | -0.593588 | -0.089128 |
| C | 0.492734 | -1.072005 | -0.437274 |
| C | 0.574838 | -2.309666 | -1.216990 |
| H | 0.540062 | -2.267786 | -2.303195 |
| H | 0.725515 | -3.275325 | -0.743913 |
| C | -3.179713 | 2.250156 | -0.823738 |
| H | -3.765889 | 1.601335 | -1.483897 |
| H | -3.864206 | 2.843595 | -0.214318 |
| H | -2.596146 | 2.921209 | -1.460757 |
| C | 1.641026 | -0.282303 | -0.105346 |
| C | 1.557523 | 0.868900 | 0.716449 |
| C | 2.918004 | -0.658820 | -0.591964 |
| C | 2.694525 | 1.602376 | 1.026788 |
| H | 0.600097 | 1.177602 | 1.124409 |
| C | 4.047509 | 0.083945 | -0.276357 |
| H | 3.009335 | -1.539114 | -1.222175 |
| C | 3.946290 | 1.219593 | 0.533587 |
| H | 2.606643 | 2.478989 | 1.661830 |
| H | 5.014770 | -0.223282 | -0.662941 |
| H | 4.831511 | 1.797520 | 0.779861 |
| C | -1.750309 | -1.490428 | 0.463380 |
| O | -2.937123 | -1.373579 | 0.229170 |
| C | -1.198684 | -2.582721 | 1.338914 |
| H | -1.887697 | -2.714905 | 2.175634 |
| H | -1.174026 | -3.518720 | 0.772603 |
| H | -0.195878 | -2.360924 | 1.707693 |

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3A_Ac_conf_6 Eopt -747.353947

| | | | |
|---|---|---|---|
| C | 2.274388 | -1.475463 | -1.385990 |
| H | 1.593704 | -0.873874 | -1.983467 |
| H | 2.960271 | -2.130178 | -1.916915 |
| C | 2.276704 | -1.429556 | -0.050845 |
| C | 1.247976 | -0.622613 | 0.677281 |
| O | 0.726463 | -1.034326 | 1.695241 |
| N | 0.807717 | 0.593682 | 0.089053 |
| C | -0.492644 | 1.071942 | 0.437248 |
| C | -0.574876 | 2.309714 | 1.216829 |
| H | -0.539632 | 2.268099 | 2.303027 |
| H | -0.726827 | 3.275136 | 0.743671 |
| C | 3.178622 | -2.251507 | 0.823600 |
| H | 3.764209 | -1.603595 | 1.485151 |
| H | 2.594337 | -2.923307 | 1.459176 |
| H | 3.863623 | -2.844293 | 0.214118 |
| C | -1.640958 | 0.282280 | 0.105300 |
| C | -1.557403 | -0.868920 | -0.716494 |
| C | -2.917951 | 0.658776 | 0.591884 |
| C | -2.694378 | -1.602412 | -1.026909 |
| H | -0.599962 | -1.177561 | -1.124437 |
| C | -4.047420 | -0.084007 | 0.276208 |
| H | -3.009348 | 1.539069 | 1.222081 |
| C | -3.946157 | -1.219638 | -0.533758 |
| H | -2.606462 | -2.479017 | -1.661954 |
| H | -5.014710 | 0.223214 | 0.662718 |
| H | -4.831364 | -1.797566 | -0.780077 |
| C | 1.750392 | 1.490635 | -0.463204 |
| O | 2.937260 | 1.373564 | -0.229348 |
| C | 1.198772 | 2.583535 | -1.337991 |
| H | 1.887211 | 2.715539 | -2.175206 |
| H | 0.195467 | 2.362675 | -1.705971 |
| H | 1.175272 | 3.519386 | -0.771384 |

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3A_Ac_conf_7 Eopt -747.354297

| | | | |
|---|---|---|---|
| C | 3.543986 | -0.050424 | -1.020849 |
| H | 2.830018 | 0.014096 | -1.839265 |
| H | 4.594139 | 0.098346 | -1.257354 |
| C | 3.157083 | -0.317792 | 0.229387 |
| C | 1.724877 | -0.668283 | 0.478685 |
| O | 1.413934 | -1.631604 | 1.153460 |
| N | 0.725553 | 0.060784 | -0.209648 |
| C | -0.414921 | -0.675107 | -0.654662 |
| C | -0.153238 | -1.757590 | -1.605364 |
| H | 0.090879 | -2.759170 | -1.263082 |
| H | -0.156128 | -1.562211 | -2.674604 |
| C | 4.079450 | -0.451262 | 1.404620 |
| H | 4.020559 | -1.458282 | 1.828422 |
| H | 5.110422 | -0.250524 | 1.106495 |

H 3.795838 0.253115 2.194427
C -1.710209 -0.364467 -0.135181
C -2.862055 -0.977462 -0.689918
C -1.889497 0.540850 0.941341
C -4.126929 -0.684697 -0.199704
H -2.746372 -1.679133 -1.511493
C -3.159789 0.822770 1.423989
H -1.024911 1.004767 1.408087
C -4.287096 0.217821 0.857280
H -4.996296 -1.161791 -0.642416
H -3.274466 1.514930 2.252915
H -5.278053 0.443331 1.238546
C 0.847155 1.448779 -0.418863
O 1.592970 2.113623 0.274663
C 0.004455 2.033122 -1.519576
H 0.448046 2.984618 -1.813929
H -0.056925 1.357953 -2.376735
H -1.010475 2.220766 -1.154565

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3A_Ac_conf_8 Eopt -747.353776

C -3.845807 0.703639 -1.513108
H -3.383474 1.085617 -2.418770
H -4.918318 0.530223 -1.523319
C -3.119856 0.437647 -0.424837
C -1.660725 0.780981 -0.459510
O -1.252808 1.825677 -0.931857
N -0.746541 -0.071616 0.206043
C 0.413440 0.558418 0.766435
C 0.168844 1.483838 1.873333
H 0.154240 1.124057 2.898817
H -0.062779 2.528892 1.687924
C -3.689870 -0.055294 0.878573
H -3.362608 0.585868 1.705307
H -4.781188 -0.036064 0.835065
H -3.374234 -1.077019 1.105617
C 1.701132 0.310608 0.198687
C 2.862469 0.832223 0.823208
C 1.864810 -0.440507 -0.992814
C 4.120924 0.601882 0.285530
H 2.759186 1.414553 1.734789
C 3.129063 -0.661985 -1.520899
H 0.993246 -0.833051 -1.509306
C 4.265380 -0.146852 -0.887521
H 4.997515 1.008341 0.781267
H 3.231821 -1.235192 -2.437531
H 5.251374 -0.323462 -1.305687
C -0.927897 -1.463706 0.275449
O -1.720053 -2.024008 -0.459296
C -0.090723 -2.195549 1.288935
H 0.914328 -2.365053 0.889163
H 0.000672 -1.629255 2.218975
H -0.558204 -3.162549 1.475841

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3A_Ac_conf_9 Eopt -747.354297

C -3.543588 -0.050664 1.021446
H -2.829264 0.013547 1.839581
H -4.593637 0.098038 1.258458
C -3.157211 -0.317553 -0.229055
C -1.725105 -0.667978 -0.479077
O -1.414498 -1.631029 -1.154415
N -0.725484 0.060714 0.209177
C 0.414847 -0.675505 0.653950
C 0.152953 -1.758630 1.603876
H -0.089962 -2.760268 1.260918
H 0.156127 -1.564099 2.673269
C -4.080029 -0.450484 -1.403991
H -3.796875 0.254469 -2.193454
H -4.021051 -1.457213 -1.828468
H -5.110926 -0.250170 -1.105328
C 1.710272 -0.364599 0.134903
C 1.889784 0.541222 -0.941146
C 2.861975 -0.977845 0.689625
C 3.160187 0.823389 -1.423366
H 1.025295 1.005334 -1.407874
C 4.126969 -0.684822 0.199853
H 2.746108 -1.679908 1.510840
C 4.287367 0.218197 -0.856664
H 3.275061 1.515935 -2.251943
H 4.996240 -1.162105 0.642549
H 5.278410 0.443908 -1.237589
C -0.847056 1.448623 0.419065
O -1.592925 2.113748 -0.274132
C -0.004301 2.032457 1.519993
H -0.447737 2.983931 1.814650
H 0.056909 1.356978 2.376924
H 1.010691 2.220027 1.155115

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3A_Bn_conf_1 Eopt -865.027438

C -3.253668 -1.497660 0.450599
H -2.971710 -1.563868 1.498227
H -4.307064 -1.352886 0.224215
C -2.355920 -1.610990 -0.532214
C -0.918641 -1.934427 -0.222040
O -0.342479 -2.816811 -0.856581
N -0.304522 -1.267402 0.809192
C -0.756909 -0.030079 1.339317
C -0.939858 0.043281 2.792322
H -0.129773 0.338859 3.453254
H -1.906648 -0.178902 3.238084
C -2.701868 -1.580735 -1.993466
H -2.464830 -2.541066 -2.461238
H -3.764662 -1.370009 -2.130978
H -2.119149 -0.812975 -2.515098
C -0.939287 1.103172 0.478375
C -0.520851 1.096962 -0.876697
C -1.534122 2.287759 0.980597
C -0.698779 2.215332 -1.680370
H -0.030298 0.219961 -1.290733
C -1.711304 3.397841 0.165286
H -1.860081 2.320699 2.016655
C -1.298094 3.372216 -1.170878
H -0.361321 2.187670 -2.712501
H -2.174891 4.291489 0.572996
H -1.436108 4.242573 -1.804575
C 1.039564 -1.710364 1.229306
H 1.096086 -1.597294 2.315913
H 1.135125 -2.765985 0.974935
C 2.104677 -0.880913 0.550565
C 2.547853 0.308361 1.138458
C 2.595527 -1.244249 -0.708308
C 3.460105 1.129992 0.475118
H 2.170244 0.592945 2.118739
C 3.510523 -0.426393 -1.371598
H 2.245859 -2.164745 -1.168357
C 3.940801 0.764510 -0.783023
H 3.795133 2.052679 0.939930
H 3.886239 -0.717159 -2.348379
H 4.650840 1.402607 -1.300875

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3A_Bn_conf_10 Eopt -865.023439

C 0.280526 -4.229744 0.557838
H -0.295237 -4.674190 -0.248801
H 0.790428 -4.896518 1.248077
C 0.364397 -2.903145 0.693784

| | | | |
|---|---|---|---|
| C | -0.428024 | -2.060595 | -0.270970 |
| O | -1.520420 | -2.424374 | -0.694332 |
| N | 0.079098 | -0.815331 | -0.596994 |
| C | 1.479202 | -0.598214 | -0.673876 |
| C | 2.313201 | -1.648055 | -1.271503 |
| H | 2.799371 | -2.411963 | -0.671494 |
| H | 2.510567 | -1.638224 | -2.340992 |
| C | 1.135023 | -2.235329 | 1.805715 |
| H | 0.585051 | -1.375846 | 2.203666 |
| H | 1.299304 | -2.949492 | 2.616261 |
| H | 2.114089 | -1.871682 | 1.477061 |
| C | 2.028311 | 0.658986 | -0.254011 |
| C | 1.267975 | 1.608143 | 0.473709 |
| C | 3.382156 | 0.972887 | -0.535122 |
| C | 1.832886 | 2.808905 | 0.883192 |
| H | 0.237196 | 1.387996 | 0.732299 |
| C | 3.935516 | 2.177046 | -0.121323 |
| H | 3.990994 | 0.260473 | -1.084935 |
| C | 3.167147 | 3.106445 | 0.587876 |
| H | 1.230004 | 3.517219 | 1.444184 |
| H | 4.974387 | 2.394679 | -0.351744 |
| H | 3.603673 | 4.046258 | 0.911096 |
| C | -0.815626 | 0.069552 | -1.357426 |
| H | -0.216360 | 0.914444 | -1.704972 |
| H | -1.170989 | -0.468962 | -2.243022 |
| C | -2.011410 | 0.585189 | -0.580544 |
| C | -2.978948 | 1.314994 | -1.280875 |
| C | -2.180595 | 0.385158 | 0.790948 |
| C | -4.089835 | 1.839900 | -0.623590 |
| H | -2.858188 | 1.471413 | -2.350797 |
| C | -3.294130 | 0.908380 | 1.451837 |
| H | -1.442712 | -0.182625 | 1.352756 |
| C | -4.251565 | 1.637904 | 0.748702 |
| H | -4.830306 | 2.404420 | -1.182864 |
| H | -3.411143 | 0.741077 | 2.518660 |
| H | -5.117693 | 2.043393 | 1.263025 |

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3A_Bn_conf_11 Eopt -865.021651

| | | | |
|---|---|---|---|
| C | -2.979584 | -2.860874 | 0.209310 |
| H | -3.360248 | -2.284587 | 1.048864 |
| H | -3.683234 | -3.485941 | -0.334947 |
| C | -1.694820 | -2.810700 | -0.144157 |
| C | -0.728942 | -1.987406 | 0.671164 |
| O | -0.351626 | -2.373360 | 1.776826 |
| N | -0.234302 | -0.846533 | 0.105165 |
| C | 0.688636 | -0.058054 | 0.866609 |
| C | 0.182353 | 0.616178 | 2.063994 |
| H | -0.239673 | 1.616496 | 1.996931 |
| H | 0.201361 | 0.124879 | 3.031734 |
| C | -1.084684 | -3.600655 | -1.270491 |
| H | -0.313500 | -4.276102 | -0.882625 |
| H | -1.847376 | -4.193904 | -1.780451 |
| H | -0.598695 | -2.946414 | -2.003341 |
| C | 2.023837 | 0.088182 | 0.376626 |
| C | 2.502016 | -0.677428 | -0.717986 |
| C | 2.916943 | 1.005243 | 0.988036 |
| C | 3.803061 | -0.522005 | -1.175986 |
| H | 1.844617 | -1.403121 | -1.188654 |
| C | 4.215068 | 1.151525 | 0.519306 |
| H | 2.573054 | 1.599987 | 1.830067 |
| C | 4.668523 | 0.393075 | -0.565832 |
| H | 4.150541 | -1.121282 | -2.012579 |
| H | 4.881319 | 1.861592 | 1.000576 |
| H | 5.684637 | 0.510805 | -0.929092 |
| C | -0.782995 | -0.212885 | -1.106478 |
| H | 0.032498 | -0.042855 | -1.816792 |
| H | -1.497856 | -0.900135 | -1.560795 |
| C | -1.459463 | 1.098019 | -0.768988 |
| C | -0.844103 | 2.314785 | -1.067265 |
| C | -2.686352 | 1.096936 | -0.096113 |
| C | -1.445850 | 3.520528 | -0.697985 |
| H | 0.111910 | 2.317815 | -1.586521 |
| C | -3.289927 | 2.297370 | 0.271878 |
| H | -3.163398 | 0.148209 | 0.142809 |
| C | -2.667847 | 3.512947 | -0.026869 |
| H | -0.957978 | 4.462117 | -0.932353 |
| H | -4.243300 | 2.287396 | 0.791946 |
| H | -3.136787 | 4.448965 | 0.261816 |

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3A_Bn_conf_12 Eopt -865.026878

| | | | |
|---|---|---|---|
| C | -2.627767 | -1.602929 | -1.988917 |
| H | -1.883335 | -1.727330 | -2.770309 |
| H | -3.658794 | -1.436042 | -2.289882 |
| C | -2.286065 | -1.643229 | -0.698228 |
| C | -0.840706 | -1.939579 | -0.382583 |
| O | -0.202484 | -2.759807 | -1.040192 |
| N | -0.284382 | -1.306919 | 0.703480 |
| C | -0.800571 | -0.109772 | 1.256966 |
| C | -1.051384 | -0.097847 | 2.701969 |
| H | -0.290758 | 0.222866 | 3.408208 |
| H | -2.022692 | -0.390528 | 3.093893 |
| C | -3.285697 | -1.482464 | 0.421074 |
| H | -4.282840 | -1.746296 | 0.059459 |
| H | -3.039674 | -2.130456 | 1.268392 |
| H | -3.327018 | -0.452957 | 0.792437 |
| C | -0.990915 | 1.049001 | 0.431464 |
| C | -1.684626 | 2.175218 | 0.942060 |
| C | -0.476479 | 1.130950 | -0.888327 |
| C | -1.859803 | 3.315690 | 0.169406 |
| H | -2.085624 | 2.138907 | 1.951512 |
| C | -0.650614 | 2.279933 | -1.647324 |
| H | 0.083583 | 0.297907 | -1.304840 |
| C | -1.345681 | 3.378759 | -1.129773 |
| H | -2.399170 | 4.163401 | 0.581835 |
| H | -0.237321 | 2.322688 | -2.650850 |
| H | -1.480162 | 4.273465 | -1.729478 |
| C | 1.051095 | -1.733365 | 1.164796 |
| H | 1.057484 | -1.658442 | 2.256232 |
| H | 1.182219 | -2.776721 | 0.877288 |
| C | 2.126070 | -0.857848 | 0.564347 |
| C | 2.700990 | -1.178214 | -0.670154 |
| C | 2.497234 | 0.330649 | 1.201723 |
| C | 3.627958 | -0.319000 | -1.260846 |
| H | 2.407639 | -2.098052 | -1.169038 |
| C | 3.420892 | 1.193710 | 0.610921 |
| H | 2.054685 | 0.581858 | 2.163768 |
| C | 3.985814 | 0.870856 | -0.623701 |
| H | 4.069551 | -0.576691 | -2.219191 |
| H | 3.699372 | 2.115173 | 1.113972 |
| H | 4.704911 | 1.541036 | -1.085479 |

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3A_Bn_conf_13 Eopt -865.025528

| | | | |
|---|---|---|---|
| C | 1.593972 | 3.107543 | 0.019053 |
| H | 1.558599 | 3.386959 | -1.030231 |
| H | 2.236107 | 3.686217 | 0.678035 |
| C | 0.880109 | 2.078980 | 0.484372 |
| C | -0.030642 | 1.380173 | -0.494489 |
| O | -0.688712 | 2.016907 | -1.314628 |
| N | -0.149555 | 0.012034 | -0.411753 |
| C | 0.723285 | -0.818151 | 0.329872 |
| C | 0.107539 | -1.705374 | 1.322794 |
| H | -0.249352 | -2.695481 | 1.052386 |
| H | 0.008566 | -1.390857 | 2.359087 |
| C | 0.892178 | 1.664236 | 1.936149 |

| | | | |
|---|---|---|---|
| H | 1.607428 | 0.858103 | 2.129264 |
| H | 1.177306 | 2.519363 | 2.554400 |
| H | -0.094293 | 1.317053 | 2.260517 |
| C | 2.129687 | -0.825552 | 0.049160 |
| C | 3.018389 | -1.517809 | 0.910995 |
| C | 2.680110 | -0.173466 | -1.083633 |
| C | 4.382584 | -1.546228 | 0.654710 |
| H | 2.621736 | -2.026531 | 1.785553 |
| C | 4.044996 | -0.215644 | -1.332885 |
| H | 2.026194 | 0.346059 | -1.777990 |
| C | 4.908163 | -0.895909 | -0.466805 |
| H | 5.043153 | -2.078906 | 1.332644 |
| H | 4.441760 | 0.282737 | -2.212606 |
| H | 5.974850 | -0.922349 | -0.666086 |
| C | -1.231023 | -0.626913 | -1.164684 |
| H | -1.248719 | -0.190118 | -2.167449 |
| H | -0.973709 | -1.684405 | -1.271730 |
| C | -2.604919 | -0.498544 | -0.533768 |
| C | -2.811607 | 0.084207 | 0.717276 |
| C | -3.706400 | -1.000369 | -1.237418 |
| C | -4.097181 | 0.163452 | 1.258934 |
| H | -1.967796 | 0.481543 | 1.274725 |
| C | -4.988655 | -0.925665 | -0.698084 |
| H | -3.554686 | -1.452441 | -2.215415 |
| C | -5.188756 | -0.341956 | 0.555368 |
| H | -4.241357 | 0.622520 | 2.232746 |
| H | -5.832382 | -1.320674 | -1.256469 |
| H | -6.187786 | -0.280350 | 0.976408 |

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3A_Bn_conf_14 Eopt -865.025313

| | | | |
|---|---|---|---|
| C | -0.529349 | 4.045038 | 0.931180 |
| H | -1.605450 | 4.103191 | 0.796457 |
| H | -0.054342 | 4.786602 | 1.568257 |
| C | 0.189396 | 3.087177 | 0.338387 |
| C | -0.558114 | 2.135892 | -0.562732 |
| O | -1.491238 | 2.528340 | -1.260126 |
| N | -0.116249 | 0.833409 | -0.610506 |
| C | 0.583521 | 0.240252 | 0.480573 |
| C | -0.019001 | 0.328152 | 1.814581 |
| H | 0.221886 | 1.139034 | 2.497101 |
| H | -0.712681 | -0.439009 | 2.152876 |
| C | 1.687073 | 2.976515 | 0.489728 |
| H | 2.156558 | 2.640255 | -0.440090 |
| H | 2.098076 | 3.954274 | 0.753587 |
| H | 1.974619 | 2.271437 | 1.276677 |
| C | 1.769475 | -0.518824 | 0.208572 |
| C | 2.422410 | -0.450880 | -1.047375 |
| C | 2.341597 | -1.337860 | 1.212888 |
| C | 3.581418 | -1.178043 | -1.283440 |
| H | 2.019303 | 0.193503 | -1.823509 |
| C | 3.499891 | -2.062591 | 0.963939 |
| H | 1.861598 | -1.401163 | 2.185802 |
| C | 4.126920 | -1.991746 | -0.284337 |
| H | 4.069296 | -1.106938 | -2.251212 |
| H | 3.918619 | -2.687981 | 1.746982 |
| H | 5.032725 | -2.558765 | -0.475074 |
| C | -0.806196 | -0.107345 | -1.518531 |
| H | -1.244198 | 0.484892 | -2.322424 |
| H | -0.057875 | -0.782662 | -1.940376 |
| C | -1.859153 | -0.902047 | -0.778984 |
| C | -3.062527 | -0.298765 | -0.392521 |
| C | -1.611688 | -2.226472 | -0.409055 |
| C | -4.000659 | -1.011108 | 0.352710 |
| H | -3.254121 | 0.733487 | -0.674914 |
| C | -2.550695 | -2.942339 | 0.337180 |
| H | -0.676578 | -2.697880 | -0.704481 |
| C | -3.745762 | -2.334703 | 0.720774 |
| H | -4.931626 | -0.534846 | 0.646486 |
| H | -2.346507 | -3.971162 | 0.619125 |
| H | -4.476992 | -2.888674 | 1.302049 |

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3A_Bn_conf_15 Eopt -865.023327

| | | | |
|---|---|---|---|
| C | -0.825886 | 2.677059 | -0.905468 |
| H | -0.050485 | 2.423697 | -1.624610 |
| H | -1.458020 | 3.532915 | -1.129219 |
| C | -0.994323 | 1.977113 | 0.219192 |
| C | -0.018859 | 0.883884 | 0.565019 |
| O | 0.601640 | 0.934329 | 1.621762 |
| N | 0.172981 | -0.128580 | -0.356776 |
| C | 1.244819 | -1.037021 | -0.188966 |
| C | 0.931551 | -2.469403 | -0.112856 |
| H | 0.786077 | -2.946912 | 0.853060 |
| H | 0.939942 | -3.103956 | -0.994609 |
| C | -2.029669 | 2.281370 | 1.263350 |
| H | -2.625529 | 3.149458 | 0.972205 |
| H | -2.699620 | 1.423467 | 1.401301 |
| H | -1.552744 | 2.482021 | 2.227884 |
| C | 2.592461 | -0.550100 | -0.113264 |
| C | 3.648208 | -1.437206 | 0.215742 |
| C | 2.929079 | 0.798758 | -0.392102 |
| C | 4.963532 | -0.994185 | 0.272497 |
| H | 3.421522 | -2.477636 | 0.431925 |
| C | 4.247406 | 1.228480 | -0.338450 |
| H | 2.150547 | 1.502653 | -0.670183 |
| C | 5.275900 | 0.340728 | -0.001834 |
| H | 5.752319 | -1.694481 | 0.531836 |
| H | 4.479030 | 2.265684 | -0.563417 |
| H | 6.304643 | 0.684399 | 0.041653 |
| C | -0.887278 | -0.466847 | -1.327317 |
| H | -0.932150 | 0.292309 | -2.111501 |
| H | -0.582157 | -1.401860 | -1.803138 |
| C | -2.249038 | -0.633495 | -0.687247 |
| C | -2.399169 | -1.342970 | 0.509391 |
| C | -3.376823 | -0.067678 | -1.286805 |
| C | -3.657779 | -1.489208 | 1.091951 |
| H | -1.526558 | -1.773335 | 0.995710 |
| C | -4.637363 | -0.211524 | -0.705674 |
| H | -3.262637 | 0.503726 | -2.205302 |
| C | -4.780754 | -0.922306 | 0.486538 |
| H | -3.760183 | -2.040814 | 2.021923 |
| H | -5.504329 | 0.240686 | -1.178447 |
| H | -5.759740 | -1.029287 | 0.944085 |

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3A_Bn_conf_16 Eopt -865.021653

| | | | |
|---|---|---|---|
| C | -1.624704 | -3.172084 | -1.467322 |
| H | -0.645915 | -3.009078 | -1.912715 |
| H | -2.328393 | -3.793341 | -2.015748 |
| C | -1.955572 | -2.644279 | -0.286545 |
| C | -0.929918 | -1.906275 | 0.533172 |
| O | -0.673963 | -2.306482 | 1.669267 |
| N | -0.263313 | -0.842664 | -0.011563 |
| C | 0.700315 | -0.174707 | 0.815243 |
| C | 0.222190 | 0.505990 | 2.021130 |
| H | 0.183913 | -0.007528 | 2.976144 |
| H | -0.094714 | 1.545655 | 1.976507 |
| C | -3.278128 | -2.856383 | 0.393842 |
| H | -3.940586 | -3.457597 | -0.232844 |
| H | -3.135420 | -3.363343 | 1.353045 |
| H | -3.764779 | -1.896683 | 0.602802 |
| C | 2.058007 | -0.126569 | 0.368612 |
| C | 2.502389 | -0.881013 | -0.747812 |
| C | 3.008813 | 0.678069 | 1.047965 |
| C | 3.826417 | -0.823059 | -1.160387 |
| H | 1.799229 | -1.521833 | -1.271880 |

| | | | |
|---|---|---|---|
| C | 4.329660 | 0.727195 | 0.624630 |
| H | 2.692147 | 1.262541 | 1.907606 |
| C | 4.749555 | -0.019087 | -0.482158 |
| H | 4.146079 | -1.412198 | -2.015082 |
| H | 5.040137 | 1.351328 | 1.158854 |
| H | 5.783552 | 0.022467 | -0.809846 |
| C | -0.699263 | -0.084900 | -1.200406 |
| H | 0.163192 | 0.058991 | -1.858518 |
| H | -1.441888 | -0.676708 | -1.732859 |
| C | -1.278114 | 1.254056 | -0.798017 |
| C | -2.503007 | 1.304792 | -0.123159 |
| C | -0.579532 | 2.438283 | -1.036165 |
| C | -3.021922 | 2.523419 | 0.307736 |
| H | -3.043064 | 0.379681 | 0.072776 |
| C | -1.096816 | 3.662950 | -0.605245 |
| H | 0.376104 | 2.400921 | -1.554659 |
| C | -2.316760 | 3.706562 | 0.068040 |
| H | -3.973232 | 2.553331 | 0.830813 |
| H | -0.544426 | 4.579091 | -0.792645 |
| H | -2.718696 | 4.657064 | 0.406144 |

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3A_Bn_conf_2 Eopt -865.026744

| | | | |
|---|---|---|---|
| C | -0.853217 | 1.561507 | 1.933621 |
| H | -0.250746 | 0.713269 | 2.248856 |
| H | -1.436061 | 2.070569 | 2.697184 |
| C | -0.875904 | 1.984585 | 0.666912 |
| C | 0.034426 | 1.369902 | -0.361281 |
| O | 0.701362 | 2.097920 | -1.093800 |
| N | 0.152941 | 0.000702 | -0.430038 |
| C | -0.702949 | -0.927565 | 0.212028 |
| C | -0.061277 | -1.946767 | 1.050100 |
| H | 0.055810 | -1.789147 | 2.119763 |
| H | 0.289428 | -2.886395 | 0.632132 |
| C | -1.656321 | 3.177979 | 0.194741 |
| H | -2.317007 | 2.905575 | -0.636155 |
| H | -2.262387 | 3.584320 | 1.007344 |
| H | -0.979868 | 3.956652 | -0.170303 |
| C | -2.118067 | -0.890037 | -0.014123 |
| C | -2.706988 | -0.060196 | -1.001570 |
| C | -2.979753 | -1.706265 | 0.761087 |
| C | -4.082432 | -0.044422 | -1.188996 |
| H | -2.077566 | 0.556360 | -1.636883 |
| C | -4.354516 | -1.678526 | 0.566973 |
| H | -2.555310 | -2.354454 | 1.522927 |
| C | -4.919287 | -0.846637 | -0.405445 |
| H | -4.507856 | 0.595893 | -1.956541 |
| H | -4.992956 | -2.308964 | 1.179215 |
| H | -5.994255 | -0.827424 | -0.554507 |
| C | 1.259683 | -0.531285 | -1.229047 |
| H | 1.026343 | -1.574545 | -1.457909 |
| H | 1.287188 | 0.015560 | -2.175757 |
| C | 2.617687 | -0.445077 | -0.557818 |
| C | 2.782057 | -0.029314 | 0.764797 |
| C | 3.747803 | -0.811304 | -1.298454 |
| C | 4.054980 | 0.018050 | 1.338995 |
| H | 1.916753 | 0.262509 | 1.354599 |
| C | 5.017477 | -0.767995 | -0.726706 |
| H | 3.628409 | -1.131322 | -2.331459 |
| C | 5.175496 | -0.352032 | 0.597551 |
| H | 4.166531 | 0.346149 | 2.368416 |
| H | 5.884189 | -1.055475 | -1.314861 |
| H | 6.164487 | -0.315012 | 1.044410 |

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3A_Bn_conf_3 Eopt -865.026750

| | | | |
|---|---|---|---|
| C | -1.312887 | 3.223011 | 0.306359 |
| H | -1.961501 | 2.600451 | -0.305183 |
| H | -1.782700 | 3.991881 | 0.914696 |
| C | 0.014199 | 3.071268 | 0.303828 |
| C | 0.663644 | 2.073315 | -0.615640 |
| O | 1.601109 | 2.416498 | -1.332839 |
| N | 0.138828 | 0.804497 | -0.640965 |
| C | -0.589419 | 0.279090 | 0.469320 |
| C | 0.041696 | 0.346458 | 1.791581 |
| H | 0.689270 | -0.460019 | 2.130169 |
| H | -0.163027 | 1.164442 | 2.476397 |
| C | 0.968917 | 3.910796 | 1.102374 |
| H | 0.426491 | 4.622384 | 1.728711 |
| H | 1.591603 | 3.275568 | 1.743998 |
| H | 1.643580 | 4.460107 | 0.438560 |
| C | -1.830748 | -0.391313 | 0.226009 |
| C | -2.493135 | -0.298633 | -1.024239 |
| C | -2.449084 | -1.149455 | 1.251784 |
| C | -3.705031 | -0.942980 | -1.233351 |
| H | -2.053317 | 0.300215 | -1.816840 |
| C | -3.659834 | -1.791513 | 1.029007 |
| H | -1.962803 | -1.230064 | 2.220356 |
| C | -4.296132 | -1.696943 | -0.213408 |
| H | -4.198499 | -0.853603 | -2.196820 |
| H | -4.113441 | -2.370517 | 1.828159 |
| H | -5.243244 | -2.199468 | -0.383121 |
| C | 0.750413 | -0.190841 | -1.545529 |
| H | -0.047401 | -0.809971 | -1.962947 |
| H | 1.230270 | 0.361843 | -2.353908 |
| C | 1.742732 | -1.055711 | -0.801063 |
| C | 1.396581 | -2.352368 | -0.412591 |
| C | 2.989272 | -0.539692 | -0.425632 |
| C | 2.281086 | -3.126730 | 0.341710 |
| H | 0.427282 | -2.755064 | -0.699108 |
| C | 3.873235 | -1.310545 | 0.327555 |
| H | 3.257821 | 0.471265 | -0.722879 |
| C | 3.519716 | -2.605885 | 0.714463 |
| H | 2.000596 | -4.133074 | 0.638801 |
| H | 4.838511 | -0.902417 | 0.612911 |
| H | 4.208511 | -3.205405 | 1.302302 |

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3A_Bn_conf_4 Eopt -865.022072

| | | | |
|---|---|---|---|
| C | 1.520597 | 2.578677 | -1.403829 |
| H | 0.547993 | 2.603673 | -1.890038 |
| H | 2.366489 | 2.989946 | -1.949397 |
| C | 1.678859 | 2.072223 | -0.179709 |
| C | 0.474173 | 1.619483 | 0.605611 |
| O | 0.123603 | 2.257773 | 1.595892 |
| N | -0.214033 | 0.514696 | 0.172175 |
| C | -1.330789 | 0.067336 | 0.936479 |
| C | -1.156452 | -0.177469 | 2.371482 |
| H | -0.878913 | -1.166130 | 2.729075 |
| H | -1.362803 | 0.595149 | 3.103585 |
| C | 2.984825 | 2.025353 | 0.562165 |
| H | 3.792138 | 2.422398 | -0.058034 |
| H | 2.921121 | 2.613869 | 1.483516 |
| H | 3.231604 | 0.995314 | 0.847556 |
| C | -2.571559 | -0.169159 | 0.259342 |
| C | -2.783426 | 0.243156 | -1.081725 |
| C | -3.643951 | -0.809366 | 0.931779 |
| C | -3.999916 | 0.015495 | -1.710877 |
| H | -1.992403 | 0.762317 | -1.614952 |
| C | -4.854601 | -1.032645 | 0.290821 |
| H | -3.509497 | -1.130606 | 1.960996 |
| C | -5.043263 | -0.626018 | -1.034706 |
| H | -4.140595 | 0.346467 | -2.735814 |
| H | -5.659679 | -1.527685 | 0.826064 |
| H | -5.991886 | -0.801855 | -1.532205 |
| C | 0.305393 | -0.357254 | -0.905818 |
| H | -0.428193 | -1.156871 | -1.030514 |

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H 1.069136 -1.629185 1.388897
C 4.171470 -2.026896 0.050134
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H -2.205010 0.222382 2.410647
H -4.041398 0.466663 2.237345
C -3.109660 -0.643978 0.705701
C -1.828591 -1.279002 0.226007
O -1.525125 -2.411276 0.598157
N -1.052181 -0.569835 -0.647319
C 0.164340 -1.143364 -1.128106
C 0.207344 -1.501948 -2.547999
H 0.528960 -0.792396 -3.305565
H -0.116856 -2.486974 -2.874550
C -4.323641 -0.939459 -0.130623
H -5.212719 -0.474944 0.302245
H -4.191875 -0.568659 -1.154128
H -4.486090 -2.020963 -0.197481
C 1.280321 -1.288291 -0.244316
C 1.248779 -0.799619 1.086378
C 2.475755 -1.899226 -0.699163
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C 0.391532 -2.041592 -0.224841
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H -2.378100 1.307401 -0.707881
C -5.173058 -0.539184 -0.122539
H -5.184446 -2.607563 0.491192
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H -6.254666 -0.449403 -0.143716
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3A_Bn_conf_8 Eopt -865.025510
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3B_Ac_conf_3 Eopt -747.412818
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3B Ac MECP Eopt -747.414424
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3B_Bn_conf_1 Eopt -865.078982
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3B_Bn_conf_2 Eopt -865.076227
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H -3.597517 -2.854086 -0.223246
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| H | -2.117847 | -4.371430 | -1.655112 |
| H | -0.369206 | -4.424013 | -1.290557 |
| H | -1.557623 | -4.997630 | -0.106695 |
| C | -1.565918 | 1.326173 | 0.039478 |
| C | -2.792032 | 2.044633 | 0.120156 |
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| C | -2.843565 | 3.417765 | -0.080896 |
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| H | 0.543083 | 1.590700 | -0.425473 |
| C | -1.687353 | 4.143193 | -0.382562 |
| H | -3.799328 | 3.927991 | 0.000371 |
| H | 0.433875 | 3.993904 | -0.748924 |
| H | -1.732028 | 5.216081 | -0.540568 |
| C | 0.724898 | -0.284648 | 1.262169 |
| H | 0.917699 | -1.006050 | 2.063527 |
| H | 0.373250 | 0.636781 | 1.730642 |
| C | 2.032957 | -0.026020 | 0.536977 |
| C | 3.106971 | 0.466200 | 1.285852 |
| C | 2.206440 | -0.242164 | -0.831252 |
| C | 4.332961 | 0.737532 | 0.679569 |
| H | 2.979922 | 0.638991 | 2.352649 |
| C | 3.431783 | 0.029952 | -1.441499 |
| H | 1.379644 | -0.622385 | -1.425543 |
| C | 4.499548 | 0.519982 | -0.689232 |
| H | 5.156366 | 1.120129 | 1.275673 |
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| H | 5.452854 | 0.730265 | -1.164759 |

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3B_Bn_conf_3 Eopt -865.079020

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| H | -2.706933 | -0.900906 | 1.931439 |
| H | -3.434751 | 0.637232 | 2.373846 |
| C | -3.385252 | 0.212744 | 0.278805 |
| C | -2.553563 | -0.237835 | -0.824410 |
| O | -3.013256 | -0.736274 | -1.858598 |
| N | -1.177074 | -0.143210 | -0.625741 |
| C | -0.652526 | 0.687213 | 0.375904 |
| C | -1.381309 | 0.793607 | 1.685075 |
| H | -0.791626 | 0.321309 | 2.485311 |
| H | -1.463890 | 1.854077 | 1.952089 |
| C | -4.852025 | 0.353294 | 0.095941 |
| H | -5.219298 | 1.239216 | 0.626240 |
| H | -5.121136 | 0.420865 | -0.959552 |
| H | -5.377161 | -0.511786 | 0.527560 |
| C | 0.562436 | 1.418431 | 0.146673 |
| C | 1.358752 | 1.840793 | 1.241363 |
| C | 0.998404 | 1.776486 | -1.154163 |
| C | 2.540445 | 2.543604 | 1.038650 |
| H | 1.058090 | 1.590321 | 2.254230 |
| C | 2.178031 | 2.484548 | -1.344387 |
| H | 0.383046 | 1.530866 | -2.013230 |
| C | 2.966559 | 2.865490 | -0.253637 |
| H | 3.137653 | 2.839444 | 1.896611 |
| H | 2.480813 | 2.752676 | -2.352826 |
| H | 3.890737 | 3.413616 | -0.407768 |
| C | -0.310055 | -1.003830 | -1.449219 |
| H | -0.957034 | -1.796395 | -1.833322 |
| H | 0.091273 | -0.473488 | -2.317031 |
| C | 0.817720 | -1.599071 | -0.635956 |
| C | 2.131730 | -1.548076 | -1.103219 |
| C | 0.555816 | -2.214109 | 0.593957 |
| C | 3.172951 | -2.105256 | -0.356828 |
| H | 2.342759 | -1.059684 | -2.051948 |
| C | 1.592633 | -2.764642 | 1.344377 |
| H | -0.466047 | -2.251919 | 0.967176 |
| C | 2.906199 | -2.710675 | 0.870264 |
| H | 4.191359 | -2.055778 | -0.730962 |
| H | 1.377408 | -3.236230 | 2.298880 |
| H | 3.715046 | -3.136754 | 1.456361 |

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3B_Bn_conf_4 Eopt -865.084117

| | | | |
|---|---|---|---|
| C | 0.674408 | 2.782662 | 1.093151 |
| H | 0.373203 | 3.450112 | 1.910605 |
| H | 1.636141 | 3.165695 | 0.718279 |
| C | -0.338355 | 2.846223 | 0.000873 |
| C | -0.755199 | 1.649363 | -0.712336 |
| O | -1.714394 | 1.644958 | -1.496678 |
| N | -0.029215 | 0.479311 | -0.498402 |
| C | 1.022570 | 0.432732 | 0.431630 |
| C | 0.864200 | 1.345847 | 1.604734 |
| H | -0.024541 | 1.056837 | 2.183096 |
| H | 1.729729 | 1.300480 | 2.265524 |
| C | -0.985691 | 4.145505 | -0.318160 |
| H | -0.237401 | 4.946346 | -0.340676 |
| H | -1.514091 | 4.110703 | -1.271911 |
| H | -1.709179 | 4.413663 | 0.465341 |
| C | 2.206646 | -0.324067 | 0.142680 |
| C | 3.111616 | -0.693709 | 1.171272 |
| C | 2.531743 | -0.716269 | -1.183164 |
| C | 4.261910 | -1.417680 | 0.887242 |
| H | 2.894830 | -0.429093 | 2.201349 |
| C | 3.686707 | -1.437739 | -1.454558 |
| H | 1.884218 | -0.416732 | -2.002245 |
| C | 4.561156 | -1.799880 | -0.424852 |
| H | 4.930393 | -1.692674 | 1.698179 |
| H | 3.913859 | -1.711697 | -2.481022 |
| H | 5.461652 | -2.365855 | -0.641489 |
| C | -0.591256 | -0.751109 | -1.073866 |
| H | -0.785767 | -0.595738 | -2.137360 |
| H | 0.162161 | -1.533635 | -0.972782 |
| C | -1.861961 | -1.181778 | -0.369803 |
| C | -3.021058 | -1.457182 | -1.097738 |
| C | -1.880341 | -1.334545 | 1.021344 |
| C | -4.182224 | -1.882094 | -0.449335 |
| H | -3.015577 | -1.329309 | -2.177463 |
| C | -3.039947 | -1.752328 | 1.672767 |
| H | -0.980837 | -1.124995 | 1.597084 |
| C | -4.195087 | -2.028553 | 0.937774 |
| H | -5.077887 | -2.090440 | -1.027474 |
| H | -3.041465 | -1.866674 | 2.752924 |
| H | -5.098814 | -2.354235 | 1.444346 |

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3B_Bn_conf_5 Eopt -865.084326

| | | | |
|---|---|---|---|
| C | -2.839295 | 1.009162 | 1.409741 |
| H | -3.460950 | 0.806536 | 2.291311 |
| H | -2.916119 | 2.090817 | 1.219695 |
| C | -3.386536 | 0.269539 | 0.237116 |
| C | -2.516698 | -0.406988 | -0.713617 |
| O | -2.968399 | -1.170287 | -1.579062 |
| N | -1.145605 | -0.158898 | -0.627356 |
| C | -0.623065 | 0.660369 | 0.386826 |
| C | -1.373258 | 0.642353 | 1.678366 |
| H | -1.332358 | -0.364368 | 2.120198 |
| H | -0.940157 | 1.344286 | 2.391777 |
| C | -4.860017 | 0.156331 | 0.075835 |
| H | -5.340916 | 1.113119 | 0.309342 |
| H | -5.135003 | -0.156690 | -0.932302 |
| H | -5.265505 | -0.580635 | 0.784436 |
| C | 0.557462 | 1.441552 | 0.146281 |

| | | | |
|---|---|---|---|
| C | 1.422330 | 1.798382 | 1.211702 |
| C | 0.905895 | 1.883000 | -1.155332 |
| C | 2.579451 | 2.530583 | 0.978642 |
| H | 1.198018 | 1.466821 | 2.221178 |
| C | 2.062871 | 2.619645 | -1.375728 |
| H | 0.236973 | 1.677172 | -1.985183 |
| C | 2.914975 | 2.943585 | -0.315215 |
| H | 3.231450 | 2.775203 | 1.812447 |
| H | 2.297800 | 2.954051 | -2.382399 |
| H | 3.821210 | 3.514114 | -0.492665 |
| C | -0.243605 | -0.981219 | -1.453992 |
| H | -0.870659 | -1.750834 | -1.907105 |
| H | 0.192654 | -0.394348 | -2.266239 |
| C | 0.854277 | -1.614395 | -0.628577 |
| C | 0.538100 | -2.346627 | 0.521598 |
| C | 2.192743 | -1.478478 | -1.000799 |
| C | 1.544967 | -2.930331 | 1.287532 |
| H | -0.503767 | -2.451421 | 0.819154 |
| C | 3.204624 | -2.067941 | -0.238923 |
| H | 2.444800 | -0.899654 | -1.886733 |
| C | 2.883165 | -2.791600 | 0.908447 |
| H | 1.287760 | -3.494363 | 2.179460 |
| H | 4.242336 | -1.952284 | -0.538083 |
| H | 3.668544 | -3.244465 | 1.506268 |

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3B_Bn_conf_6 Eopt -865.083245

| | | | |
|---|---|---|---|
| C | -2.216232 | 2.601360 | 0.536329 |
| H | -2.878025 | 3.464596 | 0.393812 |
| H | -2.376342 | 2.251309 | 1.567608 |
| C | -0.799676 | 3.025513 | 0.363788 |
| C | 0.155871 | 2.155618 | -0.299152 |
| O | 1.277431 | 2.550419 | -0.645572 |
| N | -0.210131 | 0.825240 | -0.532565 |
| C | -1.538081 | 0.395557 | -0.362699 |
| C | -2.570504 | 1.476022 | -0.445504 |
| H | -2.599051 | 1.892686 | -1.462617 |
| H | -3.561086 | 1.086841 | -0.213227 |
| C | -0.379295 | 4.388503 | 0.780668 |
| H | -0.797238 | 4.627699 | 1.765422 |
| H | 0.706684 | 4.487212 | 0.809348 |
| H | -0.774316 | 5.139841 | 0.081420 |
| C | -1.850894 | -0.975346 | -0.081724 |
| C | -3.154472 | -1.486824 | -0.325504 |
| C | -0.897539 | -1.878007 | 0.460634 |
| C | -3.472357 | -2.809752 | -0.050141 |
| H | -3.913967 | -0.846177 | -0.761028 |
| C | -1.228292 | -3.198567 | 0.733770 |
| H | 0.098603 | -1.525630 | 0.703246 |
| C | -2.515584 | -3.682006 | 0.479875 |
| H | -4.476742 | -3.167640 | -0.258505 |
| H | -0.475300 | -3.855514 | 1.160314 |
| H | -2.768975 | -4.715616 | 0.693122 |
| C | 0.756228 | 0.032313 | -1.299553 |
| H | 0.234060 | -0.848754 | -1.677865 |
| H | 1.065895 | 0.628913 | -2.164434 |
| C | 2.000018 | -0.397652 | -0.544999 |
| C | 2.225267 | -0.087931 | 0.797415 |
| C | 2.957393 | -1.149504 | -1.235001 |
| C | 3.385205 | -0.524038 | 1.440656 |
| H | 1.490824 | 0.494083 | 1.348398 |
| C | 4.116963 | -1.585461 | -0.595983 |
| H | 2.790356 | -1.395112 | -2.281802 |
| C | 4.335101 | -1.273619 | 0.747413 |
| H | 3.544846 | -0.274836 | 2.485783 |
| H | 4.849101 | -2.169327 | -1.146351 |
| H | 5.237418 | -1.611684 | 1.248166 |

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3C_Ac_conf_1 Eopt -747.393919

| | | | |
|---|---|---|---|
| C | 3.223201 | -1.973178 | -0.607690 |
| H | 3.364655 | -1.851942 | -1.676427 |
| H | 4.046089 | -2.344143 | -0.007349 |
| C | 2.011729 | -1.408326 | 0.047394 |
| C | 2.116593 | 0.120294 | 0.179182 |
| O | 3.105935 | 0.746336 | 0.481858 |
| N | 0.848246 | 0.672488 | -0.106874 |
| C | -0.068852 | -0.352205 | -0.441979 |
| C | 0.719809 | -1.578684 | -0.783857 |
| H | 0.194928 | -2.502485 | -0.531587 |
| H | 0.968073 | -1.599012 | -1.854921 |
| C | 1.832076 | -1.966039 | 1.471095 |
| H | 2.701315 | -1.721475 | 2.088682 |
| H | 0.935272 | -1.555105 | 1.946924 |
| H | 1.732076 | -3.054158 | 1.420445 |
| C | -1.466126 | -0.294950 | -0.161285 |
| C | -2.317576 | -1.300564 | -0.685477 |
| C | -2.048289 | 0.702468 | 0.660804 |
| C | -3.678775 | -1.296397 | -0.411953 |
| H | -1.901200 | -2.073603 | -1.324796 |
| C | -3.408982 | 0.689318 | 0.934472 |
| H | -1.424842 | 1.469633 | 1.107822 |
| C | -4.237366 | -0.302560 | 0.397968 |
| H | -4.310428 | -2.072905 | -0.833563 |
| H | -3.829393 | 1.457009 | 1.577741 |
| H | -5.301517 | -0.302660 | 0.612007 |
| C | 0.622765 | 2.042208 | -0.403054 |
| O | -0.328453 | 2.348135 | -1.093400 |
| C | 1.573493 | 3.050265 | 0.172157 |
| H | 1.784513 | 2.845066 | 1.222943 |
| H | 2.523388 | 3.019498 | -0.367758 |
| H | 1.117282 | 4.033187 | 0.053638 |

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3C_Ac_conf_2 Eopt -747.390634

| | | | |
|---|---|---|---|
| C | 3.375312 | -1.731891 | -0.691025 |
| H | 3.486821 | -1.556390 | -1.755796 |
| H | 4.235046 | -2.065870 | -0.121355 |
| C | 2.142154 | -1.279081 | 0.008308 |
| C | 2.151745 | 0.247524 | 0.218134 |
| O | 3.103125 | 0.925781 | 0.519894 |
| N | 0.839972 | 0.720577 | -0.020871 |
| C | -0.008099 | -0.337478 | -0.402322 |
| C | 0.849576 | -1.494448 | -0.812289 |
| H | 0.386549 | -2.459844 | -0.596761 |
| H | 1.080029 | -1.449223 | -1.886698 |
| C | 2.021326 | -1.915445 | 1.404912 |
| H | 2.883989 | -1.647337 | 2.022009 |
| H | 1.109103 | -1.583679 | 1.912360 |
| H | 1.987303 | -3.004098 | 1.302926 |
| C | -1.405545 | -0.364913 | -0.124097 |
| C | -2.212758 | -1.375963 | -0.706905 |
| C | -2.032700 | 0.563663 | 0.745775 |
| C | -3.573311 | -1.440639 | -0.441821 |
| H | -1.760218 | -2.096950 | -1.381554 |
| C | -3.393660 | 0.483197 | 1.006775 |
| H | -1.442253 | 1.325591 | 1.247048 |
| C | -4.177211 | -0.512354 | 0.413646 |
| H | -4.170860 | -2.219545 | -0.906463 |
| H | -3.847616 | 1.197541 | 1.687485 |
| H | -5.241397 | -0.567417 | 0.619697 |
| C | 0.571730 | 2.105098 | -0.205377 |
| O | 1.162936 | 2.934110 | 0.450861 |
| C | -0.425157 | 2.465274 | -1.275750 |
| H | -0.082237 | 3.393407 | -1.736676 |
| H | -0.528853 | 1.683218 | -2.029400 |
| H | -1.404126 | 2.652176 | -0.824560 |

32
3C_Ac_conf_3 Eopt -747.391375
C 1.985816 -1.752134 1.507171
H 0.998837 -1.863997 1.944652
H 2.855845 -1.779624 2.154599
C 2.137191 -1.269330 0.096731
C 2.154256 0.265320 0.192253
O 3.116004 0.969636 0.383995
N 0.825899 0.712090 -0.013107
C -0.012947 -0.362685 -0.361082
C 0.855428 -1.529825 -0.722627
H 0.396652 -2.489523 -0.475781
H 1.099659 -1.521887 -1.794827
C 3.417903 -1.787444 -0.547605
H 3.366991 -2.876771 -0.636628
H 3.551750 -1.359131 -1.545532
H 4.286335 -1.528785 0.064442
C -1.414786 -0.386620 -0.104717
C -2.208575 -1.415415 -0.675017
C -2.060998 0.563064 0.727604
C -3.574244 -1.475364 -0.436736
H -1.741241 -2.153646 -1.320309
C -3.427153 0.487538 0.961852
H -1.482838 1.337917 1.223212
C -4.197228 -0.524673 0.379504
H -4.160858 -2.267847 -0.892263
H -3.895851 1.219244 1.613511
H -5.265545 -0.575344 0.564142
C 0.537404 2.091727 -0.206014
O 1.105393 2.927900 0.461448
C -0.443420 2.437894 -1.295367
H -0.070733 3.337405 -1.789692
H -0.565679 1.632057 -2.020182
H -1.417675 2.672676 -0.856857
32
3C_Ac_conf_4 Eopt -747.394578
C 1.755542 -1.820012 1.547722
H 0.746581 -1.868114 1.944642
H 2.595700 -1.871148 2.232068
C 1.991654 -1.399167 0.128658
C 2.113721 0.130177 0.172595
O 3.115524 0.767332 0.404604
N 0.836248 0.669668 -0.106353
C -0.073595 -0.364890 -0.429402
C 0.725640 -1.596604 -0.730668
H 0.197277 -2.517623 -0.476778
H 1.008639 -1.633535 -1.792511
C 3.255350 -2.028249 -0.447902
H 3.128939 -3.113622 -0.502796
H 3.455034 -1.646032 -1.453547
H 4.117185 -1.810029 0.188725
C -1.473226 -0.309184 -0.156887
C -2.317794 -1.325403 -0.671157
C -2.063497 0.697392 0.647706
C -3.680505 -1.322741 -0.405055
H -1.894890 -2.105989 -1.296885
C -3.425703 0.683040 0.914147
H -1.445429 1.472651 1.088216
C -4.247292 -0.319534 0.387406
H -4.306806 -2.107790 -0.818742
H -3.852370 1.457941 1.544505
H -5.312542 -0.320852 0.595897
C 0.603847 2.034875 -0.414561
O -0.338354 2.330356 -1.121706
C 1.535164 3.053297 0.174800
H 1.762975 2.831185 1.218590
H 2.478680 3.058514 -0.377002
H 1.054092 4.027269 0.082497
32
3C_Ac_MECP Eopt -747.393643
C 3.226952 -1.895581 -0.694487
H 3.310051 -1.739544 -1.764664
H 4.102592 -2.219280 -0.143263
C 2.023002 -1.400547 0.034088
C 2.100226 0.125415 0.212700
O 3.079570 0.747658 0.555982
N 0.839462 0.673834 -0.088541
C -0.075134 -0.355931 -0.421073
C 0.708913 -1.594836 -0.744090
H 0.189831 -2.504671 -0.434700
H 0.908004 -1.664390 -1.824430
C 1.927958 -2.013726 1.441691
H 2.809221 -1.751003 2.033965
H 1.032413 -1.655961 1.961231
H 1.872594 -3.103116 1.357255
C -1.476746 -0.290679 -0.160859
C -2.325988 -1.296657 -0.687826
C -2.063159 0.707260 0.657858
C -3.686684 -1.299531 -0.409950
H -1.908701 -2.066118 -1.331006
C -3.422545 0.685044 0.938347
H -1.443224 1.479428 1.101182
C -4.246698 -0.313788 0.408710
H -4.316784 -2.075827 -0.834124
H -3.845031 1.451018 1.582400
H -5.308490 -0.325274 0.634255
C 0.619088 2.039360 -0.411796
O -0.328617 2.335323 -1.110295
C 1.572289 3.052379 0.150364
H 1.772627 2.866040 1.206645
H 2.526774 3.002823 -0.380353
H 1.125416 4.036098 0.007838
40
3C Bn conf 1 Eopt -865.065117
C -0.898983 3.477512 -0.815692
H -1.856359 3.099362 -1.160598
H -0.444022 4.310361 -1.341553
C -0.074595 2.673110 0.140877
C 0.727175 1.668984 -0.704463
O 1.776741 1.870726 -1.292488
N 0.050283 0.465645 -0.706184
C -1.058082 0.490947 0.144368
C -0.958167 1.729890 0.989103
H -1.934506 2.165490 1.215729
H -0.449478 1.511178 1.940511
C 0.864929 3.554222 0.959075
H 0.280424 4.222139 1.599403
H 1.516312 2.942948 1.592000
H 1.490339 4.162787 0.299826
C -2.163596 -0.404608 0.089310
C -3.044377 -0.478051 1.202157
C -2.472361 -1.201963 -1.045560
C -4.144980 -1.322356 1.188876
H -2.838460 0.123673 2.082996
C -3.578780 -2.041628 -1.043724
H -1.873601 -1.120782 -1.946947
C -4.420391 -2.118765 0.070818
H -4.794983 -1.364049 2.058325
H -3.797998 -2.630899 -1.929732
H -5.282081 -2.778666 0.064300
C 0.717650 -0.722418 -1.233559
H 0.006142 -1.548343 -1.221169
H 1.004239 -0.535874 -2.271629
C 1.938034 -1.106110 -0.417153

| | | | |
|---|---|---|---|
| C | 3.041290 | -1.677484 | -1.055658 |
| C | 1.965021 | -0.941173 | 0.971020 |
| C | 4.155482 | -2.082174 | -0.319539 |
| H | 3.030125 | -1.799380 | -2.136245 |
| C | 3.079754 | -1.340909 | 1.707979 |
| H | 1.114934 | -0.494029 | 1.482070 |
| C | 4.178076 | -1.914323 | 1.065258 |
| H | 5.008397 | -2.520467 | -0.829551 |
| H | 3.089379 | -1.203915 | 2.785383 |
| H | 5.046682 | -2.223065 | 1.639127 |

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3C_Bn_conf_2 Eopt -865.068139

| | | | |
|---|---|---|---|
| C | 3.872135 | 1.017139 | -0.724777 |
| H | 3.379461 | 1.838519 | -1.235524 |
| H | 4.819424 | 0.653086 | -1.108408 |
| C | 3.118170 | 0.195179 | 0.275306 |
| C | 2.357837 | -0.868522 | -0.526556 |
| O | 2.808513 | -1.919180 | -0.953745 |
| N | 1.059788 | -0.427492 | -0.718325 |
| C | 0.796075 | 0.745272 | -0.006180 |
| C | 1.965021 | 0.997455 | 0.906402 |
| H | 2.204702 | 2.059714 | 0.998495 |
| H | 1.750273 | 0.609445 | 1.914231 |
| C | 4.055528 | -0.458468 | 1.286892 |
| H | 4.550664 | 0.314447 | 1.882775 |
| H | 3.500114 | -1.118438 | 1.960661 |
| H | 4.821559 | -1.046829 | 0.774133 |
| C | -0.364965 | 1.562227 | -0.080370 |
| C | -0.568531 | 2.532790 | 0.943119 |
| C | -1.337795 | 1.506847 | -1.117087 |
| C | -1.673677 | 3.370139 | 0.935251 |
| H | 0.145511 | 2.607238 | 1.757332 |
| C | -2.438136 | 2.353263 | -1.111040 |
| H | -1.219196 | 0.823833 | -1.948112 |
| C | -2.624955 | 3.289226 | -0.088378 |
| H | -1.798924 | 4.091399 | 1.737981 |
| H | -3.157313 | 2.286818 | -1.922766 |
| H | -3.489699 | 3.945040 | -0.092068 |
| C | 0.093698 | -1.304969 | -1.372674 |
| H | -0.268321 | -0.863290 | -2.303439 |
| H | 0.659695 | -2.200484 | -1.644633 |
| C | -1.060004 | -1.681562 | -0.467842 |
| C | -2.339097 | -1.844867 | -1.004494 |
| C | -0.859575 | -1.902521 | 0.898145 |
| C | -3.404832 | -2.230148 | -0.190315 |
| H | -2.502006 | -1.660907 | -2.064132 |
| C | -1.924790 | -2.280461 | 1.714987 |
| H | 0.132483 | -1.773364 | 1.326797 |
| C | -3.200652 | -2.445781 | 1.172785 |
| H | -4.395176 | -2.351277 | -0.619352 |
| H | -1.758152 | -2.445358 | 2.775467 |
| H | -4.030440 | -2.737142 | 1.809739 |

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3C_Bn_conf_3 Eopt -865.068914

| | | | |
|---|---|---|---|
| C | 1.172824 | 2.572605 | 1.746847 |
| H | 1.214196 | 1.723376 | 2.420556 |
| H | 0.647180 | 3.469706 | 2.057087 |
| C | 1.627439 | 2.442001 | 0.323766 |
| C | 0.360182 | 2.178669 | -0.496445 |
| O | -0.452818 | 3.001155 | -0.887748 |
| N | 0.249935 | 0.816499 | -0.695503 |
| C | 1.364550 | 0.120146 | -0.228682 |
| C | 2.420128 | 1.139736 | 0.107679 |
| H | 3.003824 | 0.862459 | 0.988973 |
| H | 3.115674 | 1.261968 | -0.736115 |
| C | 2.339219 | 3.704993 | -0.155872 |
| H | 3.262796 | 3.846799 | 0.413678 |
| H | 2.590019 | 3.628819 | -1.218577 |
| H | 1.701852 | 4.581353 | -0.008384 |
| C | 1.519544 | -1.287529 | -0.109502 |
| C | 2.834224 | -1.803372 | 0.085022 |
| C | 0.454916 | -2.232989 | -0.138050 |
| C | 3.063060 | -3.164021 | 0.221415 |
| H | 3.677499 | -1.119993 | 0.109079 |
| C | 0.702144 | -3.591557 | 0.001583 |
| H | -0.573011 | -1.903902 | -0.227762 |
| C | 2.002576 | -4.076638 | 0.177090 |
| H | 4.080353 | -3.519557 | 0.359445 |
| H | -0.136316 | -4.282359 | -0.015138 |
| H | 2.184845 | -5.141121 | 0.284116 |
| C | -0.898717 | 0.296611 | -1.418267 |
| H | -1.169862 | 1.054962 | -2.159131 |
| H | -0.593672 | -0.600376 | -1.962242 |
| C | -2.102365 | 0.012490 | -0.538715 |
| C | -3.235684 | -0.562244 | -1.125114 |
| C | -2.116790 | 0.305784 | 0.825927 |
| C | -4.366167 | -0.837897 | -0.359134 |
| H | -3.227634 | -0.795953 | -2.187567 |
| C | -3.250597 | 0.030956 | 1.594542 |
| H | -1.241596 | 0.746411 | 1.298740 |
| C | -4.377048 | -0.540915 | 1.005965 |
| H | -5.238260 | -1.285890 | -0.826446 |
| H | -3.248377 | 0.263738 | 2.655380 |
| H | -5.257135 | -0.756159 | 1.604477 |

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3C_Bn_conf_4 Eopt -865.067641

| | | | |
|---|---|---|---|
| C | 3.969033 | -0.559956 | 1.368408 |
| H | 3.510704 | -0.975949 | 2.259740 |
| H | 5.001865 | -0.805817 | 1.148204 |
| C | 3.120453 | 0.101538 | 0.339029 |
| C | 2.347785 | -0.931851 | -0.493211 |
| O | 2.786797 | -1.978214 | -0.942959 |
| N | 1.059268 | -0.469456 | -0.687561 |
| C | 0.813358 | 0.712684 | 0.014054 |
| C | 1.978929 | 0.949757 | 0.934336 |
| H | 2.250216 | 2.006744 | 1.001451 |
| H | 1.735316 | 0.599876 | 1.949292 |
| C | 3.973209 | 0.922619 | -0.644343 |
| H | 4.690418 | 0.276648 | -1.159540 |
| H | 3.342020 | 1.414762 | -1.391972 |
| H | 4.524959 | 1.690697 | -0.094007 |
| C | -0.328947 | 1.553935 | -0.075144 |
| C | -0.518414 | 2.536138 | 0.940102 |
| C | -1.294593 | 1.513688 | -1.119373 |
| C | -1.604655 | 3.397532 | 0.918270 |
| H | 0.190802 | 2.600016 | 1.759430 |
| C | -2.375635 | 2.384549 | -1.127532 |
| H | -1.185568 | 0.822017 | -1.944513 |
| C | -2.549302 | 3.331397 | -0.112563 |
| H | -1.719933 | 4.126695 | 1.715359 |
| H | -3.089720 | 2.328943 | -1.944552 |
| H | -3.399034 | 4.006383 | -0.127308 |
| C | 0.081526 | -1.326430 | -1.352940 |
| H | -0.254970 | -0.880478 | -2.291197 |
| H | 0.629707 | -2.236653 | -1.612196 |
| C | -1.094435 | -1.669126 | -0.463588 |
| C | -2.370585 | -1.795479 | -1.016787 |
| C | -0.918247 | -1.895223 | 0.904905 |
| C | -3.457798 | -2.147912 | -0.216233 |
| H | -2.514427 | -1.607385 | -2.078456 |
| C | -2.004815 | -2.240004 | 1.708213 |
| H | 0.071628 | -1.795632 | 1.346235 |
| C | -3.277917 | -2.367442 | 1.149687 |
| H | -4.445625 | -2.240084 | -0.658052 |

H -1.856959 -2.408667 2.770878
H -4.124347 -2.632693 1.776070
40
3C_Bn_conf_5 Eopt -865.064621
C 0.841436 3.467988 1.007601
H 1.302633 3.025572 1.884766
H 1.212434 4.421226 0.647608
C -0.078812 2.655252 0.165456
C 0.708812 1.650381 -0.695313
O 1.741814 1.858237 -1.310448
N 0.046451 0.441389 -0.676388
C -1.072572 0.469100 0.158573
C -0.997912 1.720069 0.987486
H -1.981286 2.163506 1.165657
H -0.537709 1.508916 1.964687
C -0.893517 3.540727 -0.792491
H -0.227113 4.091481 -1.463256
H -1.578352 2.935935 -1.396660
H -1.481606 4.260367 -0.214998
C -2.169436 -0.436230 0.103137
C -3.067794 -0.494365 1.203079
C -2.455076 -1.257268 -1.021179
C -4.162474 -1.346151 1.188492
H -2.880194 0.125444 2.075410
C -3.556223 -2.103745 -1.020842
H -1.842115 -1.190018 -1.914163
C -4.414946 -2.165624 0.081648
H -4.825945 -1.375713 2.048239
H -3.757565 -2.711137 -1.898831
H -5.272222 -2.831230 0.074100
C 0.722895 -0.749074 -1.186493
H 0.028892 -1.587598 -1.123721
H 0.974683 -0.594563 -2.238941
C 1.974300 -1.082934 -0.395255
C 3.045704 -1.705074 -1.040808
C 2.063279 -0.824954 0.975835
C 4.188463 -2.069546 -0.328090
H 2.986587 -1.899419 -2.109192
C 3.206981 -1.184456 1.689094
H 1.240910 -0.335133 1.492996
C 4.272663 -1.809550 1.040046
H 5.015486 -2.548631 -0.843993
H 3.264623 -0.974936 2.753258
H 5.163566 -2.086972 1.595474
40
3C_Bn_conf_6 Eopt -865.067865
C 2.425564 3.621193 -0.308298
H 2.951676 3.533398 -1.253123
H 2.277432 4.606796 0.118656
C 1.702758 2.445839 0.250578
C 0.391325 2.180739 -0.501511
O -0.432995 3.006839 -0.860127
N 0.257160 0.820096 -0.685390
C 1.370972 0.108994 -0.239809
C 2.452802 1.109597 0.065704
H 3.028506 0.841635 0.955740
H 3.153180 1.180130 -0.779901
C 1.327968 2.670347 1.726442
H 0.667136 3.536678 1.826517
H 0.820999 1.790802 2.137993
H 2.236332 2.851764 2.308922
C 1.504114 -1.299582 -0.111476
C 2.812535 -1.835715 0.071620
C 0.423503 -2.227317 -0.118666
C 3.020288 -3.198831 0.216254
H 3.667311 -1.166392 0.080901
C 0.649852 -3.588587 0.029178
H -0.599771 -1.881821 -0.199523
C 1.944212 -4.093919 0.192638
H 4.033099 -3.570199 0.345255
H -0.200033 -4.265498 0.028214
H 2.110081 -5.160392 0.306329
C -0.898516 0.313756 -1.409173
H -1.158731 1.075822 -2.150174
H -0.601493 -0.586355 -1.952763
C -2.109273 0.040993 -0.536789
C -3.246100 -0.517318 -1.132156
C -2.127128 0.326823 0.829003
C -4.383674 -0.783617 -0.373462
H -3.235295 -0.745518 -2.195796
C -3.267818 0.061160 1.590602
H -1.248527 0.753187 1.307079
C -4.398002 -0.493949 0.993194
H -5.258558 -1.218797 -0.847606
H -3.268179 0.287834 2.652760
H -5.283606 -0.702083 1.586040
46
3TS-I_2ab_conf_1 Eopt -1054.929854
C 3.463794 -1.781995 1.088538
H 3.506036 -0.741134 1.390710
H 3.994606 -2.497138 1.711969
C 3.051366 -2.133769 -0.159853
C 2.292966 -1.142404 -0.940035
O 2.194502 -1.138214 -2.152029
N 1.559431 -0.228456 -0.109919
C 0.710766 -0.867556 0.861603
C 1.339580 -1.430249 2.066732
H 1.619478 -0.763013 2.881020
H 1.141007 -2.463454 2.333996
C 3.254080 -3.485283 -0.775610
H 2.298653 -3.929901 -1.076371
H 3.870226 -3.408010 -1.677912
H 3.752913 -4.156329 -0.073088
C -0.685905 -0.949232 0.592922
C -1.584336 -1.465406 1.568608
C -1.246503 -0.514612 -0.634224
C -2.941227 -1.533315 1.328686
H -1.198341 -1.804146 2.525614
C -2.610227 -0.589000 -0.882907
H -0.600275 -0.124796 -1.415459
C -3.470966 -1.096320 0.101203
H -3.620597 -1.923704 2.080439
H -2.991564 -0.251415 -1.839725
C 1.493659 1.123747 -0.413744
O 2.156607 1.647692 -1.286376
O 0.652097 1.740259 0.417185
C 0.318996 3.158025 0.250151
C 1.555652 4.019144 0.478023
H 2.285228 3.892834 -0.323329
H 1.252836 5.070100 0.516006
H 2.023406 3.762531 1.434024
C -0.308475 3.383311 -1.120675
H -1.154929 2.703433 -1.264672
H -0.681412 4.410682 -1.174178
H 0.414640 3.232561 -1.924089
C -0.708088 3.385677 1.351692
H -0.267993 3.187508 2.333768
H -1.052519 4.423102 1.324839
H -1.569944 2.725222 1.211540
O -4.812526 -1.205042 -0.039600
C -5.390969 -0.767288 -1.263952
H -5.004203 -1.346456 -2.109062
H -6.462787 -0.936416 -1.165285
H -5.200901 0.298728 -1.427715

29
3TS-I_2af_conf_1 Eopt -708.040417
C 2.593491 2.157445 -0.116464
H 2.708504 1.631814 -1.059695
H 2.900082 3.199182 -0.096268
C 2.375670 1.478665 1.039114
C 1.918806 0.089030 0.990293
O 2.125041 -0.751823 1.846063
N 1.119334 -0.192713 -0.167116
C 0.055727 0.744757 -0.413089
C 0.390001 2.073395 -0.949485
H 0.576337 2.180875 -2.017183
H 0.040033 2.956847 -0.425099
C -1.282071 0.350089 -0.094869
C -2.373745 1.186803 -0.441811
C -1.565596 -0.865636 0.579335
C -3.676898 0.819716 -0.135096
H -2.186543 2.121982 -0.961615
C -2.871573 -1.215488 0.889283
H -0.752672 -1.524204 0.870533
C -3.937304 -0.380935 0.532901
H -4.496959 1.473813 -0.416258
H -3.064440 -2.147284 1.412805
H -4.957236 -0.662687 0.775055
C 1.204466 -1.364631 -0.913888
O 0.422130 -1.567234 -1.829515
C 2.307362 -2.329309 -0.568237
H 3.243163 -1.818026 -0.333163
H 2.016670 -2.918780 0.305327
H 2.446454 -2.991914 -1.422332
H 2.483882 1.936425 2.017404
35
3TS-I_2d_conf_1 Eopt -1084.299047
C -3.984887 -1.447897 -0.764153
H -4.005154 -0.650762 -1.500094
H -4.471621 -2.380949 -1.036785
C -3.649861 -1.201984 0.530196
C -2.958042 0.061665 0.826632
O -2.985495 0.636640 1.898554
N -2.149562 0.541290 -0.258918
C -1.249394 -0.423289 -0.828368
C -1.793483 -1.513510 -1.652172
H -1.998828 -1.323010 -2.704559
H -1.578040 -2.540501 -1.374773
C -3.886563 -2.143923 1.671549
H -2.950194 -2.380799 2.188968
H -4.556821 -1.690358 2.409496
H -4.340622 -3.070762 1.315053
C 0.145254 -0.301864 -0.532853
C 1.085578 -1.134709 -1.194119
C 0.630818 0.621052 0.426920
C 2.437061 -1.039890 -0.914827
H 0.742593 -1.849375 -1.935677
C 1.984419 0.705041 0.711846
H -0.060870 1.261745 0.964121
C 2.888737 -0.120209 0.039089
H 3.144622 -1.679927 -1.434429
H 2.335735 1.411941 1.456018
C -2.074872 1.879045 -0.642384
O -1.286786 2.226235 -1.507562
C -3.023239 2.841626 0.020710
H -4.017865 2.411554 0.156538
H -2.636398 3.116753 1.005460
H -3.082284 3.731042 -0.606379
C 4.354140 -0.060755 0.333902
F 4.680277 0.930907 1.180439
F 4.811252 -1.206686 0.889737
F 5.093685 0.122334 -0.782428
36
3TS-I_2g_conf_1 Eopt -861.828364
C -3.437181 -1.437557 -0.579698
H -3.544541 -0.656975 -1.325436
H -3.938108 -2.381417 -0.779903
C -2.979212 -1.155748 0.670382
C -2.273900 0.119482 0.873137
O -2.196184 0.711842 1.935897
N -1.579127 0.570399 -0.295752
C -0.724345 -0.434232 -0.878155
C -1.348097 -1.477054 -1.704947
H -1.680116 -1.231117 -2.712262
H -1.117432 -2.519106 -1.508078
C -3.093461 -2.074327 1.849552
H -2.108900 -2.287312 2.281102
H -3.697279 -1.613022 2.638417
H -3.565369 -3.015285 1.558953
C 0.664365 -0.394771 -0.574341
C 1.565988 -1.319396 -1.175695
C 1.215724 0.548657 0.330140
C 2.914144 -1.296333 -0.887825
H 1.187827 -2.054512 -1.879749
C 2.570602 0.568604 0.629029
H 0.567288 1.270025 0.818038
C 3.432909 -0.354607 0.019461
H 3.595316 -2.002956 -1.352341
H 2.946803 1.302013 1.332768
C -1.516109 1.891031 -0.714704
O -0.782195 2.215544 -1.637120
C -2.408890 2.878315 -0.009424
H -3.387914 2.454675 0.224797
H -1.940572 3.186991 0.929101
H -2.522268 3.746959 -0.658052
O 4.765535 -0.415424 0.242227
C 5.331221 0.517347 1.156463
H 6.397111 0.293842 1.189285
H 5.182367 1.545290 0.809641
H 4.899883 0.396964 2.155708
32
3TS-I_2l_conf_1 Eopt -846.553931
C -3.004494 -1.436045 -0.911496
H -2.984681 -0.633433 -1.641373
H -3.472024 -2.368235 -1.218471
C -2.747865 -1.197810 0.402617
C -2.079121 0.065639 0.749757
O -2.170278 0.629909 1.824939
N -1.211441 0.552704 -0.283533
C -0.275170 -0.416221 -0.789549
C -0.765734 -1.481354 -1.677105
H -0.913407 -1.263492 -2.733899
H -0.571278 -2.517002 -1.416371
C -3.048964 -2.149476 1.520769
H -2.143408 -2.390148 2.088974
H -3.760692 -1.702705 2.223223
H -3.480676 -3.073899 1.131514
C 1.089406 -0.318929 -0.371978
C 2.070624 -1.173507 -0.937812
C 1.507539 0.610114 0.616177
C 3.399002 -1.103938 -0.544200
H 1.782465 -1.891983 -1.698829
C 2.831446 0.678251 1.020825
H 0.783384 1.271615 1.080709
C 3.751583 -0.178814 0.429297
H 4.154060 -1.752035 -0.976821
H 3.156307 1.380127 1.781847
C -1.114193 1.888690 -0.656485

O -0.271666 2.243045 -1.467069
C -2.104310 2.847810 -0.050582
H -3.103136 2.413358 0.028635
H -1.776064 3.125870 0.954529
H -2.131568 3.737005 -0.680265
F 5.046430 -0.110450 0.821885
32
3TS-I_2n_conf_1 Eopt -1206.912860
C -3.385394 -1.442378 -0.813632
H -3.405064 -0.638527 -1.542186
H -3.862958 -2.376271 -1.099274
C -3.067542 -1.204697 0.487076
C -2.388698 0.061564 0.803267
O -2.434608 0.627219 1.880225
N -1.569104 0.551171 -0.267702
C -0.656485 -0.414062 -0.820416
C -1.186134 -1.479349 -1.685098
H -1.383380 -1.258637 -2.733113
H -0.974565 -2.514437 -1.436194
C -3.312050 -2.158147 1.617301
H -2.380450 -2.393831 2.143921
H -3.993793 -1.715221 2.351229
H -3.756035 -3.084726 1.247566
C 0.725037 -0.313824 -0.469311
C 1.681800 -1.160421 -1.085470
C 1.188823 0.609556 0.502898
C 3.026695 -1.084928 -0.757453
H 1.362039 -1.877990 -1.834807
C 2.530367 0.680876 0.840428
H 0.487721 1.265047 1.009722
C 3.441645 -0.164194 0.204543
H 3.747984 -1.735313 -1.241439
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29
3TS-II_2af_conf_1 Eopt -708.039911
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35
3TS-II_2d_conf_1 Eopt -1084.297699
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3TS-II_2g_conf_1 Eopt -861.825000
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C 0.624289 -0.366813 -0.538875
C 1.233231 -1.578996 -1.127541
H 0.816660 -2.551413 -0.891011
H 1.746622 -1.488379 -2.085894
C 3.948894 -2.281370 -0.017809
H 4.102551 -2.136501 -1.089822
H 4.880693 -2.019226 0.494439
H 3.737086 -3.336530 0.170791
C -0.756082 -0.197432 -0.269979
C -1.709198 -1.066698 -0.861003
C -1.254544 0.797554 0.621021
C -3.069588 -0.947136 -0.606974
H -1.371192 -1.842549 -1.541793
C -2.602894 0.907153 0.886441
H -0.566481 1.465431 1.130141
C -3.528527 0.044890 0.269725
H -3.760075 -1.629382 -1.089465
H -2.972178 1.657812 1.578982
C 1.446684 1.970130 -0.395918
O 0.572386 2.344693 -1.151574
C 2.345095 2.930821 0.333615
H 2.688112 2.536844 1.290340
H 3.221041 3.150256 -0.281842
H 1.778399 3.852040 0.480642
O -4.831122 0.242365 0.590632
C -5.797580 -0.602977 -0.020357
H -6.765014 -0.276317 0.360185
H -5.777691 -0.497379 -1.110427
H -5.631617 -1.650871 0.252019
32
3TS-II_2l_conf_1 Eopt -846.551326
C 1.826572 -1.694027 1.616712
H 1.091532 -1.034607 2.069889
H 1.967264 -2.676989 2.056744
C 2.528218 -1.328037 0.503620
C 2.492147 0.124011 0.133218
O 3.490462 0.808029 0.039810
N 1.191783 0.607730 -0.127990
C 0.277770 -0.396190 -0.538255
C 0.950201 -1.578689 -1.118105
H 0.588599 -2.569532 -0.868495
H 1.447581 -1.467682 -2.082556
C 3.704844 -2.117480 -0.008881
H 3.848599 -1.971678 -1.082071
H 4.620969 -1.799724 0.500081
H 3.552343 -3.181301 0.187799
C -1.116070 -0.302249 -0.276785
C -2.010631 -1.212957 -0.900942
C -1.661557 0.644336 0.632659
C -3.373765 -1.169213 -0.650825
H -1.623163 -1.950189 -1.597461
C -3.021356 0.681345 0.897157
H -1.008909 1.332931 1.159398
C -3.852736 -0.220952 0.244000

H -4.061100 -1.856308 -1.133544
H -3.441146 1.392197 1.601569
C 0.954009 1.985534 -0.389962
O 0.054048 2.306967 -1.138836
C 1.798473 2.994293 0.337768
H 2.166036 2.618197 1.292643
H 2.658641 3.263435 -0.280178
H 1.180892 3.881549 0.487954
F -5.184824 -0.179191 0.498678
32
3TS-II_2n_conf_1 Eopt -1206.910723
C 2.120940 -1.702748 1.632447
H 1.380451 -1.036524 2.066396
H 2.241206 -2.686993 2.075558
C 2.855674 -1.342610 0.539019
C 2.841613 0.109330 0.167366
O 3.847001 0.785051 0.096886
N 1.551009 0.604566 -0.123532
C 0.640581 -0.390805 -0.558013
C 1.318256 -1.575240 -1.126256
H 0.939360 -2.564251 -0.896314
H 1.848774 -1.459621 -2.072094
C 4.037406 -2.142920 0.056328
H 4.209807 -1.998307 -1.012790
H 4.943132 -1.833794 0.588636
H 3.869912 -3.205237 0.248746
C -0.756774 -0.287096 -0.334351
C -1.642546 -1.189492 -0.982702
C -1.321987 0.661054 0.561421
C -3.010211 -1.133904 -0.769729
H -1.244743 -1.929724 -1.670267
C -2.687006 0.706586 0.787901
H -0.681111 1.344448 1.109003
C -3.525457 -0.184800 0.114490
H -3.673870 -1.822640 -1.282452
H -3.102328 1.425973 1.486423
C 1.329592 1.986055 -0.385589
O 0.450755 2.316264 -1.154809
C 2.165473 2.984745 0.364848
H 2.504734 2.603354 1.328077
H 3.043775 3.245430 -0.230811
H 1.553632 3.878215 0.500634
Cl -5.250892 -0.117161 0.393311
33
3TS-II 2p conf 1 Eopt -839.564680
C 1.971532 -1.690669 1.635503
H 1.228648 -1.020069 2.058514
H 2.085215 -2.672517 2.085373
C 2.721281 -1.338132 0.549697
C 2.713090 0.110040 0.163849
O 3.717444 0.784743 0.088711
N 1.420900 0.604989 -0.131723
C 0.515629 -0.391156 -0.562236
C 1.196503 -1.567318 -1.137569
H 0.805040 -2.557964 -0.939536
H 1.763748 -1.429840 -2.057945
C 3.904053 -2.145644 0.083356
H 4.086488 -2.009236 -0.985121
H 4.805488 -1.834581 0.621746
H 3.731667 -3.205776 0.282747
C -0.875126 -0.294381 -0.333718
C -1.762254 -1.192220 -0.995518
C -1.434457 0.642526 0.584244
C -3.122872 -1.139142 -0.776608
H -1.362597 -1.917990 -1.696722
C -2.791949 0.681535 0.816818
H -0.786863 1.312293 1.140316
C -3.651722 -0.201621 0.132090
H -3.789040 -1.818389 -1.298667
H -3.204094 1.387361 1.530836
C 1.189370 1.990050 -0.382466
O 0.304303 2.318135 -1.143454
C 2.030025 2.984653 0.366052
H 2.360694 2.603568 1.332568
H 2.913948 3.233516 -0.226301
H 1.425698 3.884036 0.494692
C -5.061135 -0.152472 0.369732
N -6.205161 -0.112664 0.562592
44
3TS-II_2y_conf_1 Eopt -1128.701799
C 0.595759 3.372543 1.779301
H 0.726079 2.376388 2.192591
H 1.115200 4.195642 2.261062
C -0.157408 3.590562 0.660350
C -1.065591 2.476328 0.237459
O -2.264358 2.596612 0.109192
N -0.368846 1.277874 -0.048476
C 0.969174 1.461315 -0.488856
C 1.223204 2.834578 -0.972928
H 2.141056 3.335066 -0.685719
H 0.782811 3.137055 -1.924687
C -0.540299 4.972924 0.198426
H -0.733354 4.997599 -0.876599
H -1.449578 5.302694 0.711927
H 0.261856 5.677175 0.431185
C 1.939468 0.437170 -0.362391
C 3.206744 0.577374 -0.999493
C 1.733035 -0.737544 0.406569
C 4.178899 -0.393635 -0.885528
H 3.407493 1.462782 -1.595839
C 2.715804 -1.710634 0.531929
H 0.803618 -0.881815 0.949717
C 3.945909 -1.551101 -0.120317
H 5.138001 -0.280061 -1.382006
H 2.516259 -2.584288 1.141478
C -1.081493 0.111132 -0.382492
O -0.810512 -0.612341 -1.306556
O -2.053674 -0.110621 0.516106
O 4.962875 -2.445606 -0.066032
C 4.763959 -3.628630 0.698080
H 5.684948 -4.203581 0.605063
H 4.585852 -3.389877 1.752124
H 3.925420 -4.213187 0.304541
C -2.945904 -1.151211 0.239645
C -2.823531 -2.328074 0.964617
C -3.954865 -0.953589 -0.694731
C -3.750183 -3.347336 0.741643
H -2.019782 -2.436400 1.686510
C -4.871259 -1.981838 -0.910119
H -4.014665 -0.015118 -1.237690
C -4.771016 -3.176438 -0.193815
H -3.670897 -4.274379 1.300773
H -5.666025 -1.846391 -1.637041
H -5.489459 -3.972148 -0.363849
32
3TS-II_Ac_conf_1 Eopt -747.340148
C 1.582305 -1.667923 1.601473
H 0.849109 -1.023537 2.078693
H 1.760772 -2.645691 2.039403
C 2.234698 -1.291264 0.462215
C 2.153090 0.158070 0.087762
O 3.131736 0.864485 -0.042651
N 0.834710 0.611040 -0.129916
C -0.072343 -0.413394 -0.501431

C 0.604258 -1.584322 -1.099739
H 0.271995 -2.581336 -0.834653
H 1.065240 -1.466725 -2.081352
C 3.409343 -2.056840 -0.089677
H 3.510923 -1.912719 -1.167892
H 4.335903 -1.716482 0.384577
H 3.287913 -3.122879 0.116371
C -1.457590 -0.345496 -0.189780
C -2.356699 -1.276650 -0.775835
C -1.988857 0.594424 0.734440
C -3.709525 -1.250194 -0.469638
H -1.977360 -2.009816 -1.481987
C -3.340516 0.597560 1.042971
H -1.328726 1.299510 1.230741
C -4.215525 -0.315404 0.440681
H -4.377406 -1.965860 -0.940343
H -3.720132 1.316724 1.763137
H -5.273352 -0.302125 0.683271
C 0.559871 1.982795 -0.391155
O -0.359982 2.281666 -1.124420
C 1.395806 3.011209 0.318721
H 1.803686 2.639499 1.258784
H 2.227435 3.310907 -0.323817
H 0.757108 3.878615 0.495008
32
3TS-II_Ac_conf_2 Eopt -747.337248
C 1.711545 -1.715000 1.504795
H 0.949786 -1.155364 2.040630
H 1.940155 -2.719523 1.848962
C 2.338096 -1.201201 0.405516
C 2.183560 0.274639 0.171638
O 3.124482 1.036665 0.126714
N 0.840287 0.665314 -0.034375
C -0.008756 -0.372453 -0.479445
C 0.718128 -1.453952 -1.176621
H 0.427347 -2.484038 -1.006250
H 1.179684 -1.226335 -2.138477
C 3.547799 -1.851122 -0.214772
H 3.636262 -1.604515 -1.275453
H 4.457720 -1.506838 0.288001
H 3.483519 -2.936406 -0.106396
C -1.393191 -0.391487 -0.160196
C -2.264303 -1.290793 -0.834316
C -1.953112 0.438083 0.851021
C -3.615917 -1.335365 -0.527657
H -1.862486 -1.940474 -1.606730
C -3.304045 0.371243 1.154913
H -1.313562 1.109885 1.417490
C -4.150515 -0.507319 0.467002
H -4.262191 -2.023363 -1.065056
H -3.704048 1.005555 1.940714
H -5.207755 -0.551204 0.708087
C 0.517724 2.048522 -0.175724
O 1.041579 2.868384 0.545138
C -0.462338 2.414432 -1.258519
H -0.438023 1.706803 -2.089471
H -1.478419 2.441292 -0.852752
H -0.206530 3.417564 -1.603308
32
3TS-II_Ac_conf_3 Eopt -747.337826
C 3.467934 -1.861935 -0.290932
H 4.002910 -1.371524 -1.098018
H 3.758194 -2.873237 -0.022914
C 2.400897 -1.266911 0.310623
C 2.188713 0.199192 0.032066
O 3.101675 0.996738 -0.058967
N 0.845280 0.578356 -0.138332
C -0.058152 -0.456864 -0.468156
C 0.584737 -1.686247 -0.970742
H 0.342440 -2.635624 -0.503351
H 0.871654 -1.728926 -2.021972
C 1.799645 -1.808440 1.592672
H 2.338711 -1.387904 2.448595
H 0.743222 -1.550942 1.707182
H 1.901143 -2.895905 1.621644
C -1.452286 -0.360484 -0.176689
C -2.347416 -1.307205 -0.740002
C -1.990279 0.609338 0.709601
C -3.704927 -1.263584 -0.456062
H -1.960987 -2.067497 -1.413225
C -3.347122 0.629759 0.999200
H -1.336235 1.325852 1.197872
C -4.218727 -0.296067 0.414398
H -4.369273 -1.991997 -0.911936
H -3.731374 1.373086 1.691812
H -5.279825 -0.268975 0.641151
C 0.523485 1.950737 -0.391933
O -0.346290 2.220578 -1.190891
C 1.241611 2.998015 0.411592
H 1.664803 2.600304 1.333420
H 2.048890 3.425312 -0.188360
H 0.517007 3.785129 0.631474
32
3TS-II_Ac_conf_4 Eopt -747.334950
C 3.586016 -1.632339 -0.425787
H 4.080786 -1.035015 -1.185214
H 3.930226 -2.650226 -0.269271
C 2.503188 -1.158049 0.248926
C 2.213562 0.320147 0.134111
O 3.082844 1.165728 0.164235
N 0.849673 0.631286 -0.037609
C 0.003583 -0.419622 -0.440302
C 0.696678 -1.565886 -1.056363
H 0.498043 -2.565370 -0.682314
H 0.984881 -1.493138 -2.105661
C 1.952985 -1.857087 1.476230
H 2.484618 -1.496907 2.363807
H 0.886993 -1.667202 1.628925
H 2.110072 -2.935188 1.393681
C -1.391636 -0.403644 -0.142952
C -2.259052 -1.320202 -0.795668
C -1.959662 0.463319 0.829649
C -3.616426 -1.342244 -0.511938
H -1.849567 -2.002662 -1.535387
C -3.317008 0.418918 1.113353
H -1.326088 1.147245 1.387744
C -4.160046 -0.474621 0.442960
H -4.259169 -2.044535 -1.034877
H -3.722756 1.083008 1.871085
H -5.221403 -0.501057 0.668042
C 0.466177 2.008981 -0.166919
O 0.899075 2.831455 0.605421
C -0.447438 2.357126 -1.312308
H -0.426843 1.606276 -2.103346
H -1.474583 2.463737 -0.950495
H -0.123801 3.325780 -1.698653
40
3TS-II_Bn_conf_1 Eopt -865.012827
C 3.535627 1.655616 -0.299911
H 2.919565 2.080891 -1.087647
H 4.303223 2.285632 0.140968
C 3.320449 0.394339 0.169226
C 2.459006 -0.509280 -0.674229
O 2.927822 -1.476683 -1.261955

| | | | |
|---|---|---|---|
| N | 1.130108 | -0.142460 | -0.742783 |
| C | 0.666839 | 0.720935 | 0.266614 |
| C | 1.499017 | 0.721113 | 1.486897 |
| H | 1.742069 | 1.665630 | 1.961428 |
| H | 1.443799 | -0.149179 | 2.145211 |
| C | 4.284641 | -0.294545 | 1.103064 |
| H | 3.785191 | -1.057115 | 1.705727 |
| H | 5.074944 | -0.786879 | 0.526739 |
| H | 4.747782 | 0.436979 | 1.769782 |
| C | -0.549762 | 1.456722 | 0.138196 |
| C | -1.239112 | 1.880662 | 1.306216 |
| C | -1.100332 | 1.823732 | -1.118811 |
| C | -2.431071 | 2.584589 | 1.216354 |
| H | -0.833332 | 1.627206 | 2.282115 |
| C | -2.287085 | 2.540575 | -1.192824 |
| H | -0.568355 | 1.583180 | -2.033089 |
| C | -2.971790 | 2.916588 | -0.032006 |
| H | -2.946503 | 2.878722 | 2.126311 |
| H | -2.679416 | 2.818296 | -2.167179 |
| H | -3.902083 | 3.471726 | -0.098167 |
| C | 0.209384 | -0.980621 | -1.528379 |
| H | 0.833388 | -1.750500 | -1.987262 |
| H | -0.249965 | -0.404567 | -2.332999 |
| C | -0.856700 | -1.613673 | -0.661265 |
| C | -2.199105 | -1.560364 | -1.039557 |
| C | -0.508398 | -2.260655 | 0.529827 |
| C | -3.183819 | -2.150017 | -0.243442 |
| H | -2.475643 | -1.045904 | -1.957170 |
| C | -1.489106 | -2.844731 | 1.329037 |
| H | 0.535527 | -2.300540 | 0.836308 |
| C | -2.831137 | -2.790703 | 0.943526 |
| H | -4.225250 | -2.098816 | -0.547308 |
| H | -1.207677 | -3.342498 | 2.252458 |
| H | -3.595872 | -3.243266 | 1.567697 |

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3TS-II_Bn_conf_2 Eopt -865.012815

| | | | |
|---|---|---|---|
| C | 0.784453 | 2.593053 | 1.819380 |
| H | 0.384314 | 1.655093 | 2.195497 |
| H | 1.281191 | 3.252617 | 2.525561 |
| C | 0.727530 | 2.911402 | 0.495837 |
| C | -0.221879 | 2.109368 | -0.353023 |
| O | -1.246411 | 2.591396 | -0.820208 |
| N | 0.125465 | 0.787006 | -0.537930 |
| C | 1.469809 | 0.443561 | -0.320996 |
| C | 2.387667 | 1.603157 | -0.340836 |
| H | 3.136968 | 1.697915 | 0.437149 |
| H | 2.642047 | 2.037141 | -1.309686 |
| C | 1.084986 | 4.283329 | -0.019348 |
| H | 1.426735 | 4.247516 | -1.056546 |
| H | 0.207324 | 4.936960 | 0.022303 |
| H | 1.872198 | 4.722366 | 0.598446 |
| C | 1.911923 | -0.897334 | -0.125303 |
| C | 3.294454 | -1.202734 | -0.273712 |
| C | 1.049404 | -1.960079 | 0.265001 |
| C | 3.770691 | -2.489467 | -0.074126 |
| H | 3.983669 | -0.413621 | -0.561008 |
| C | 1.543689 | -3.240203 | 0.471079 |
| H | -0.003608 | -1.769521 | 0.443698 |
| C | 2.903161 | -3.523915 | 0.297905 |
| H | 4.829886 | -2.691093 | -0.207165 |
| H | 0.861037 | -4.026726 | 0.780484 |
| H | 3.280761 | -4.528502 | 0.459429 |
| C | -0.807923 | -0.036893 | -1.307335 |
| H | -0.261934 | -0.904046 | -1.683358 |
| H | -1.127778 | 0.552352 | -2.172944 |
| C | -2.035327 | -0.479370 | -0.535764 |
| C | -3.055470 | -1.135270 | -1.234068 |
| C | -2.180465 | -0.269321 | 0.836608 |
| C | -4.198833 | -1.576416 | -0.571350 |
| H | -2.950519 | -1.299144 | -2.304453 |
| C | -3.327635 | -0.707630 | 1.502157 |
| H | -1.395702 | 0.237878 | 1.392744 |
| C | -4.339164 | -1.362787 | 0.801946 |
| H | -4.981779 | -2.084606 | -1.126666 |
| H | -3.427128 | -0.534573 | 2.569791 |
| H | -5.231064 | -1.702919 | 1.319586 |

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3TS-II_Bn_conf_4 Eopt -865.011714

| | | | |
|---|---|---|---|
| C | 4.170082 | -0.495616 | 1.117147 |
| H | 4.023883 | -1.555472 | 1.302752 |
| H | 4.937408 | 0.021820 | 1.685641 |
| C | 3.357928 | 0.189682 | 0.269170 |
| C | 2.458137 | -0.613188 | -0.643983 |
| O | 2.885337 | -1.549565 | -1.309630 |
| N | 1.142786 | -0.194821 | -0.701616 |
| C | 0.697776 | 0.700126 | 0.283098 |
| C | 1.539220 | 0.774573 | 1.489377 |
| H | 1.900355 | 1.741285 | 1.828373 |
| H | 1.393809 | 0.021659 | 2.266335 |
| C | 3.684190 | 1.595281 | -0.194135 |
| H | 4.305174 | 1.542666 | -1.095579 |
| H | 2.788581 | 2.172132 | -0.441402 |
| H | 4.243735 | 2.126882 | 0.579535 |
| C | -0.511390 | 1.456104 | 0.135139 |
| C | -1.206158 | 1.893868 | 1.292767 |
| C | -1.034298 | 1.837048 | -1.127445 |
| C | -2.383164 | 2.621328 | 1.187961 |
| H | -0.818328 | 1.632251 | 2.273868 |
| C | -2.206579 | 2.577465 | -1.217853 |
| H | -0.492594 | 1.590285 | -2.034297 |
| C | -2.900103 | 2.964602 | -0.067078 |
| H | -2.904749 | 2.924699 | 2.091334 |
| H | -2.578119 | 2.865122 | -2.197463 |
| H | -3.818621 | 3.537562 | -0.145329 |
| C | 0.195314 | -0.987304 | -1.503141 |
| H | 0.791957 | -1.771657 | -1.972459 |
| H | -0.243120 | -0.385516 | -2.299928 |
| C | -0.893196 | -1.595558 | -0.645499 |
| C | -2.229739 | -1.515946 | -1.039922 |
| C | -0.572092 | -2.249626 | 0.549303 |
| C | -3.235352 | -2.086299 | -0.256042 |
| H | -2.485261 | -0.995957 | -1.960531 |
| C | -1.573749 | -2.814663 | 1.336190 |
| H | 0.466985 | -2.309446 | 0.868894 |
| C | -2.909750 | -2.734220 | 0.934743 |
| H | -4.271831 | -2.014478 | -0.572472 |
| H | -1.313181 | -3.317861 | 2.262789 |
| H | -3.690736 | -3.171646 | 1.549510 |

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3TS-II_Bn_conf_5 Eopt -865.012490

| | | | |
|---|---|---|---|
| C | 0.923681 | 4.249472 | -0.131219 |
| H | 0.702186 | 4.514784 | -1.160575 |
| H | 1.453596 | 4.973915 | 0.480371 |
| C | 0.629953 | 3.015641 | 0.355971 |
| C | -0.291857 | 2.133128 | -0.450333 |
| O | -1.360693 | 2.532666 | -0.897314 |
| N | 0.111867 | 0.821841 | -0.609578 |
| C | 1.446940 | 0.497958 | -0.335580 |
| C | 2.348476 | 1.662265 | -0.245020 |
| H | 2.946641 | 1.803391 | 0.650385 |
| H | 2.773441 | 2.057499 | -1.168323 |
| C | 0.701918 | 2.696010 | 1.836130 |
| H | -0.264250 | 2.922111 | 2.301810 |
| H | 0.923451 | 1.641676 | 2.025632 |

| | | | |
|---|---|---|---|
| H | 1.468575 | 3.308264 | 2.317618 |
| C | 1.917327 | -0.839231 | -0.140376 |
| C | 3.313204 | -1.096008 | -0.241364 |
| C | 1.081941 | -1.933863 | 0.214797 |
| C | 3.828418 | -2.367103 | -0.037071 |
| H | 3.984521 | -0.280913 | -0.496937 |
| C | 1.613986 | -3.198850 | 0.426960 |
| H | 0.018548 | -1.784191 | 0.365448 |
| C | 2.986278 | -3.434829 | 0.296016 |
| H | 4.898100 | -2.529326 | -0.135541 |
| H | 0.948649 | -4.010198 | 0.708770 |
| H | 3.393014 | -4.427308 | 0.461747 |
| C | -0.802513 | -0.052830 | -1.344088 |
| H | -0.230411 | -0.904058 | -1.716955 |
| H | -1.161546 | 0.508774 | -2.211969 |
| C | -1.997773 | -0.526090 | -0.540160 |
| C | -2.988213 | -1.263267 | -1.198705 |
| C | -2.141096 | -0.265803 | 0.823878 |
| C | -4.101163 | -1.734431 | -0.505280 |
| H | -2.884260 | -1.467580 | -2.262202 |
| C | -3.257222 | -0.734998 | 1.520079 |
| H | -1.379461 | 0.304420 | 1.350892 |
| C | -4.239609 | -1.470835 | 0.859336 |
| H | -4.861394 | -2.305584 | -1.030157 |
| H | -3.355532 | -0.522938 | 2.580758 |
| H | -5.107457 | -1.834960 | 1.400954 |

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3TS-II_Bn_conf_6 Eopt -865.010652

| | | | |
|---|---|---|---|
| C | 0.918130 | 3.655982 | 0.812119 |
| H | 1.884400 | 3.279673 | 1.135135 |
| H | 0.576839 | 4.603742 | 1.218410 |
| C | 0.112303 | 2.920523 | -0.000451 |
| C | 0.723868 | 1.725685 | -0.696224 |
| O | 1.762981 | 1.802536 | -1.341023 |
| N | 0.023316 | 0.544211 | -0.589134 |
| C | -1.037909 | 0.479368 | 0.325564 |
| C | -1.023260 | 1.520498 | 1.370044 |
| H | -1.900417 | 2.146789 | 1.504875 |
| H | -0.421503 | 1.349430 | 2.263878 |
| C | -1.116077 | 3.508663 | -0.664973 |
| H | -0.827945 | 3.956770 | -1.622707 |
| H | -1.880583 | 2.753119 | -0.868551 |
| H | -1.550173 | 4.289106 | -0.035056 |
| C | -2.116587 | -0.450787 | 0.176805 |
| C | -2.937937 | -0.756722 | 1.293960 |
| C | -2.460256 | -1.036132 | -1.071133 |
| C | -4.008552 | -1.630693 | 1.176021 |
| H | -2.710098 | -0.307196 | 2.256912 |
| C | -3.542286 | -1.900599 | -1.176550 |
| H | -1.900513 | -0.772947 | -1.963903 |
| C | -4.319342 | -2.216319 | -0.057371 |
| H | -4.610164 | -1.858001 | 2.051518 |
| H | -3.790205 | -2.324363 | -2.145698 |
| H | -5.161254 | -2.895442 | -0.146812 |
| C | 0.660117 | -0.652243 | -1.148557 |
| H | 0.893410 | -0.471819 | -2.200445 |
| H | -0.055356 | -1.472611 | -1.096125 |
| C | 1.918481 | -1.051216 | -0.399878 |
| C | 2.081569 | -0.788992 | 0.963082 |
| C | 2.920708 | -1.747603 | -1.081359 |
| C | 3.229512 | -1.214912 | 1.632579 |
| H | 1.315866 | -0.243174 | 1.509243 |
| C | 4.066615 | -2.178258 | -0.412909 |
| H | 2.804472 | -1.947804 | -2.144066 |
| C | 4.224966 | -1.912640 | 0.947951 |
| H | 3.344432 | -1.000109 | 2.691084 |
| H | 4.838662 | -2.714402 | -0.957240 |
| H | 5.118686 | -2.242117 | 1.469348 |

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