

**Computational Mechanistic Study on *N*-Nitrosation Reaction of
Secondary Amines**

Meire Y. Kawamura¹, David J. Ponting¹, Chris G. Barber¹, Michael J. Burns^{1*}

¹Lhasa Limited, Granary Wharf House, 2 Canal Wharf, Leeds, United Kingdom

*Corresponding authors.

E-mail address: michael.burns@lhasalimited.org

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1. Computational Details

The DFT calculations were performed with Gaussian 16 [1] suite of program using an ultrafine grid. Full optimization was conducted using B3LYP/def2-tzvp[2–5] level of theory with Grimme D3 empirical dispersion [6]. The IEF-PCM [7, 8] was used for inclusion of the solvent effect for all optimizations. Visualizations were done with GaussView 6.1.1. [9] and CYLview [10]. Frequency calculations at 298.15 K (1 atm) ensured that the stationary points represent either minima (no imaginary frequency) or transition states (single imaginary frequency) on the potential-energy surface, providing also the zero-point vibrational energies, the thermal and entropic correction from which the Gibbs free energies were determined. The IRC calculations were performed ensuring that each transition state connects reagents and products.

The structures of the 24 secondary amines evaluated are depicted in **Figure 1** and the energies for all calculated structures are in **Table 1**, **Table 2** and **Table 3**.

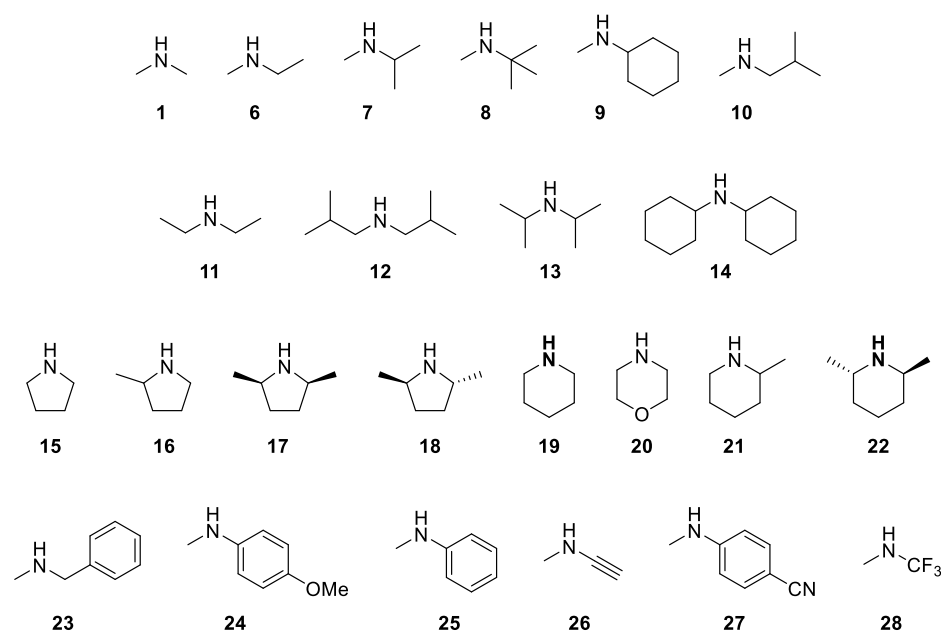


Figure 1. 24 secondary amines evaluated.

Table 1. Energies (in Hartree) at B3LYP-D3/def2-TZVP/IEFPCM for mechanism study using DMA and nitrosating agents.

Name	Electronic Energy	Gibbs Energy	Imaginary Frequency (cm ⁻¹)
1 (DMA)	-135.2282197	-135.1616177	-
<i>asym</i>-N₂O₃ (2)	-335.1364784	-335.1477264	-
PC-1	-470.3875286	-470.3119166	-
TS-1	-470.3767078	-470.3046158	-286.18
3 (NDMA)	-264.5985551	-264.5380771	-
HNO₂	-205.8012817	-205.8051727	-
<i>trans-cis</i>-N₂O₃ (4)	-335.1233496	-335.1377516	-
PC-2	-470.3818847	-470.3077367	-
TS-2	-470.3770759	-470.3042629	-108.82
<i>sym</i>-N₂O₃ (5)	-335.1249557	-335.1385747	-
PC-3	-470.3769404	-470.3037684	-
TS-3	-470.3728416	-470.3006666	-254.78

NOCl	-590.1801713	-590.1992933	-
H₂O	-76.47045997	-76.46766497	-
TS-4	-801.9050534	-801.8211414	-923.62
HCl	-460.8381714	-460.8494194	-
TS-5	-417.4925135	-417.3949525	-832.69

Table 2. Energies (in Hartree) at B3LYP-D3/def2-TZVP/IEFPCM for 24 amines evaluated.

Name*	Electronic Energy	Gibbs Energy	Imaginary Frequency (cm-1)
6	-174.5617911	-174.4691281	-
TS-6	-509.7088913	-509.6109923	-322.24
NO-6	-303.9295846	-303.8424646	-
7	-213.8950507	-213.7762247	-
TS-7	-549.0433171	-548.9175531	-259.14
NO-7	-343.263477	-343.149982	-
8	-253.2266404	-253.0816044	-
TS-8	-588.3739193	-588.2226793	-296.01
NO-8	-382.5949547	-382.4545947	-
9	-330.6793422	-330.4967702	-
TS-9	-665.8268092	-665.6375982	-265.25
NO-9	-460.0482778	-459.8709118	-
10	-253.2243694	-253.0794674	-
TS-10	-588.3706042	-588.2201972	-497.4
NO-10	-382.5946933	-382.4546613	-
11	-213.8953097	-213.7765577	-
TS-11	-549.0402242	-548.9155032	-452.92
NO-11	-343.262189	-343.148446	-
12	-371.2207114	-370.9973154	-
TS-12	-706.3682008	-706.1359028	-400.23
NO-12	-500.5888744	-500.3683984	-
13	-292.5611701	-292.3902121	-
TS-13	-627.7039918	-627.5248248	-492.97
NO-13	-421.9251998	-421.7582138	-

14	-526.1290162	-525.8301402	-
TS-14	-861.2689706	-860.9626006	-380.58
NO-14	-655.4983601	-655.2045021	-
15	-212.6777857	-212.5779527	-
TS-15	-547.8293416	-547.7225466	-311.81
NO-15	-342.0504681	-341.9543171	-
16	-252.0130136	-251.8860176	-
TS-16	-587.1617604	-587.0286974	-277.91
NO-16	-381.3852864	-381.2628154	-
17	-291.3480702	-291.1954202	-
TS-17	-626.4980217	-626.3379877	-433.26
NO-17	-420.7185202	-420.5696772	-
18	-291.347205	-291.194425	-
TS-18	-626.4966835	-626.3369095	-276.98
NO-18	-420.7185925	-420.5693225	-
19	-252.0166468	-251.8865308	-
TS-19	-587.1584769	-587.0237219	-313.33
NO-19	-381.3866774	-381.2623634	-
20	-287.9264613	-287.8201513	-
TS-20	-623.0635302	-622.9532432	-330.21
NO-20	-417.2933453	-417.1930773	-
21	-291.352464	-291.196311	-
TS-21	-626.4907996	-626.3290126	-220.21
NO-21	-420.7133959	-420.5633819	-
22	-330.6838768	-330.5012508	-
TS-22	-665.823185	-665.633784	-292.91
NO-22	-460.0476737	-459.8705557	-
23	-366.3738408	-366.2343998	-
TS-23	-701.5192106	-701.3737586	-317.32
NO-23	-495.7390314	-495.6054234	-
24	-441.6251302	-441.4825632	-
TS-24	-776.764537	-776.618896	-949.9
NO-24	-570.9860748	-570.8491888	-

25	-327.052842	-326.939142	-
TS-25	-662.1879436	-662.0707086	-961.25
NO-25	-456.4101075	-456.3021305	-
26	-172.0735508	-172.0280398	-
TS-26	-507.2029793	-507.1543573	-1061.78
NO-26	-301.4247188	-301.3849428	-
27	-419.343563	-419.234956	-
TS-27	-754.470622	-754.357024	-1051.76
NO-27	-548.6932895	-548.5894265	-
28	-433.1123414	-433.0733534	-
TS-28	-768.2329943	-768.1911873	-1093.82
NO-28	-562.453777	-562.421917	-

*The *N*-nitrosated amines have the prefix “NO-” in the name (e.g diethylamine is **11** and *N*-nitroso-diethylamine is **NO-11**).

Table 3. Energies (in Hartree) at B3LYP-D3/def2-TZVP/IEFPCM for PABA, varenicline and the degradant of sitagliptin (NTTP).

Name	Electronic Energy	Gibbs Energy	Imaginary Frequency (cm-1)
PABA	-476.4045706	-476.3066146	-
TS-29	-811.5266824	-811.4257104	-925.25
NO-PABA	-605.7515918	-605.6598498	-
H₃O⁺	-76.86145861	-76.84594661	-
4-Carboxybenzenediazonium	-529.7191912	-529.6407112	-
Aniline	-287.7323115	-287.6446435	-
TS-30	-622.8607356	-622.7700626	-755.37
NO-Aniline	-417.0844714	-417.0029034	-
Benzenediazonium	-341.0607167	-340.9918307	-
Varenicline	-667.7335617	-667.5290397	-
TS-31	-1002.883364	-1002.672845	-329.5
NO-Varenicline	-797.1035485	-796.9050655	-
TTP	-751.6988595	-751.5900745	-
TS-32	-1086.834079	-1086.721627	-596.25
NTTP	-881.0575148	-880.9552508	-

References:

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9. GaussView, Version 6.1.1, Roy Dennington, Todd Keith, and John Millam, Semichem Inc., Shawnee Mission, KS, 2019
10. CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (<http://www.cylview.org>)

2. IRC (Intrinsic Reaction Coordinate)

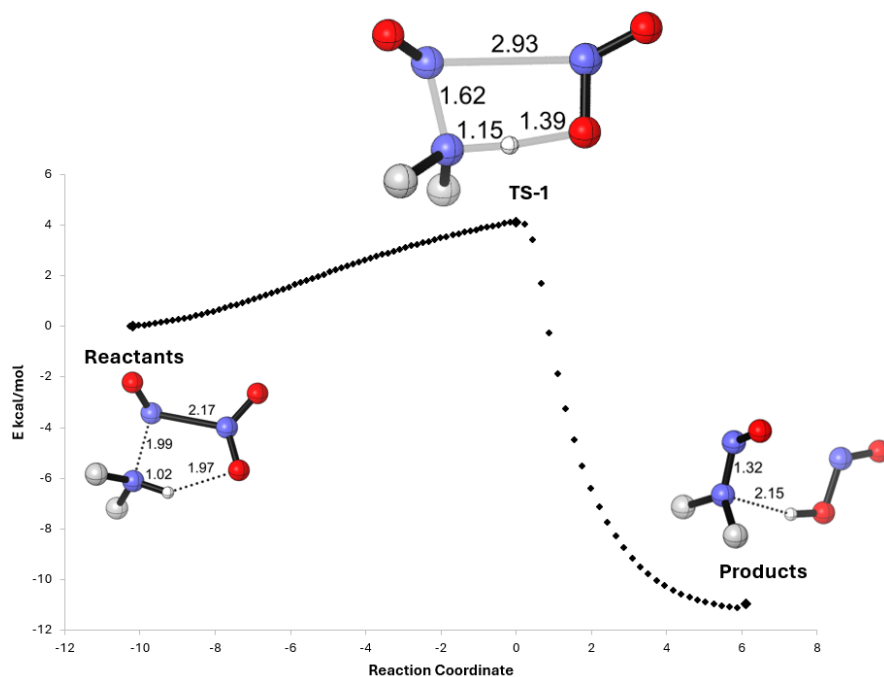


Figure 2. IRC for *N*-nitrosation of DMA (1) by *asym*-N₂O₃ (2).

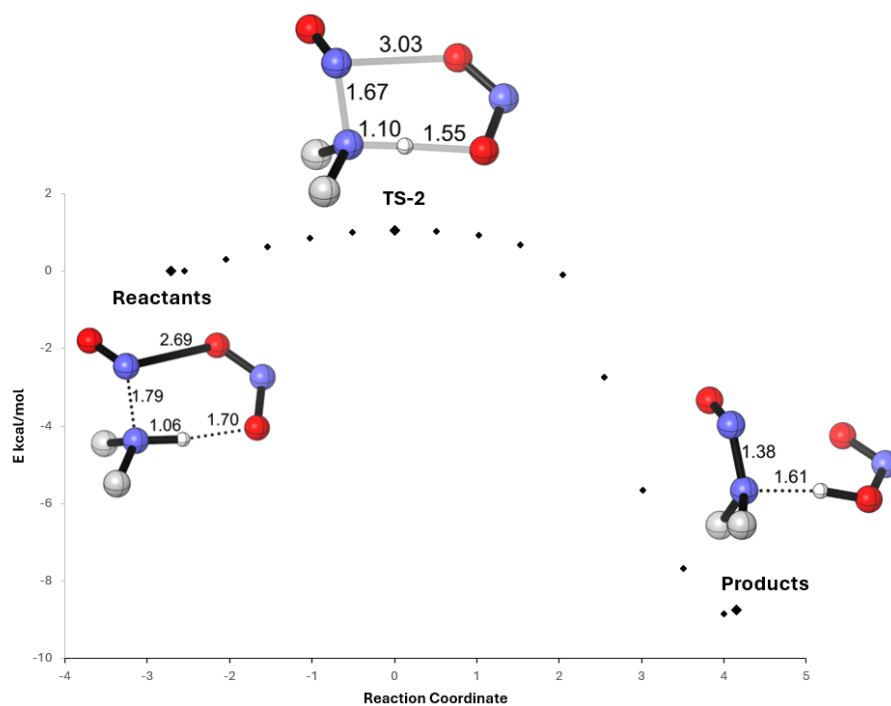


Figure 3. IRC for *N*-nitrosation of DMA (1) by *trans-cis*-N₂O₃ (4).

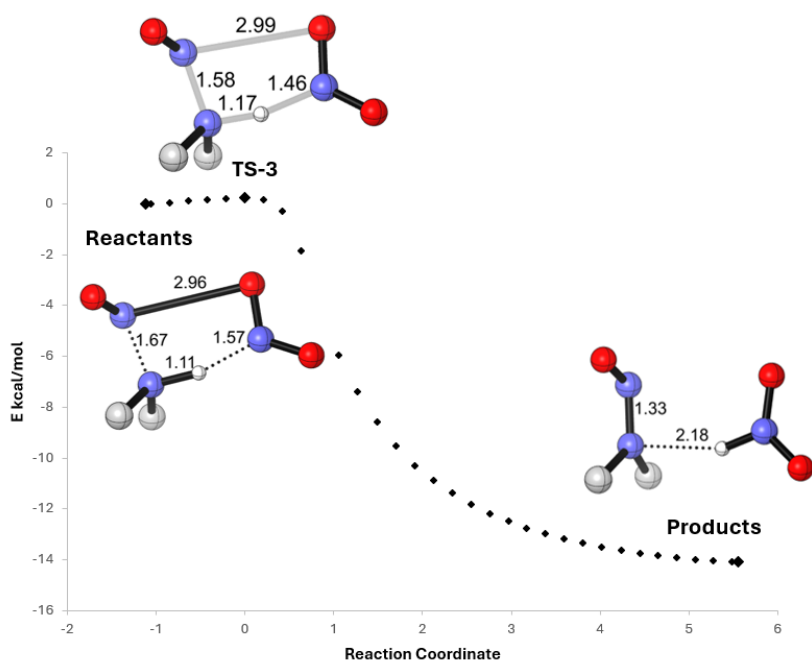


Figure 4. IRC for *N*-nitrosation of DMA (1) by *sym*-N₂O₃ (5).

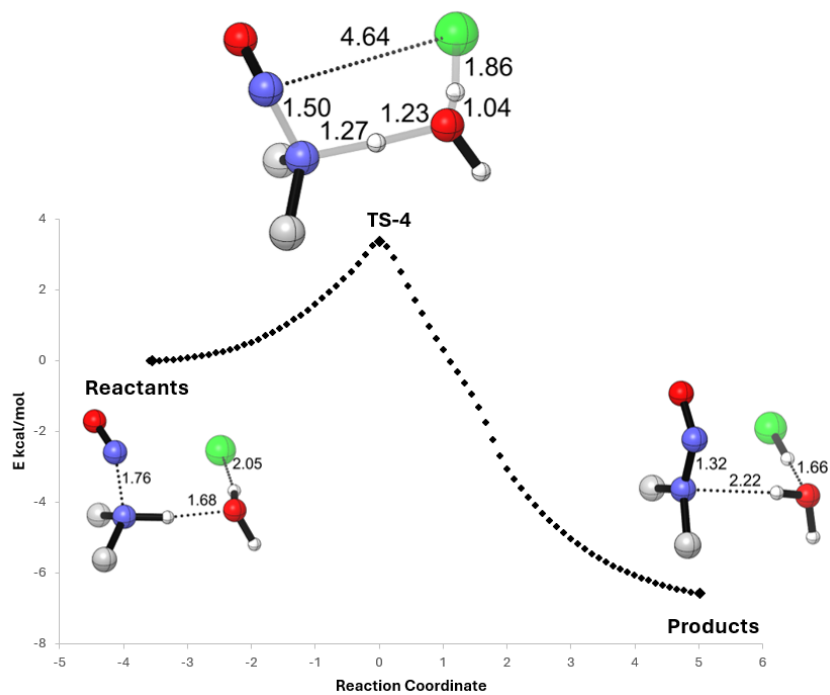


Figure 5. IRC for *N*-nitrosation of DMA (1) by NOCl.

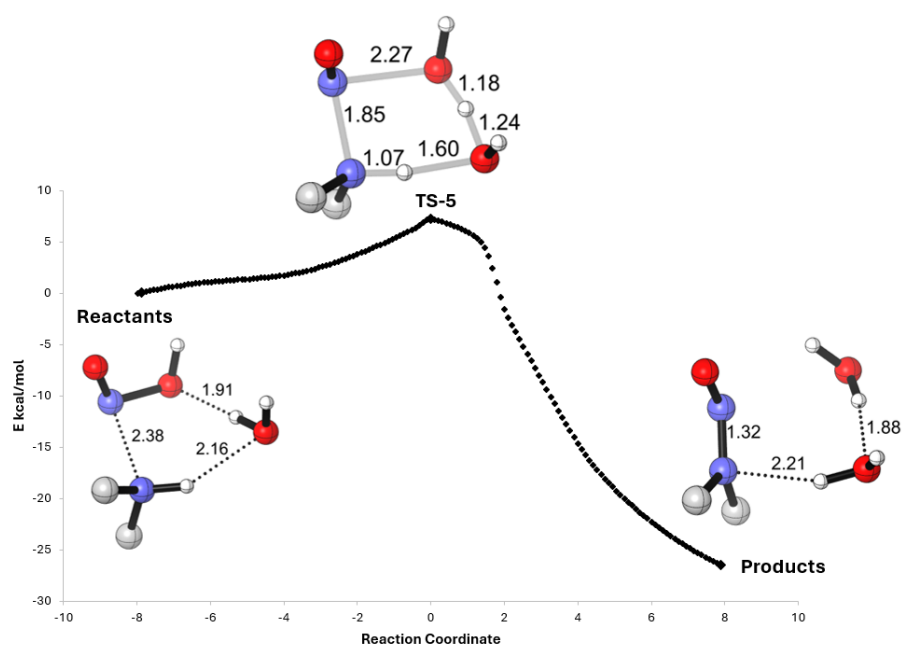


Figure 6. IRC for *N*-nitrosation of DMA (1) by HNO₂.

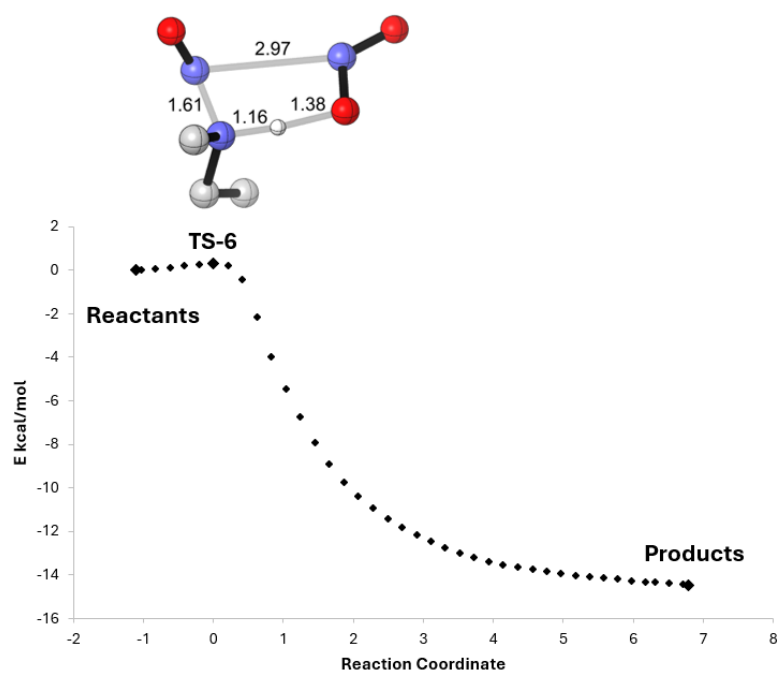


Figure 7. IRC for *N*-nitrosation of 6 by asym-N₂O₃ (2).

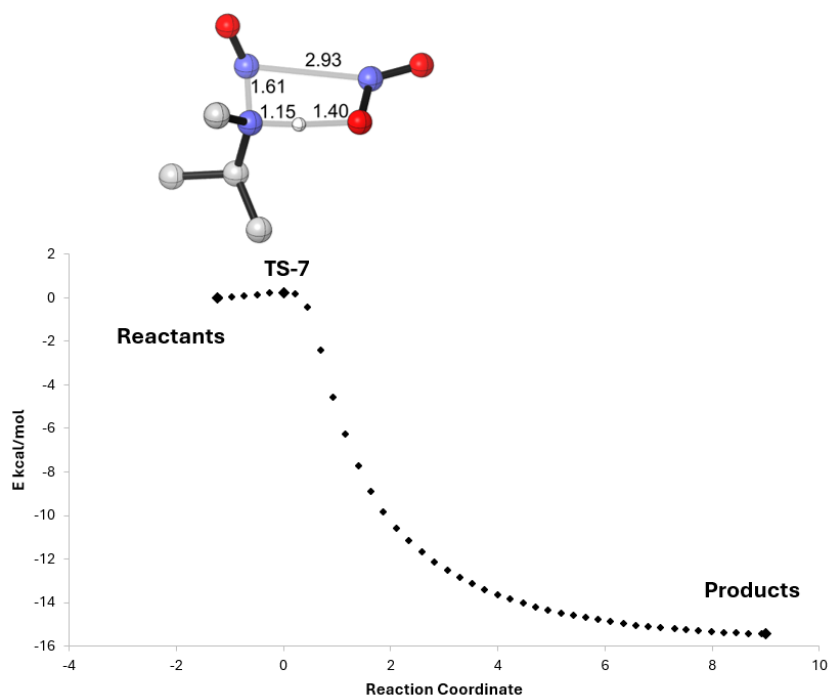


Figure 8. IRC for *N*-nitrosation of **7** by *asym*-N₂O₃ (**2**).

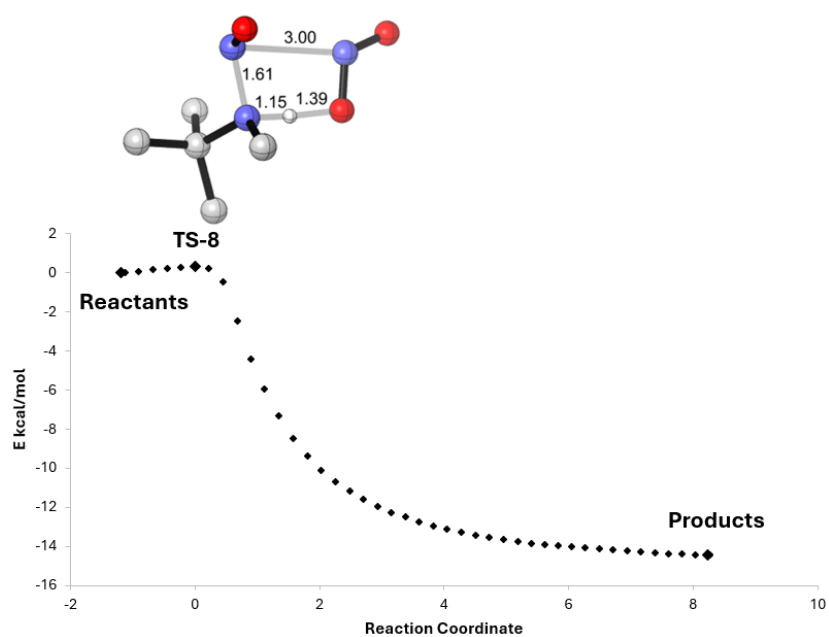


Figure 9. IRC for *N*-nitrosation of **8** by *asym*-N₂O₃ (**2**).

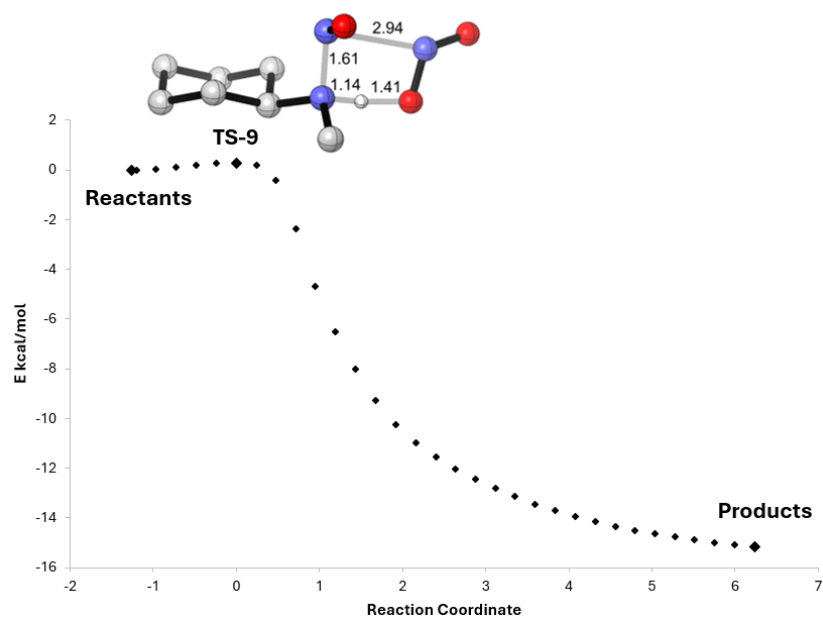


Figure 10. IRC for *N*-nitrosation of **9** by *asym*-N₂O₃ (**2**).

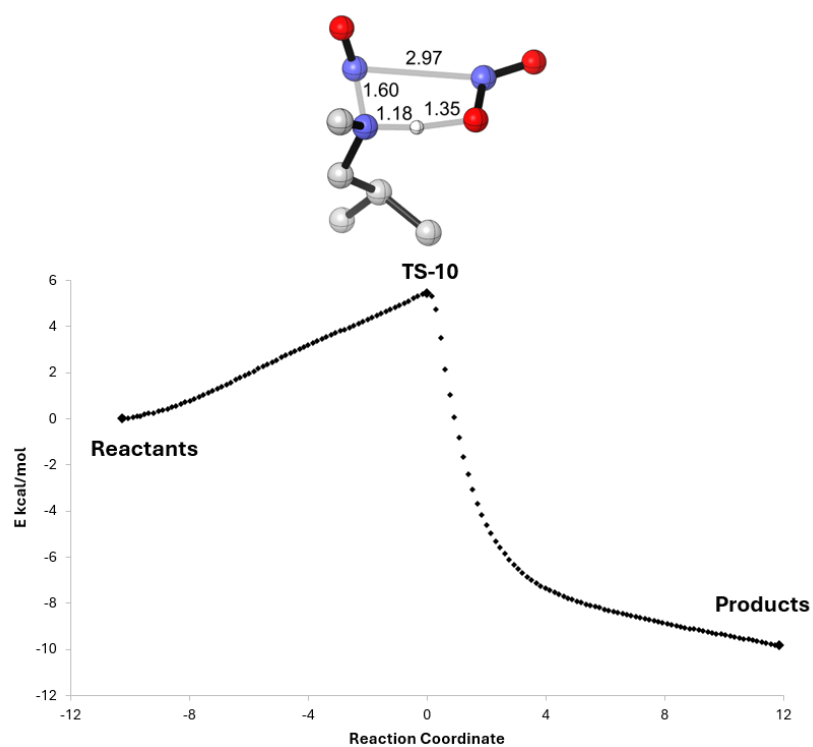


Figure 11. IRC for *N*-nitrosation of **10** by *asym*-N₂O₃ (**2**).

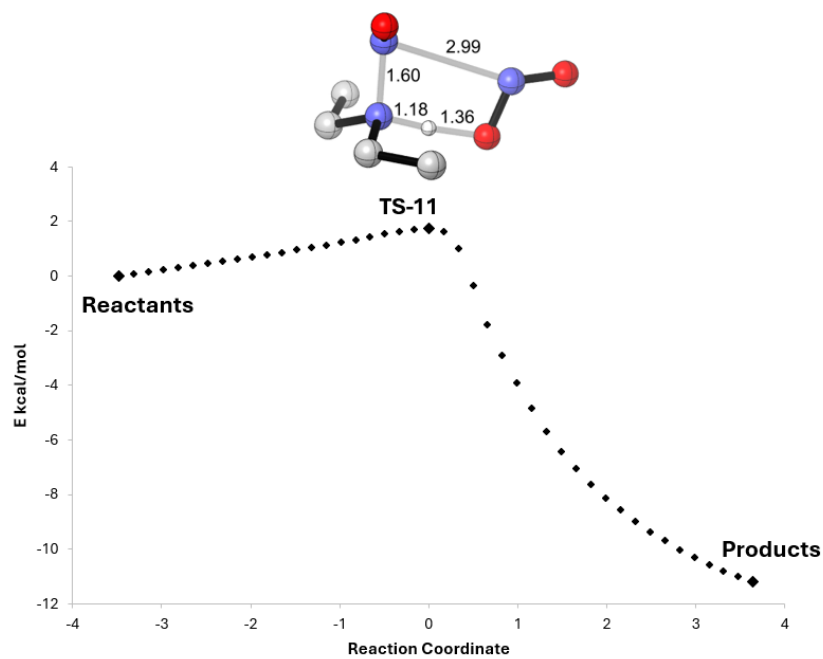


Figure 12. IRC for *N*-nitrosation of **11** by *asym*-N₂O₃ (**2**).

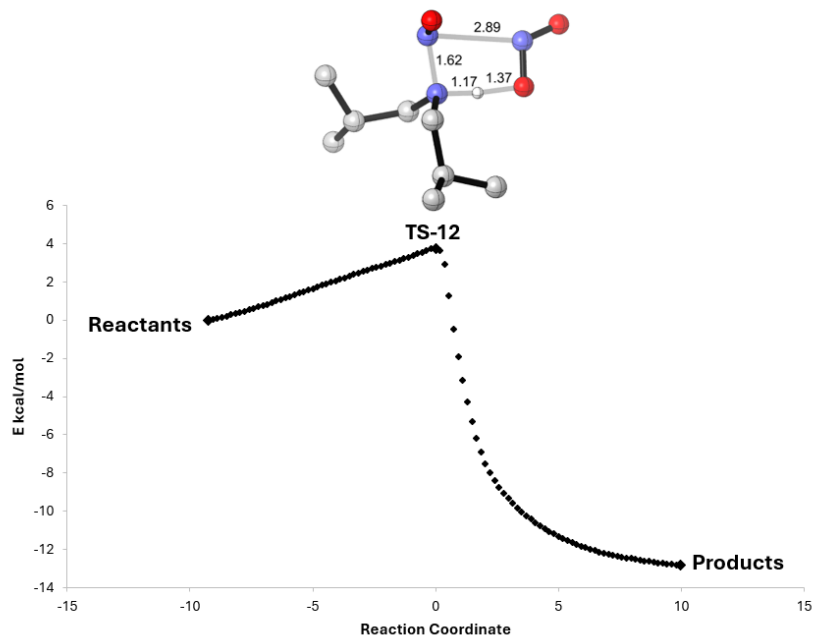


Figure 13. IRC for *N*-nitrosation of **12** by *asym*-N₂O₃ (**2**).

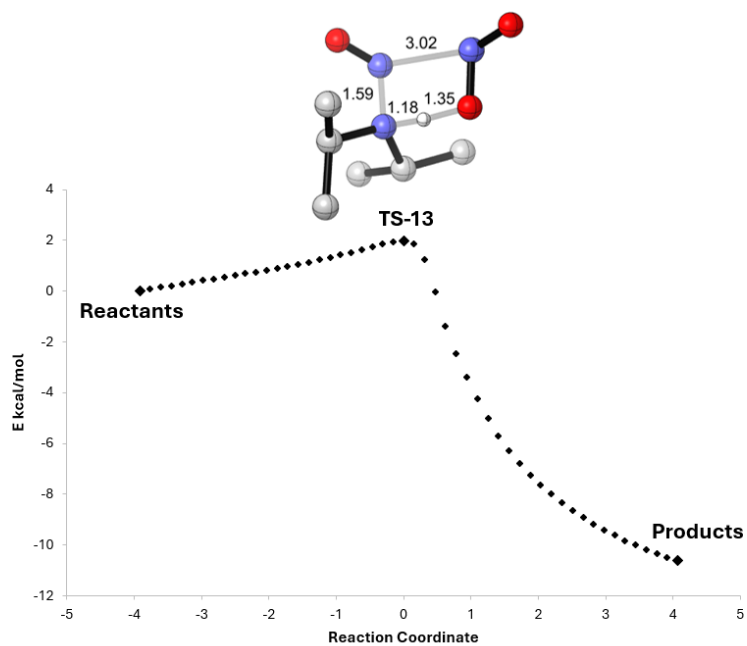


Figure 14. IRC for *N*-nitrosation of **13** by *asym*-N₂O₃ (**2**).

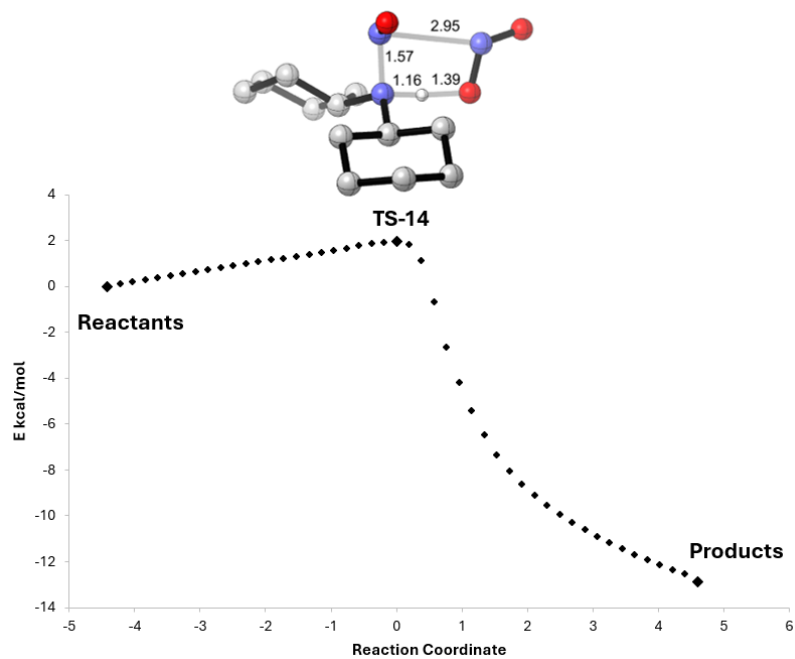


Figure 15. IRC for *N*-nitrosation of **14** by *asym*-N₂O₃ (**2**).

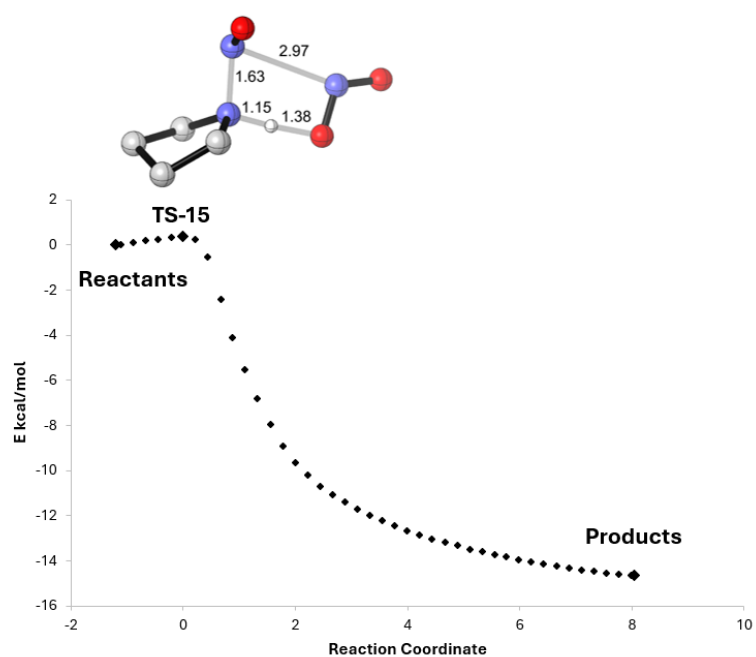


Figure 16. IRC for *N*-nitrosation of **15** by *asym*-N₂O₃ (**2**).

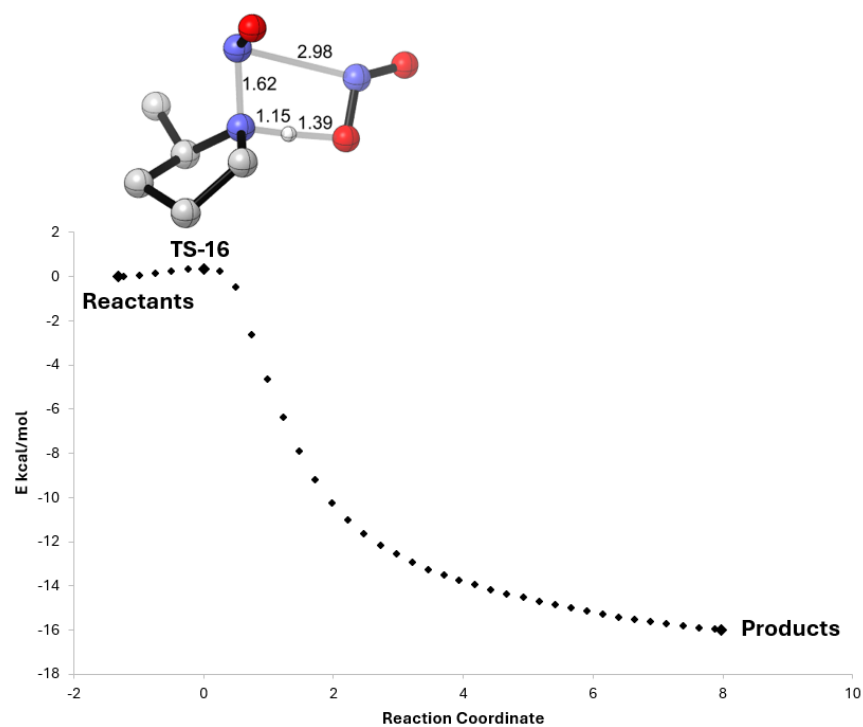


Figure 17. IRC for *N*-nitrosation of **16** by *asym*-N₂O₃ (**2**).

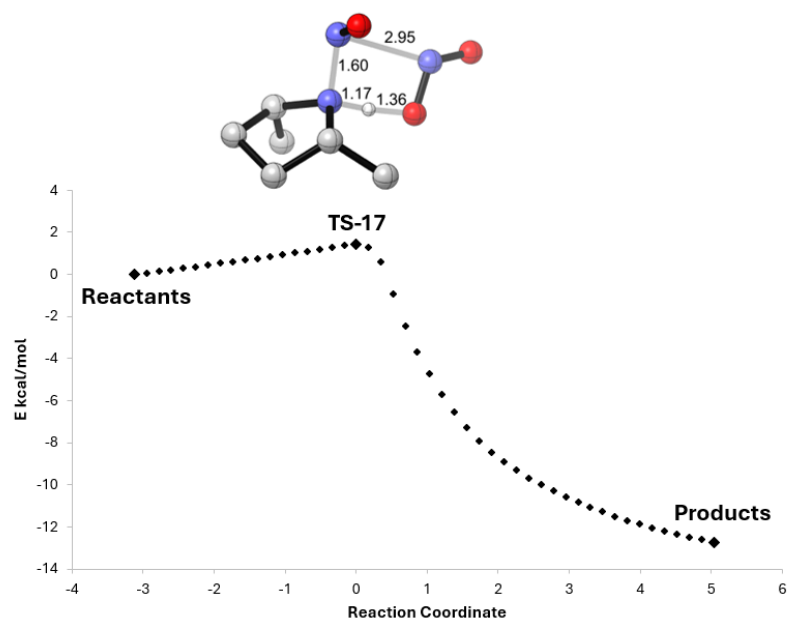


Figure 18. IRC for *N*-nitrosation of **17** by *asym*-N₂O₃ (**2**).

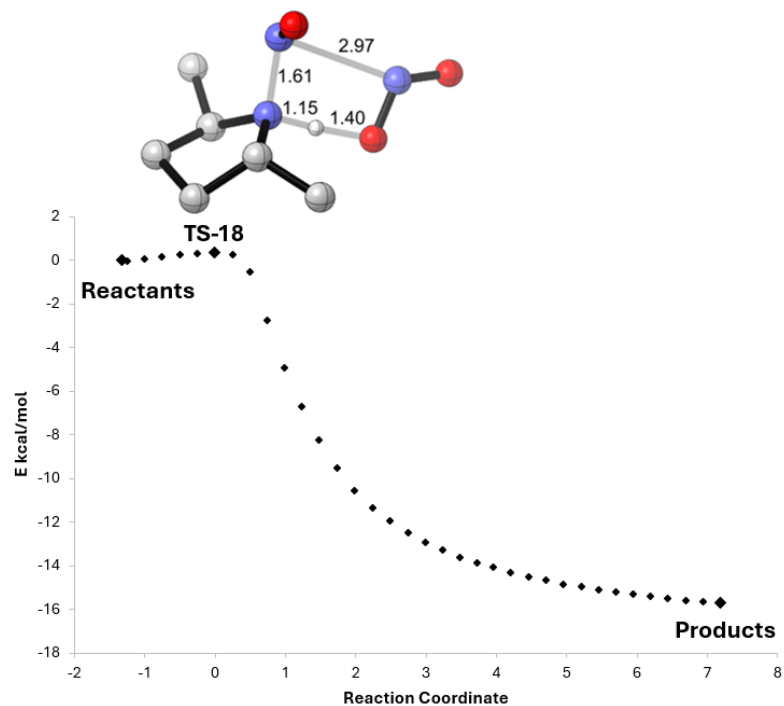


Figure 19. IRC for *N*-nitrosation of **18** by *asym*-N₂O₃ (**2**).

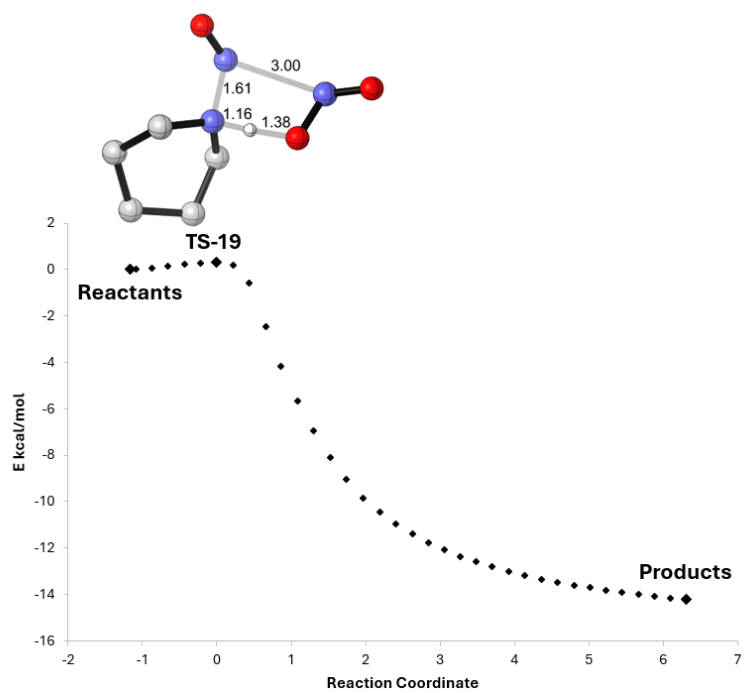


Figure 20. IRC for *N*-nitrosation of **19** by *asym*-N₂O₃ (**2**).

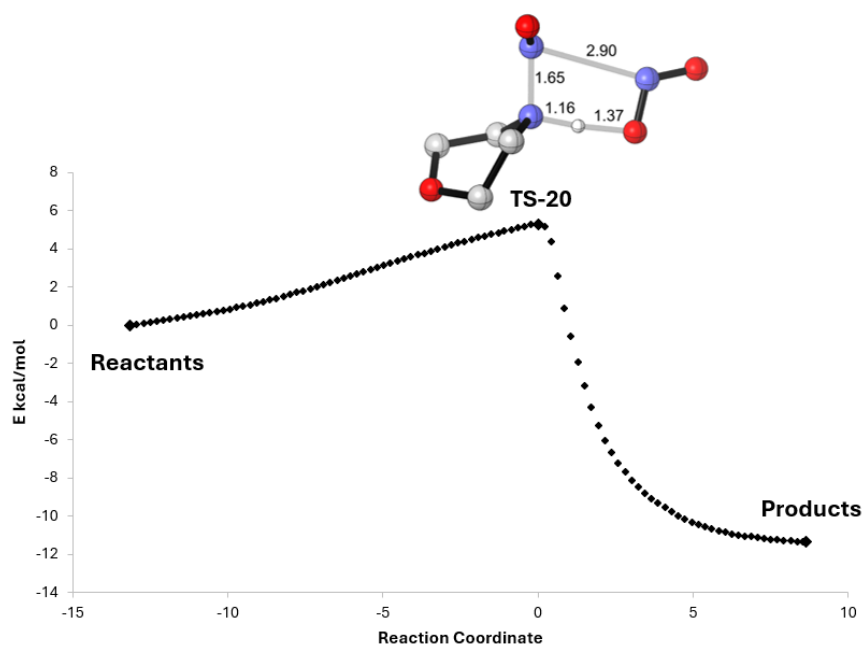


Figure 21. IRC for *N*-nitrosation of **20** by *asym*-N₂O₃ (**2**).

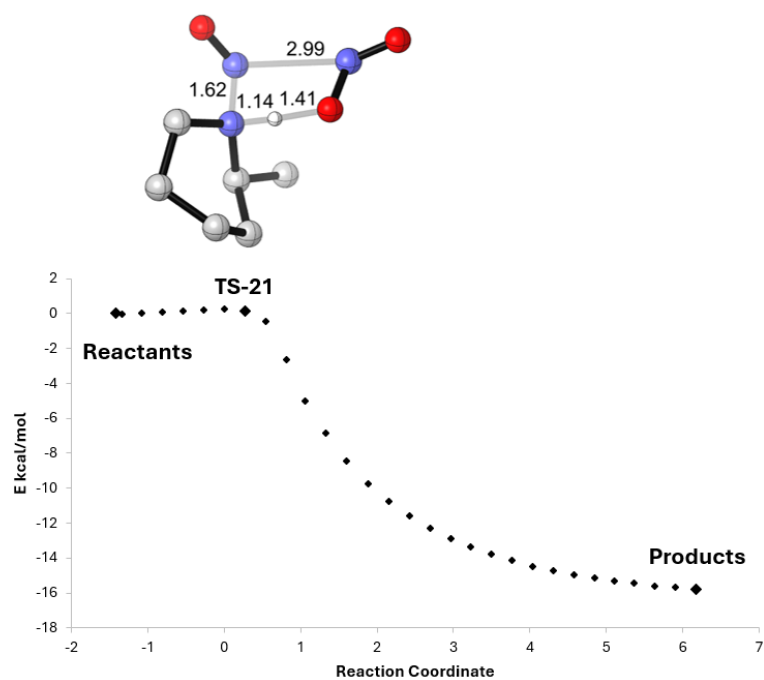


Figure 22. IRC for *N*-nitrosation of **21** by *asym*-N₂O₃ (**2**).

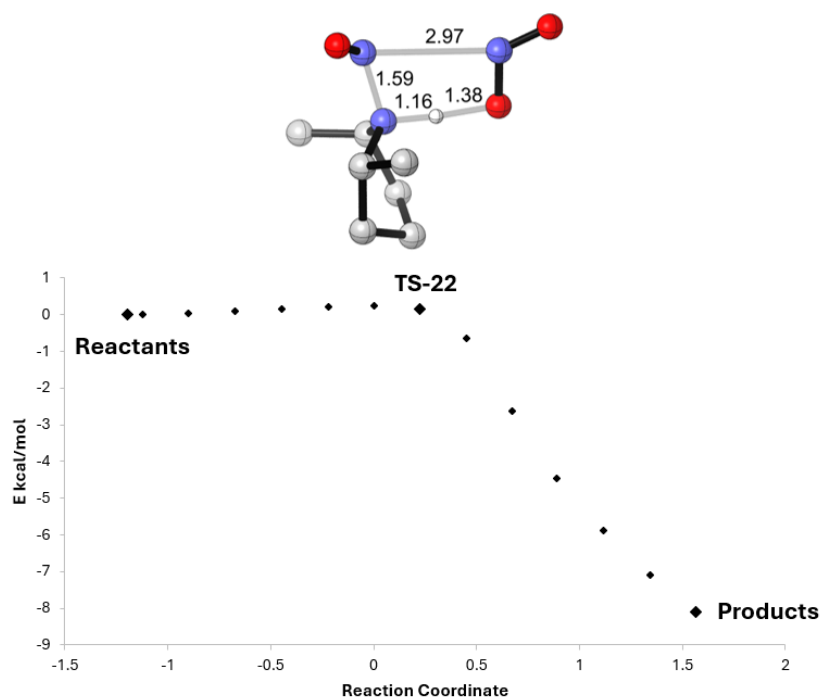


Figure 23. IRC for *N*-nitrosation of **22** by *asym*-N₂O₃ (**2**).

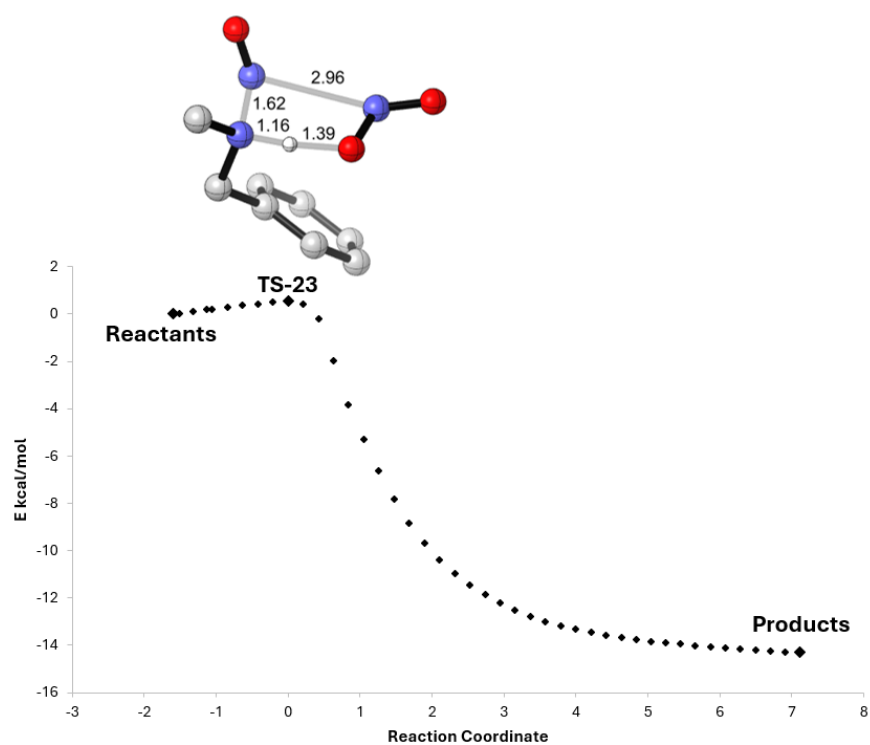


Figure 24. IRC for *N*-nitrosation of **23** by *asym*-N₂O₃ (**2**).

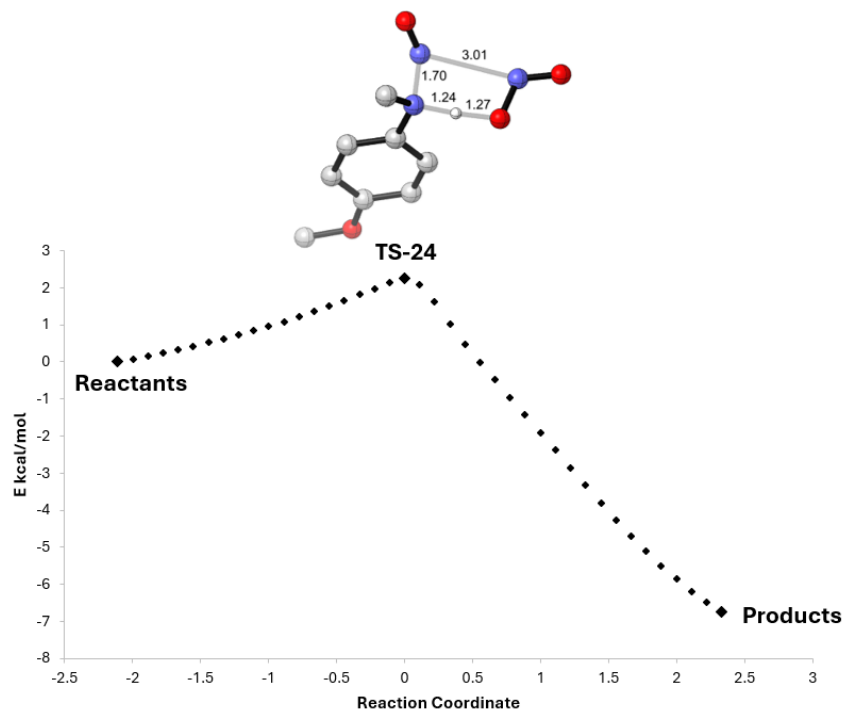


Figure 25. IRC for *N*-nitrosation of **24** by *asym*-N₂O₃ (**2**).

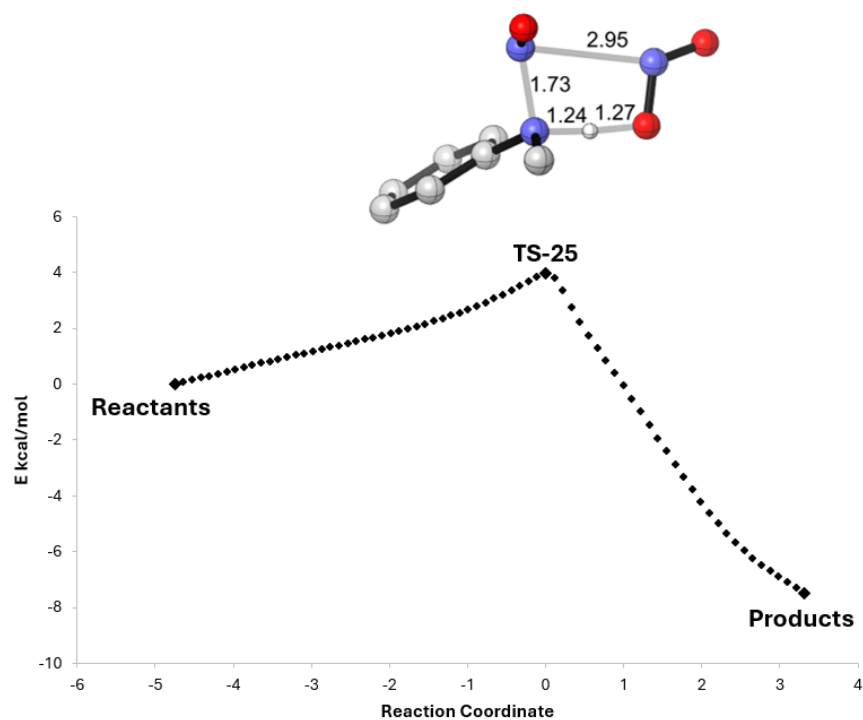


Figure 26. IRC for *N*-nitrosation of **25** by *asym*-N₂O₃ (**2**).

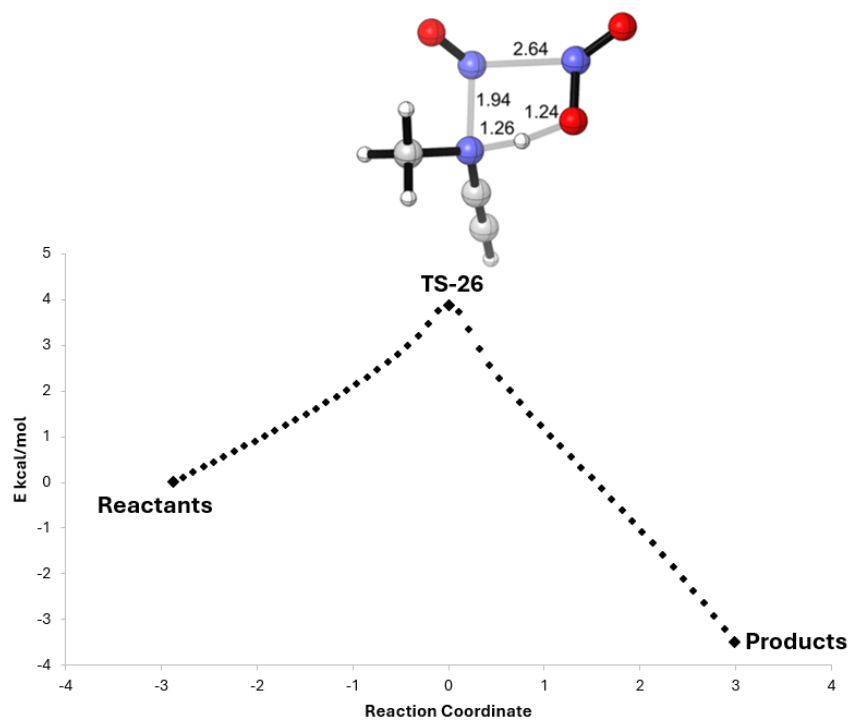


Figure 27. IRC for *N*-nitrosation of **26** by *asym*-N₂O₃ (**2**).

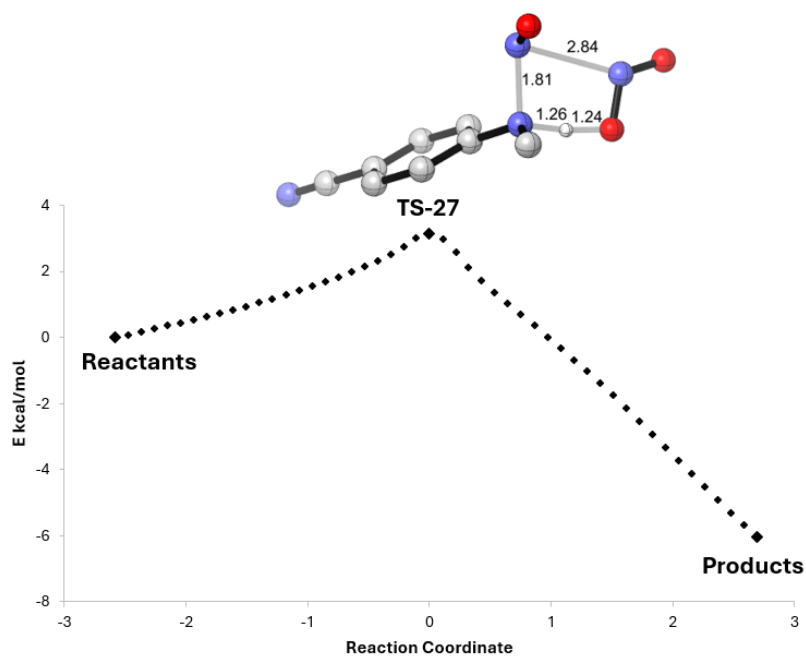


Figure 28. IRC for *N*-nitrosation of **27** by *asym*-N₂O₃ (**2**).

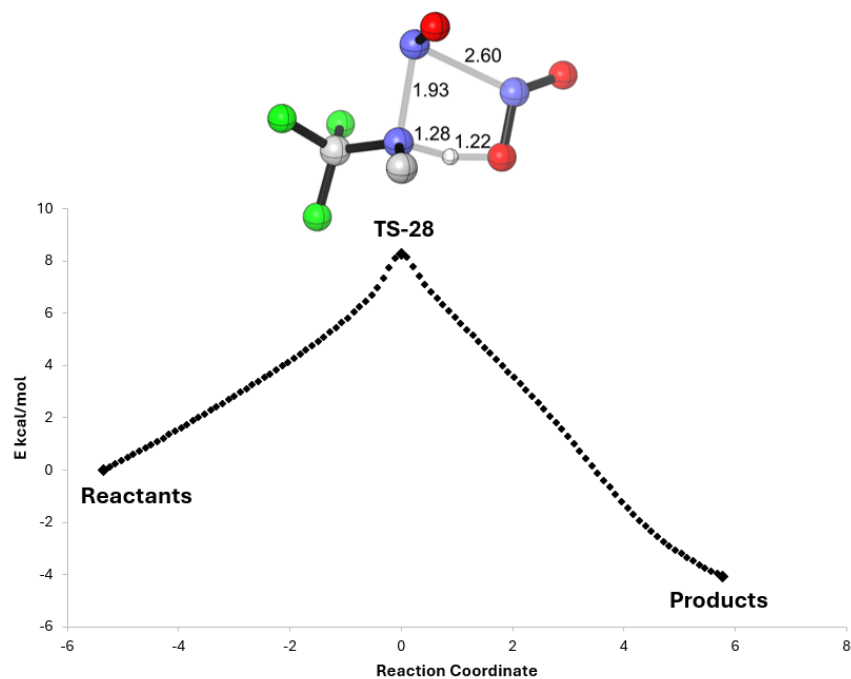


Figure 29. IRC for *N*-nitrosation of **28** by *asym*-N₂O₃ (**2**).

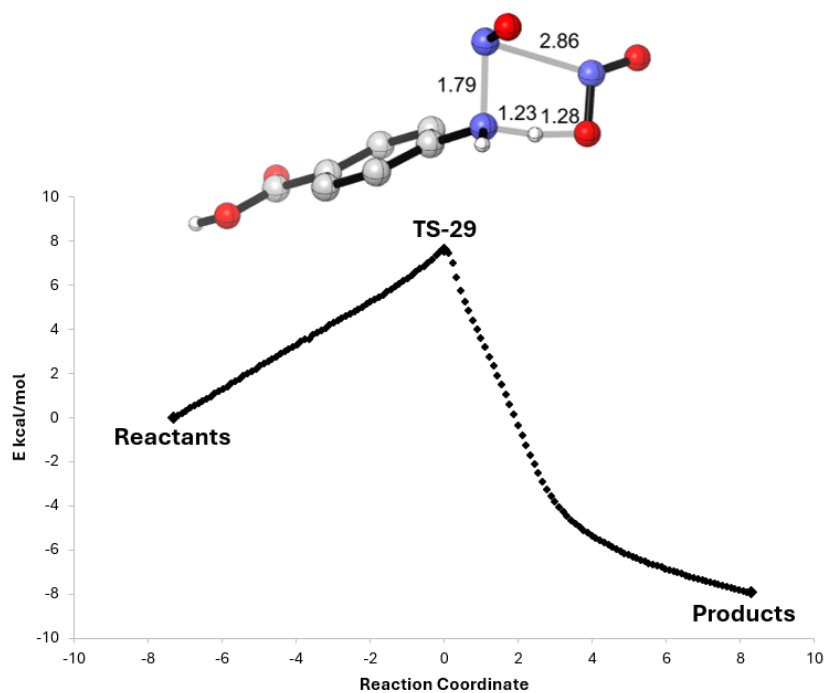


Figure 30. IRC for *N*-nitrosation of PABA by *asym*-N₂O₃ (2).

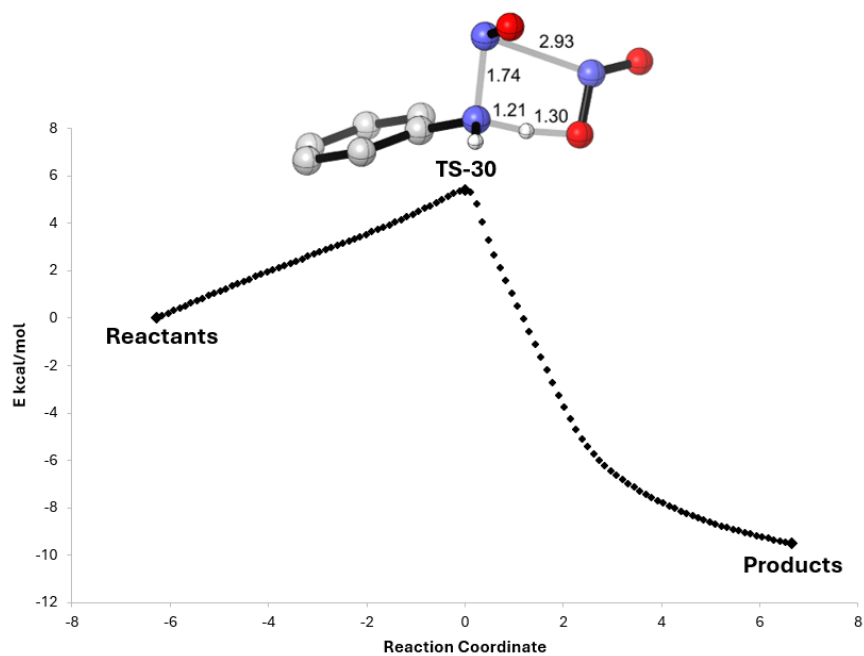


Figure 31. IRC for *N*-nitrosation of aniline by *asym*-N₂O₃ (2).

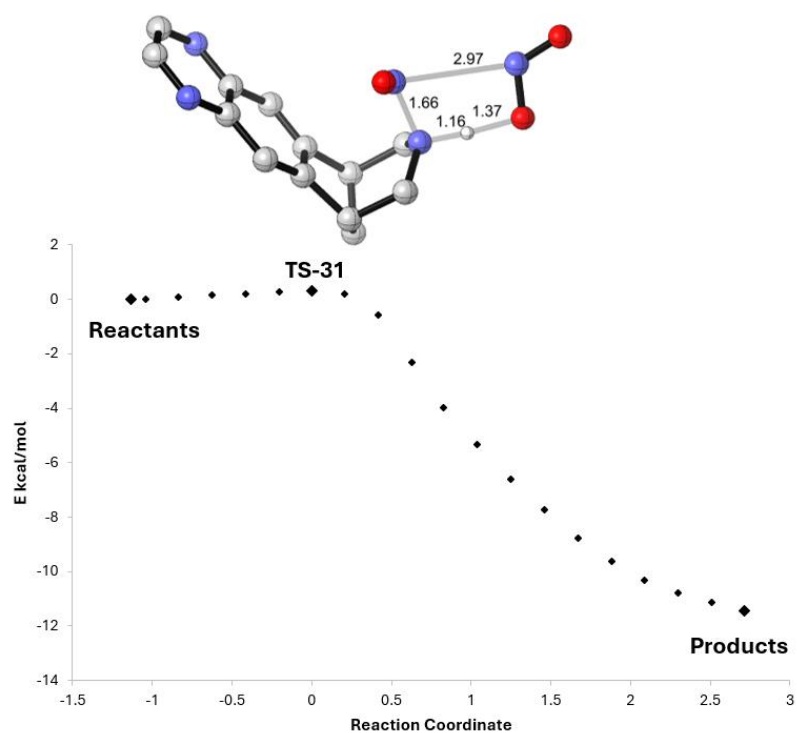


Figure 32. IRC for *N*-nitrosation of varenicline by *asym*-N₂O₃ (2).

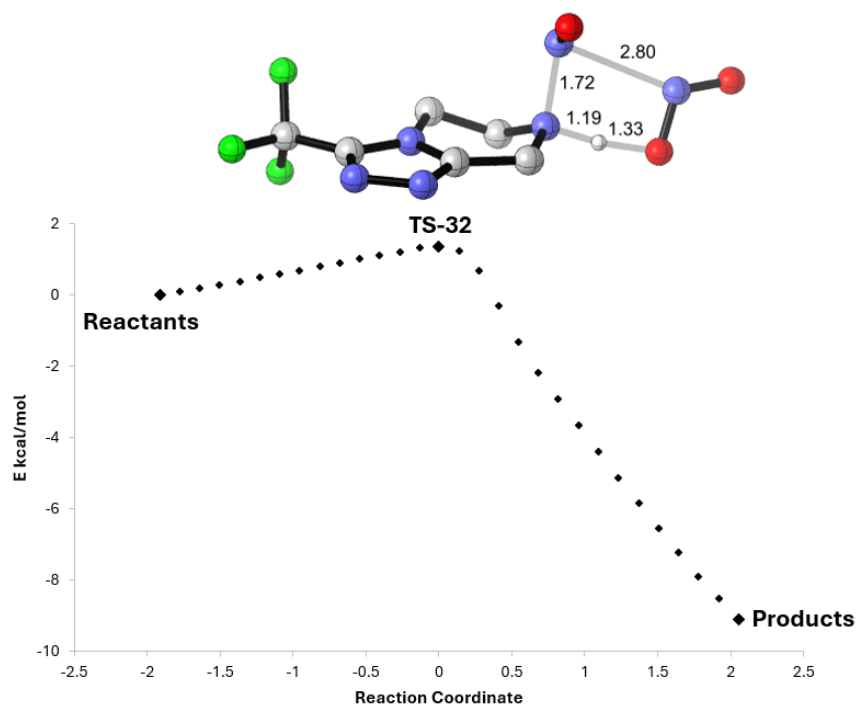


Figure 33. IRC for *N*-nitrosation of TTP by *asym*-N₂O₃ (2).

Cartesian Coordinates

Cartesian Coordinates (Å) and computed energies (in Hartrees) for all optimised structures:

1

Eopt -135.228220

N	-0.515397	0.239664	-0.288016
C	-0.883137	1.391052	0.548627
H	0.002346	1.912283	0.847187
H	-1.514109	2.050611	-0.009725
H	-1.405323	1.048347	1.417405
C	-1.731902	-0.476420	-0.698187
H	-2.362874	0.183139	-1.256539
H	-1.464227	-1.314506	-1.307172
H	-2.254088	-0.819125	0.170591
H	-0.027373	0.559949	-1.099958

asym-N₂O₃ (2)

Eopt -335.136478

O	1.283421	-1.447869	0.389002
N	0.942341	-0.480426	-0.227479
O	3.055747	-0.147401	-1.031782
N	1.876895	0.227349	-0.992766
O	1.524187	1.227773	-1.630263

PC-1

N	-1.248331	0.625364	0.360186
O	0.582300	-1.209248	1.176125
C	-1.754780	1.237247	1.576704
H	-1.083697	2.050362	1.886626
H	-2.774684	1.642013	1.443364
H	-1.785950	0.482523	2.378397
C	-1.966724	-0.528996	-0.133213
H	-3.060942	-0.378677	-0.127192
H	-1.641641	-0.766985	-1.154728
H	-1.738928	-1.398406	0.512392
N	0.670014	-0.091176	0.919689
H	-1.016126	1.306335	-0.361743
O	1.138389	1.005447	-1.574063
N	1.081343	-0.047199	-0.972738
O	1.254763	-1.157239	-1.422083

TS-1

Eopt -470.376708

N	-0.511942	0.303377	-0.288914
O	0.408826	-1.739877	0.353756
C	-0.843936	1.411364	0.616579
H	0.091699	1.851299	0.987466

H	-1.405332	2.174816	0.059649
H	-1.448770	1.054866	1.462879
C	-1.630975	-0.493026	-0.789582
H	-2.298355	0.163365	-1.365411
H	-1.246050	-1.281278	-1.449356
H	-2.188114	-0.948432	0.042440
N	0.602008	-0.602390	0.485627
H	0.128326	0.713738	-1.170904
O	1.088796	1.043681	-2.074690
N	2.012165	0.321845	-1.554187
O	3.099751	0.336235	-2.088590

3

Eopt -264.598555

N	-0.470292	0.265649	-0.311177
O	0.437557	-1.747063	0.127745
C	-0.867188	1.381197	0.559986
H	0.002111	1.932676	0.851689
H	-1.537614	2.025815	0.030933
H	-1.354959	0.997098	1.431449
C	-1.664563	-0.491990	-0.711927
H	-2.334988	0.152628	-1.240980
H	-1.375665	-1.303988	-1.346039
H	-2.152334	-0.876089	0.159536
N	0.406900	-0.577776	0.381042

HNO₂

Eopt -205.801282

O	0.855968	0.874968	0.792680
N	0.257566	0.207207	0.000000
O	-0.674257	0.701562	-0.647280
H	-1.044625	0.037846	-1.233717

trans-cis-N₂O₃ (4)

Eopt -335.123350

N	-1.680221	-1.743224	0.532317
O	-1.493981	-1.338712	-0.585184
O	-2.817695	-2.404606	0.766427
N	-3.910837	-2.612823	-0.562502
O	-4.797586	-3.190732	-0.150570

PC-2

Eopt -470.381885

N	-1.008717	-0.315090	-0.201646
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O	0.467594	-1.532875	1.481386
C	-1.621892	0.308318	0.951647
H	-1.010881	1.164774	1.265056
H	-2.649609	0.639070	0.730099
H	-1.665014	-0.420830	1.780928
C	-1.779608	-1.329425	-0.904864
H	-2.678545	-0.887563	-1.366778
H	-1.158201	-1.777761	-1.692678
H	-2.096788	-2.113720	-0.200330
N	0.593052	-1.188041	0.404123
H	-0.498593	0.349108	-0.814067
O	1.572423	0.756406	0.570753
N	1.627098	1.581445	-0.369086
O	0.848710	1.437080	-1.321542

TS-2

Eopt -470.377076

N	-0.547257	0.195458	-0.603987
O	0.689115	-0.898357	1.030272
C	-1.230325	0.829405	0.521455
H	-0.491687	1.417384	1.082679
H	-2.007214	1.497066	0.123871
H	-1.689838	0.076717	1.177616
C	-1.376430	-0.598360	-1.524932
H	-2.063749	0.077490	-2.052437
H	-0.719708	-1.087192	-2.257501
H	-1.952140	-1.355585	-0.973390
N	0.654276	-0.780299	-0.116898
H	0.053176	0.989936	-1.179813
O	1.995567	1.557293	-0.135654
N	1.857348	2.239990	-1.153390
O	0.795967	2.012645	-1.826092

sym-N₂O₃ (5)

Eopt -335.124956

N	-2.674022	-3.387438	-1.578794
O	-1.985421	-4.366291	-1.576578
N	-0.630859	-4.244794	-1.577092
O	0.057742	-5.223647	-1.574877
O	-4.028584	-3.508935	-1.578280

PC-3

Eopt -470.376940

N	-0.668009	-0.791115	0.118899
O	-1.368295	2.051695	-0.214140
C	-1.185099	-1.539421	-1.035898
H	-0.788394	-1.122287	-1.937854
H	-0.890226	-2.564988	-0.957388
H	-2.253061	-1.475675	-1.053017

C	-1.476597	-0.674434	1.340976
H	-1.252450	-1.490129	1.996186
H	-1.250641	0.249376	1.831300
H	-2.515263	-0.697620	1.084979
N	-0.782554	1.032443	-0.438561
H	0.262531	-0.499307	0.126178
O	1.180266	0.847356	0.085537
N	1.785975	-0.206643	-0.146534
O	2.976753	-0.318929	0.171419

TS-3

Eopt -470.372842

N	-0.584543	0.309656	-0.276089
O	0.527555	-1.685314	0.151956
C	-0.904666	1.413595	0.639043
H	0.036628	1.865991	0.978728
H	-1.496577	2.166699	0.100214
H	-1.474736	1.045045	1.503314
C	-1.706274	-0.509610	-0.741024
H	-2.379105	0.121643	-1.337960
H	-1.321063	-1.320850	-1.372219
H	-2.253154	-0.931790	0.114437
N	0.587411	-0.560298	0.432324
H	0.000724	0.729485	-1.178132
O	2.105677	0.506080	-1.392126
N	1.173455	1.026396	-2.027367
O	1.366268	1.606272	-3.089597

NOCI

Eopt -590.180171

Cl	-1.432432	0.207207	0.000000
N	0.257566	0.207207	0.000000
O	0.855968	0.874968	0.792680

H₂O

Eopt -76.470460

O	-1.972973	0.135135	0.000000
H	-1.012973	0.135135	0.000000
H	-2.293428	1.040071	0.000000

TS-4

Eopt -801.905053

H	-1.522571	0.186343	0.200137
N	-1.423772	-2.849984	0.032273
N	-2.980815	-3.100251	-0.182246
O	-3.359978	-2.624877	-1.171589
Cl	-3.526743	-1.301817	2.222544
H	-1.331504	-1.590265	0.370103
H	-2.184260	-0.657921	1.502756

C	-1.027939	-3.674843	1.178928
H	-1.059543	-4.736748	0.927162
H	-0.014825	-3.402905	1.475082
H	-1.712798	-3.457697	1.996988
C	-0.658538	-3.071629	-1.197205
H	-1.109494	-2.502525	-2.008417
H	0.360324	-2.714926	-1.045071
H	-0.634095	-4.131412	-1.461432
O	-1.281776	-0.493969	0.841358

HCl

Eopt -460.838171			
Cl	-0.783784	-2.117117	0.000000
H	-2.073784	-2.117117	0.000000

TS-5

Eopt -417.492513			
N	-0.566564	0.345187	-0.633565
O	1.239493	-1.116877	0.084780
C	-1.366170	1.318583	0.096356
H	-0.683040	2.067346	0.517187
H	-2.081938	1.808687	-0.582666
H	-1.923170	0.827780	0.909452
C	-1.266766	-0.796458	-1.201506
H	-1.924728	-1.268526	-0.455576
H	-1.870767	-0.475077	-2.065107
H	-0.524228	-1.528185	-1.554935
N	0.632883	-0.252392	0.547576
H	0.107536	0.835718	-1.375329
O	1.742824	1.612606	0.251407
O	1.185281	1.537166	-2.087963
H	1.593677	1.638991	-0.922472
H	1.723715	0.832602	-2.477891
H	2.605039	1.204120	0.417705

6

Eopt -174.561791			
N	-0.515397	0.239664	-0.288016
C	-0.883137	1.391052	0.548627
H	0.002346	1.912283	0.847187
H	-1.514109	2.050611	-0.009725
H	-1.405323	1.048347	1.417405
C	-1.731902	-0.476420	-0.698187
H	-2.362874	0.183139	-1.256539
H	-2.254088	-0.819125	0.170591
H	-0.027373	0.559949	-1.099958
C	-1.346651	-1.682636	-1.574671
H	-2.223770	-2.250232	-1.805747
H	-0.897274	-1.335491	-2.481562

H	-0.651233	-2.300271	-1.045689
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7

Eopt -213.895051			
N	-0.515397	0.239664	-0.288016
C	-0.883137	1.391052	0.548627
H	0.002346	1.912283	0.847187
H	-1.514109	2.050611	-0.009725
H	-1.405323	1.048347	1.417405
C	-1.731902	-0.476420	-0.698187
H	-2.362874	0.183139	-1.256539
H	-0.027373	0.559949	-1.099958
C	-1.346651	-1.682636	-1.574671
H	-2.223770	-2.250232	-1.805747
H	-0.897274	-1.335491	-2.481562
H	-0.651233	-2.300271	-1.045689
C	-2.483459	-0.969659	0.552204
H	-1.777831	-1.305012	1.283318
H	-3.064352	-0.168165	0.958493
H	-3.130381	-1.778505	0.283579

8

Eopt -253.226640			
N	-0.696239	0.593706	-0.026402
C	-1.642591	1.624194	0.424610
H	-1.108941	2.401969	0.929768
H	-2.153816	2.033782	-0.421432
H	-2.353856	1.186916	1.093780
C	-1.429383	-0.474826	-0.720405
C	-0.437967	-1.554385	-1.192893
H	0.073258	-1.963973	-0.346851
H	-0.971617	-2.332160	-1.698051
H	0.273298	-1.117107	-1.862063
C	-2.165165	0.114675	-1.938072
H	-2.854007	0.864758	-1.609785
H	-1.453900	0.551953	-2.607243
H	-2.698815	-0.663100	-2.443231
C	-2.453074	-1.104180	0.242700
H	-2.986723	-1.881954	-0.262458
H	-1.941849	-1.513768	1.088742
H	-3.141915	-0.354096	0.570988
H	-0.031505	1.002377	-0.651795

9

Eopt -330.679342			
N	-0.545020	0.236576	-0.256670
C	-0.876117	1.414808	0.537291
H	0.034838	1.960390	0.787436
H	-1.565545	2.108732	0.030718

H	-1.349292	1.104430	1.472210
H	-0.008550	0.523495	-1.068904
C	-1.732698	-0.501750	-0.709654
C	-1.727805	-0.593178	-2.222065
C	-1.747127	-1.878474	-0.076435
H	-2.635579	0.072729	-0.373576
C	-2.892627	-1.418967	-2.728828
H	-0.765470	-1.057228	-2.564019
H	-1.779351	0.437201	-2.660580
C	-2.912439	-2.703968	-0.582608
H	-0.785849	-2.406873	-0.311141
H	-1.813557	-1.778798	1.038058
C	-2.909082	-2.794867	-2.094946
H	-2.824996	-1.519642	-3.843178
H	-3.853905	-0.889743	-2.495922
H	-2.860667	-3.734465	-0.144496
H	-3.874400	-2.239880	-0.239499
H	-3.816221	-3.356135	-2.439436
H	-2.007751	-3.371393	-2.431942

10

Eopt -253.224369

N	-0.515397	0.239664	-0.288016
C	-0.883137	1.391052	0.548627
H	0.002346	1.912283	0.847187
H	-1.514109	2.050611	-0.009725
H	-1.405323	1.048347	1.417405
C	-1.731902	-0.476420	-0.698187
H	-2.362874	0.183139	-1.256539
H	-2.254088	-0.819125	0.170591
H	-0.027373	0.559949	-1.099958
C	-1.346651	-1.682636	-1.574671
H	-0.897274	-1.335491	-2.481562
C	-2.609047	-2.499550	-1.907248
H	-2.344359	-3.326242	-2.532883
H	-3.047151	-2.863652	-1.001491
H	-3.312752	-1.876350	-2.418445
C	-0.345769	-2.571568	-0.813332
H	0.625281	-2.123286	-0.845050
H	-0.659658	-2.670927	0.204755
H	-0.307512	-3.538125	-1.270720

11

Eopt -213.895310

N	-0.515397	0.239664	-0.288016
C	-0.883137	1.391052	0.548627
H	-1.514109	2.050611	-0.009725
H	-1.405323	1.048347	1.417405
C	-1.731902	-0.476420	-0.698187

H	-2.362874	0.183139	-1.256539
H	-2.254088	-0.819125	0.170591
H	-0.027373	0.559949	-1.099958
C	-1.346651	-1.682636	-1.574671
H	-2.223770	-2.250232	-1.805747
H	-0.897274	-1.335491	-2.481562
H	-0.651233	-2.300271	-1.045689
C	0.391296	2.141235	0.978330
H	0.874470	2.547455	0.114369
H	0.129812	2.934683	1.646885
H	1.055090	1.462798	1.472295

12

Eopt -292.561170

N	-0.515397	0.239664	-0.288016
C	-0.883137	1.391052	0.548627
H	-1.405323	1.048347	1.417405
C	-1.731902	-0.476420	-0.698187
H	-2.362874	0.183139	-1.256539
H	-0.027373	0.559949	-1.099958
C	-1.346651	-1.682636	-1.574671
H	-2.223770	-2.250232	-1.805747
H	-0.897274	-1.335491	-2.481562
H	-0.651233	-2.300271	-1.045689
C	-2.483459	-0.969659	0.552204
H	-1.777831	-1.305012	1.283318
H	-3.064352	-0.168165	0.958493
H	-3.130381	-1.778505	0.283579
C	0.391296	2.141235	0.978330
H	0.870906	2.553113	0.115062
H	0.130519	2.930496	1.652097
H	1.057947	1.461328	1.466390
C	-1.791265	2.340324	-0.254982
H	-1.724183	3.327633	0.151983
H	-1.476864	2.353965	-1.277658
H	-2.803717	1.998931	-0.197622

13

Eopt -371.220711

N	-0.526713	0.309998	-0.308684
C	-0.870922	1.481654	0.488084
H	-1.654465	2.109890	0.034568
H	-1.231786	1.163555	1.469416
C	-1.686991	-0.513968	-0.636409
H	-2.473267	0.074048	-1.140902
H	-2.123656	-0.870554	0.304199
H	-0.085816	0.612194	-1.171165
C	-1.331294	-1.719847	-1.510485
H	-0.838989	-1.337366	-2.414060

C	-2.603962	-2.451794	-1.942360
H	-2.366877	-3.299479	-2.588600
H	-3.140986	-2.837858	-1.070840
H	-3.281097	-1.790573	-2.487833
C	-0.364068	-2.672868	-0.805566
H	0.549686	-2.159440	-0.506675
H	-0.827323	-3.088008	0.094875
H	-0.093918	-3.506857	-1.457349
C	0.380532	2.352954	0.703254
H	0.734357	2.708552	-0.241869
C	1.480071	1.513782	1.380311
H	2.017183	0.963002	0.636637
H	2.154152	2.161981	1.900265
H	1.032841	0.833303	2.074453
C	0.023205	3.551630	1.601638
H	0.884778	4.173946	1.725388
H	-0.762701	4.117037	1.146042
H	-0.300736	3.196753	2.557684

14

Eopt -526.129016

N	-0.676434	0.622624	-0.782951
H	-0.453071	1.158752	-1.613507
C	-1.792424	-0.270383	-1.109477
C	-1.524799	-0.949435	-2.455006
C	-2.020122	-1.323256	-0.019717
H	-2.731443	0.305341	-1.207220
C	-2.644448	-1.918757	-2.841473
H	-0.575144	-1.491445	-2.385088
H	-1.400580	-0.187828	-3.231624
C	-3.144295	-2.292537	-0.397163
H	-1.084759	-1.874941	0.126468
H	-2.254237	-0.836983	0.929696
C	-2.878190	-2.963248	-1.746867
H	-2.403735	-2.406680	-3.789449
H	-3.570346	-1.355738	-3.004587
H	-3.263214	-3.045696	0.385981
H	-4.091620	-1.743765	-0.449649
H	-3.711419	-3.617095	-2.017837
H	-1.990198	-3.600356	-1.662632
C	-0.897219	1.552199	0.337910
C	-0.101368	1.134332	1.581859
C	-0.530336	2.985117	-0.062229
H	-1.965068	1.551939	0.604595
C	-0.303529	2.109679	2.744493
H	0.959029	1.100907	1.307797
H	-0.381047	0.121115	1.876477
C	-0.716898	3.973023	1.092922
H	0.517136	2.997904	-0.388130

H	-1.136529	3.289716	-0.920891
C	0.061831	3.539386	2.337600
H	0.290846	1.795047	3.606302
H	-1.352791	2.082614	3.061426
H	-0.409439	4.974306	0.780117
H	-1.782606	4.035128	1.340739
H	-0.128336	4.231814	3.162011
H	1.136051	3.588040	2.124957

15

Eopt -212.677786

C	0.591110	-0.262672	0.149100
C	1.988323	-0.217754	-0.387493
C	2.369988	1.123083	0.282472
C	0.072821	1.162183	-0.167679
H	-0.047318	-1.041619	-0.212220
H	0.693562	-0.371907	1.208567
H	2.025577	-0.156994	-1.455117
H	2.589159	-1.053126	-0.094150
H	2.285523	1.057906	1.347140
H	3.359407	1.458373	0.051106
H	-0.581012	1.443846	0.631113
H	-0.450891	1.260319	-1.095577
N	1.330141	1.971685	-0.303893
H	1.571415	2.053337	-1.270909

16

Eopt -252.013014

C	0.218000	-1.124000	0.419000
C	-1.193200	-1.100500	-0.114000
C	-1.504900	0.358600	-0.366700
N	-0.244300	1.083900	-0.388100
C	0.649100	0.324200	0.471100
C	2.075300	0.457700	-0.021300
H	0.242700	-1.569800	1.424300
H	0.885200	-1.727900	-0.213600
H	-1.260700	-1.675700	-1.049200
H	-1.904200	-1.553600	0.592500
H	-2.017500	0.470000	-1.333500
H	-2.162800	0.753600	0.421500
H	0.129400	1.129800	-1.346800
H	0.603700	0.701300	1.503500
H	2.756200	0.521500	0.840300
H	2.336400	-0.419900	-0.630900
H	2.168900	1.368600	-0.630900

17

Eopt -291.348070

C	0.807400	-1.221000	0.139100
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C	-0.698900	-1.276100	0.211900
C	-1.143200	0.154900	0.419300
N	-0.034900	1.022700	0.053800
C	1.163900	0.239500	0.307700
C	2.248600	0.624100	-0.676900
C	-2.342900	0.455900	-0.454900
H	1.254000	-1.821800	0.944900
H	1.186400	-1.627800	-0.810000
H	-1.115100	-1.676600	-0.724300
H	-1.045700	-1.933900	1.022500
H	-1.429900	0.318600	1.468600
H	-0.092500	1.282200	-0.941300
H	1.537600	0.427400	1.325100
H	3.146600	0.942600	-0.127200
H	2.493700	-0.241900	-1.309300
H	1.893300	1.451100	-1.309300
H	-3.213900	0.674400	0.180400
H	-2.124500	1.327100	-1.090000
H	-2.561600	-0.415200	-1.090000

18

Eopt -291.347205

C	0.531169	-0.345741	-0.438473
C	1.922836	-0.289972	0.199089
C	2.301958	1.214707	0.180991
C	-0.071355	0.984206	0.023730
H	0.606692	-0.357819	-1.529577
H	-0.048693	-1.217042	-0.128702
H	2.660848	-0.903530	-0.318310
H	1.870341	-0.643958	1.232767
H	2.971657	1.413042	-0.660201
N	1.030025	1.961702	-0.046933
C	2.991379	1.663548	1.464308
H	3.895773	1.076427	1.645589
H	3.271730	2.717132	1.409928
H	2.323328	1.531245	2.319252
H	0.941343	2.943275	-0.216197
H	-0.427308	0.899713	1.029244
C	-1.217674	1.404498	-0.914837
H	-1.972911	0.646533	-0.917064
H	-1.638874	2.326675	-0.572669
H	-0.837703	1.532307	-1.906899

19

Eopt -252.016647

C	-1.368932	-1.615598	0.032353
C	-0.787534	-0.206083	0.030787
C	-2.780994	0.572214	1.149915
C	-3.319237	-0.854127	1.127111

H	0.301204	-0.250298	0.103634
H	-1.026863	-2.158932	0.925588
H	-1.059503	-2.174193	-0.852611
H	-3.143687	1.094923	2.037525
H	-3.155677	1.106850	0.271389
H	-3.049655	-1.369641	2.060773
H	-4.405717	-0.867291	1.025441
H	-1.039111	0.280472	-0.916847
N	-1.314386	0.623344	1.121123
H	-0.953017	0.277116	2.005328
C	-2.797083	-1.579921	0.012724
H	-3.170220	-2.582223	0.045260
H	-3.120429	-1.108144	-0.891585

20

Eopt -287.926461

C	-1.368429	-1.614006	0.044665
C	-0.803658	-0.181555	0.015426
C	-2.773915	0.587875	1.121396
C	-3.309006	-0.856166	1.133975
H	0.265227	-0.216353	0.049662
H	-1.056401	-2.101970	0.944348
H	-1.002743	-2.157313	-0.801497
H	-3.154001	1.118933	1.968988
H	-3.089181	1.077549	0.223772
H	-2.993663	-1.345425	2.031797
H	-4.378094	-0.839162	1.093198
H	-1.115342	0.306720	-0.884209
O	-2.800092	-1.568210	-0.000851
N	-1.308291	0.560109	1.176071
H	-1.012605	0.107809	2.017495

21

Eopt -291.352464

C	-0.988300	1.254300	-0.634800
C	-1.573400	-0.033600	-1.210000
C	-1.226000	-1.203900	-0.295400
C	0.280900	-1.264300	-0.065800
C	0.772700	0.085900	0.451200
N	0.464600	1.136200	-0.518400
C	2.269500	0.025600	0.670900
H	-1.233000	2.094700	-1.301000
H	-1.416800	1.431200	0.362700
H	-2.666800	0.061600	-1.284000
H	-1.152000	-0.212700	-2.210200
H	-1.735700	-1.073800	0.670600
H	-1.554300	-2.140200	-0.770400
H	0.507700	-2.045100	0.675000
H	0.786600	-1.499700	-1.013900

H	0.267100	0.314000	1.401200
H	0.860600	2.031200	-0.197700
H	2.481600	0.017100	1.750200
H	2.671000	-0.889400	0.211100
H	2.743300	0.905400	0.211100

22

Eopt -330.683877

C	-0.990900	0.862500	-0.787700
C	-1.512000	-0.568700	-0.955400
C	-0.834200	-1.520000	0.026800
C	0.678200	-1.404500	-0.096900
C	1.090100	0.044900	0.133200
N	0.474600	0.916500	-0.872000
C	2.597100	0.160300	0.045000
C	-1.503000	1.509000	0.492200
H	-1.390900	1.450900	-1.626500
H	-2.597000	-0.579300	-0.774800
H	-1.286500	-0.904500	-1.978400
H	-1.136700	-1.261300	1.052200
H	-1.137600	-2.552300	-0.202300
H	1.159100	-2.047500	0.654900
H	0.992500	-1.723100	-1.101800
H	0.749700	0.357400	1.131400
H	0.785700	1.885500	-0.713800
H	3.022300	0.192900	1.059000
H	3.000500	-0.709500	-0.494000
H	2.863400	1.081500	-0.494000
H	-1.085000	0.981400	1.362200
H	-1.192800	2.564000	0.519500
H	-2.601000	1.448800	0.519500

23

Eopt -366.373841

N	-0.515906	0.262502	-0.316928
C	-0.881688	1.407229	0.529657
H	-0.000161	1.956034	0.787769
H	-1.555224	2.044728	-0.004051
H	-1.355928	1.054159	1.421474
C	-1.726976	-0.491465	-0.671531
H	-2.400512	0.146035	-1.205239
H	-2.201217	-0.844534	0.220286
H	-0.072691	0.592473	-1.150402
C	-1.343777	-1.690702	-1.558429
C	-1.307848	-1.548322	-2.952115
C	-1.030993	-2.924387	-0.971821
C	-0.959136	-2.639627	-3.759192
H	-1.546665	-0.606376	-3.400003
C	-0.682280	-4.015692	-1.778899

H	-1.058426	-3.033097	0.092288
C	-0.646353	-3.873313	-3.172584
H	-0.931705	-2.530917	-4.823302
H	-0.443462	-4.957638	-1.331011
H	-0.380104	-4.706549	-3.788806

24

Eopt -441.625130

N	-1.168445	1.079641	-0.873459
C	-0.372865	0.994074	0.359680
H	0.319797	1.808879	0.394512
H	-1.023346	1.042412	1.207877
H	0.164048	0.068649	0.374242
C	-2.120046	-0.039763	-0.921312
C	-1.798481	-1.259392	-0.310555
C	-3.348805	0.112701	-1.577688
C	-2.705675	-2.326556	-0.356173
H	-0.860296	-1.375801	0.190602
C	-4.256000	-0.954463	-1.623304
H	-3.594327	1.043915	-2.044014
C	-3.934435	-2.174091	-1.012546
H	-2.460153	-3.257769	0.110154
H	-5.194185	-0.838052	-2.124459
H	-0.560519	1.034466	-1.666167
O	-4.860145	-3.263033	-1.059091
C	-4.607956	-4.053599	-2.223696
H	-5.300620	-4.868402	-2.258523
H	-4.725278	-3.448115	-3.098066
H	-3.609268	-4.435824	-2.185915

25

Eopt -327.052842

N	-1.163117	1.073391	-0.878841
C	-0.380570	1.010810	0.363980
H	0.307654	1.829567	0.393728
H	-1.040457	1.068849	1.204266
H	0.160702	0.088462	0.398585
C	-2.108620	-0.051443	-0.919710
C	-1.787711	-1.259902	-0.286808
C	-3.330910	0.084674	-1.591574
C	-2.689090	-2.332245	-0.325771
H	-0.854465	-1.363831	0.226175
C	-4.232289	-0.987669	-1.630539
H	-3.575933	1.007360	-2.074807
C	-3.911378	-2.196129	-0.997639
H	-2.444068	-3.254931	0.157463
H	-5.165535	-0.883741	-2.143522
H	-4.599600	-3.014888	-1.027392
H	-0.546399	1.019149	-1.664155

26

Eopt -172.073551

N	-0.532284	0.290292	-0.332168
C	-0.921518	1.448819	0.484662
H	-0.048327	2.006902	0.751083
H	-1.586495	2.072710	-0.075218
H	-1.413052	1.110127	1.372683
H	-0.072906	0.606826	-1.162095
C	-1.731902	-0.476420	-0.698187
C	-2.737552	-1.018894	-1.068689
H	-3.633361	-1.502116	-1.398723

27

Eopt -419.343563

N	-1.168445	1.079641	-0.873459
C	-0.372865	0.994074	0.359680
H	0.319797	1.808879	0.394512
H	-1.023346	1.042412	1.207877
H	0.164048	0.068649	0.374242
C	-2.120046	-0.039763	-0.921312
C	-1.798481	-1.259392	-0.310555
C	-3.348805	0.112701	-1.577688
C	-2.705675	-2.326556	-0.356173
H	-0.860296	-1.375801	0.190602
C	-4.256000	-0.954463	-1.623304
H	-3.594327	1.043915	-2.044014
C	-3.934435	-2.174091	-1.012546
H	-2.460153	-3.257769	0.110154
H	-5.194185	-0.838052	-2.124459
H	-0.560519	1.034466	-1.666167
C	-4.931354	-3.346798	-1.062671
N	-5.673605	-4.219931	-1.099992

28

Eopt -433.112341

N	-0.515397	0.239664	-0.288016
C	-0.883137	1.391052	0.548627
H	0.002346	1.912283	0.847187
H	-1.514109	2.050611	-0.009725
H	-1.405323	1.048347	1.417405
C	-1.731902	-0.476420	-0.698187
H	-0.027373	0.559949	-1.099958
F	-2.390735	-0.908805	0.397935
F	-1.394182	-1.533818	-1.466533
F	-2.527988	0.355733	-1.402650

TS-6

Eopt -509.708891

N	-0.479922	0.222802	-0.213771
O	0.191638	-1.924113	0.325469
C	-0.800904	1.320551	0.741680
H	-1.539666	1.947685	0.242276
H	-1.281788	0.878337	1.615869
C	-1.640988	-0.422916	-0.836151
H	-2.157747	0.321293	-1.438861
H	-1.303281	-1.229671	-1.481957
H	-2.313458	-0.814309	-0.073925
N	0.446029	-0.827914	0.585002
H	0.235078	0.603538	-1.039440
O	1.167581	0.953782	-2.000843
N	2.171996	0.270338	-1.567704
O	3.199518	0.369736	-2.213438
C	0.423165	2.137942	1.122084
H	0.873719	2.598658	0.243187
H	0.116930	2.929827	1.805651
H	1.176420	1.530220	1.620796

TS-7

Eopt -549.043317

N	-0.513901	0.200390	-0.203449
O	0.273946	-1.907694	0.356377
C	-0.843578	1.335210	0.729615
H	0.045710	1.934961	0.519595
C	-1.646087	-0.515700	-0.801238
H	-2.109169	0.120499	-1.550678
H	-1.276815	-1.411593	-1.294708
H	-2.374293	-0.788359	-0.038522
N	0.455716	-0.797396	0.615180
H	0.189001	0.580834	-1.058963
O	1.068090	0.946083	-2.034170
N	2.138688	0.372644	-1.591515
O	3.137128	0.527944	-2.268919
C	-0.922641	1.021007	2.221656
H	-1.793616	0.400873	2.437479
H	-0.029112	0.466694	2.507864
H	-0.975068	1.918910	2.832817
C	-1.837539	2.286646	0.067719
H	-1.439083	2.671141	-0.873109
H	-2.801784	1.818361	-0.121351
H	-2.003608	3.131583	0.735904

TS-8

Eopt -588.373919

N	-0.514327	0.181518	-0.176387
O	0.315540	-1.920402	0.309775
C	-0.861368	1.311949	0.788257
C	-1.609822	-0.563925	-0.809803

H	-2.208755	0.124376	-1.398511
H	-1.182454	-1.306338	-1.479226
H	-2.229939	-1.061155	-0.068049
N	0.517126	-0.810344	0.560497
H	0.144419	0.616318	-1.017002
O	0.988447	1.049738	-2.035105
N	2.051870	0.391860	-1.718450
O	3.014602	0.559954	-2.445474
C	0.447498	2.001935	1.193105
H	0.979158	2.376930	0.318717
H	0.205316	2.849010	1.834222
H	1.108004	1.337576	1.745805
C	-1.749908	2.310754	0.038762
H	-1.282998	2.634812	-0.892406
H	-2.734585	1.900996	-0.181685
H	-1.890699	3.187784	0.670291
C	-1.584267	0.752954	2.014037
H	-0.961321	0.039566	2.555678
H	-1.815395	1.575348	2.690846
H	-2.524204	0.269375	1.749189

TS-9

Eopt -665.826809

N	-0.501539	0.272370	-0.249838
O	0.312875	-1.778755	0.471010
C	-1.628625	-0.491562	-0.790854
H	-2.240184	0.182124	-1.388450
H	-1.250620	-1.288795	-1.426447
H	-2.225127	-0.912317	0.017664
N	0.524910	-0.652948	0.600583
H	0.173885	0.645690	-1.102585
O	1.089042	1.018157	-2.082876
N	2.111020	0.367755	-1.644575
O	3.134784	0.481107	-2.294418
C	-0.849562	1.401689	0.624473
C	-0.268223	1.173369	2.004938
C	-0.334059	2.691288	0.018062
H	-1.968386	1.442987	0.693013
C	-0.532524	2.353793	2.917237
H	0.838095	1.008155	1.920505
H	-0.714013	0.246786	2.451422
C	-0.599102	3.871830	0.930025
H	0.768954	2.602080	-0.165649
H	-0.827969	2.864170	-0.973203
C	-0.019247	3.643858	2.311053
H	-0.037204	2.181171	3.907866
H	-1.635357	2.441948	3.102616
H	-0.152934	4.798317	0.483817
H	-1.705558	4.037054	1.013252

H	-0.287031	4.504488	2.977538
H	1.099824	3.604876	2.243928

TS-10

Eopt -588.370604

N	-0.500105	0.246843	-0.225833
O	0.370670	-1.903881	-0.322484
C	-0.721910	1.003068	1.034643
H	-1.639194	1.597061	0.895705
H	-0.934426	0.265555	1.825888
C	-1.699300	-0.359804	-0.809936
H	-2.374009	0.445929	-1.129805
H	-1.413809	-0.955917	-1.685773
H	-2.209380	-1.002299	-0.077068
N	0.624072	-0.862805	0.126730
H	0.053237	0.855955	-1.073041
O	0.842207	1.303051	-2.064170
N	1.858813	0.549878	-1.814843
O	2.831842	0.693965	-2.519965
C	0.443844	1.919878	1.437384
C	0.329952	2.243712	2.932830
H	0.374238	1.332921	3.551134
H	1.147743	2.909733	3.248618
H	-0.622238	2.756761	3.151801
C	0.486452	3.206009	0.601796
H	0.601115	2.999274	-0.470961
H	-0.437863	3.791067	0.746045
H	1.334337	3.836709	0.912673
H	1.382407	1.362315	1.277793

TS-11

Eopt -549.040224

N	-0.430906	0.161352	-0.145533
O	0.192474	-1.859414	0.778852
C	-0.817014	1.355611	0.667525
H	-1.473534	1.945975	0.028797
H	-1.404715	1.010911	1.520161
C	-1.567282	-0.587933	-0.730347
H	-2.323612	0.151426	-0.990116
H	-1.989347	-1.226255	0.048749
N	0.489720	-0.740879	0.797306
H	0.327910	0.501180	-0.976428
O	1.280987	0.826214	-1.886012
N	2.230766	0.038880	-1.499964
O	3.261088	0.102355	-2.143156
C	-1.171044	-1.399048	-1.955812
H	-0.801361	-0.751430	-2.750126
H	-0.401871	-2.135004	-1.725975
H	-2.048307	-1.930479	-2.324922

C	0.377562	2.190101	1.104492
H	0.957125	2.522608	0.243458
H	0.009382	3.071490	1.629824
H	1.035660	1.643811	1.777237

TS-12

Eopt -706.368201

N	-0.517034	0.363651	-0.072256
O	0.680659	-1.568262	0.401190
C	-0.908742	1.495404	0.803484
H	-1.336173	2.256128	0.149126
C	-1.571904	-0.526711	-0.598290
H	-1.996460	-1.084397	0.237505
N	0.659216	-0.448551	0.684838
H	0.110803	0.817426	-0.944484
O	0.970346	1.349548	-1.873031
N	2.097536	1.062675	-1.315926
O	3.092837	1.427021	-1.913346
C	-2.682970	0.194568	-1.373825
H	-3.157086	0.919906	-0.707627
C	-1.874359	1.180573	1.948607
H	-2.796850	0.774396	1.525404
C	-3.741202	-0.842755	-1.761811
H	-4.569650	-0.359955	-2.281853
H	-3.318902	-1.597485	-2.430230
H	-4.143432	-1.352326	-0.884082
C	-2.162031	0.936516	-2.605335
H	-2.995524	1.377595	-3.154070
H	-1.473311	1.741093	-2.348243
H	-1.638907	0.251782	-3.277381
H	-1.078440	-1.242974	-1.255942
C	-1.313277	0.166014	2.946501
H	-0.359253	0.506209	3.355962
H	-2.008639	0.034720	3.777122
H	-1.160539	-0.818750	2.502593
C	-2.226146	2.497905	2.647936
H	-2.949230	2.323145	3.445578
H	-1.336511	2.950297	3.093759
H	-2.659456	3.217498	1.950491
H	0.025433	1.901183	1.197689

TS-13

Eopt -627.703992

N	-0.488462	0.199966	-0.138094
O	0.205542	-1.874854	0.647048
C	-0.796768	1.346834	0.790733
H	-1.438781	2.015835	0.200672
C	-1.618616	-0.551494	-0.770749
H	-1.981310	-1.268783	-0.015694

N	0.516727	-0.752527	0.670252
H	0.236203	0.604385	-0.976841
O	1.220866	0.888821	-1.847456
N	2.032250	-0.040720	-1.471754
O	3.093996	-0.105259	-2.050031
C	-1.098025	-1.326430	-1.988200
H	-0.803996	-0.634385	-2.791119
H	-0.231467	-1.956061	-1.748288
H	-1.898020	-1.979547	-2.365929
C	0.481179	2.118819	1.131254
H	1.025426	2.410222	0.222088
H	0.203525	3.032056	1.677794
H	1.156158	1.530423	1.768346
C	-2.769112	0.372367	-1.178038
H	-3.267769	0.843992	-0.321089
H	-2.422851	1.159570	-1.865764
H	-3.522453	-0.228943	-1.707620
C	-1.552986	0.885526	2.035564
H	-0.923865	0.237060	2.665344
H	-1.834903	1.763987	2.634478
H	-2.474505	0.339081	1.788249

TS-14

Eopt -861.268971

N	-0.355502	0.221797	-0.224965
O	0.823078	-1.612084	0.507990
N	0.882097	-0.452738	0.457365
H	0.138135	0.575604	-1.216985
O	0.798798	0.914304	-2.390251
N	1.959097	0.403096	-2.156943
O	2.791458	0.560210	-3.032703
C	-0.697152	1.454920	0.597079
C	-0.555277	1.241112	2.110220
C	0.123067	2.663356	0.141676
H	-1.748202	1.642963	0.368326
C	-1.018384	2.493546	2.860934
H	0.493423	1.053298	2.353042
H	-1.122400	0.370910	2.437786
C	-0.304162	3.919630	0.909025
H	1.184142	2.460238	0.315810
H	-0.001159	2.819713	-0.929849
C	-0.221724	3.724123	2.423775
H	-0.913765	2.329447	3.935329
H	-2.084224	2.658493	2.668342
H	0.317399	4.761115	0.596026
H	-1.334388	4.170125	0.633434
H	-0.587674	4.615177	2.939027
H	0.826128	3.595503	2.716269
C	-1.525337	-0.644590	-0.627596

C	-1.152274	-1.650310	-1.726365
C	-2.260627	-1.306984	0.541131
H	-2.204856	0.084629	-1.080814
C	-2.411681	-2.368859	-2.221964
H	-0.450545	-2.390572	-1.343032
H	-0.663013	-1.131460	-2.550399
C	-3.498332	-2.054225	0.027854
H	-1.597501	-2.005432	1.054174
H	-2.572635	-0.556052	1.265932
C	-3.148024	-3.057430	-1.071662
H	-2.132651	-3.094058	-2.989180
H	-3.080390	-1.644397	-2.699792
H	-3.985256	-2.556112	0.866527
H	-4.216836	-1.326142	-0.364142
H	-4.054742	-3.543723	-1.438916
H	-2.510896	-3.845372	-0.655069

TS-15

Eopt -547.829342

N	-0.434922	0.208253	-0.258716
O	0.118698	-1.760419	0.762798
C	-0.834721	1.505617	0.353232
H	-0.577483	2.289780	-0.346324
C	-1.632709	-0.454309	-0.843104
H	-1.835696	-1.355684	-0.282038
N	0.327310	-0.648034	0.853171
H	0.420780	0.360383	-1.050109
O	1.488843	0.475926	-1.879105
N	2.402915	-0.100108	-1.222487
O	3.472844	-0.123913	-1.749917
H	-0.274408	1.657946	1.264668
H	-1.420462	-0.730719	-1.865126
C	-2.343008	1.386617	0.534033
H	-2.572094	0.846697	1.447259
H	-2.819500	2.356805	0.584415
C	-2.759012	0.573248	-0.692962
H	-3.719933	0.088582	-0.580458
H	-2.802616	1.211679	-1.568350

TS-16

Eopt -587.161760

C	0.441104	-0.621015	0.273998
C	1.949802	-0.543490	0.028364
C	2.335293	0.675208	0.852751
C	-0.039586	0.837502	0.227411
H	-0.087158	-1.235274	-0.453947
H	0.245671	-1.030742	1.269697
H	2.162269	-0.355958	-1.027317
H	2.491537	-1.436519	0.335974

H	2.285748	0.459812	1.924307
H	3.300435	1.121966	0.625554
H	-0.325036	1.111259	-0.789598
N	1.247447	1.621090	0.508483
H	1.493377	2.207985	-0.533031
N	1.057823	2.831726	1.502486
O	2.027461	3.055850	2.143340
N	1.738236	4.131073	-1.027846
O	1.934491	5.010282	-1.819976
O	1.694955	2.914248	-1.612000
C	-1.162171	1.175503	1.189682
H	-1.482306	2.213412	1.098984
H	-2.019415	0.539241	0.959992
H	-0.870249	0.975759	2.223442

TS-17

Eopt -626.498022

C	0.474420	-0.627787	0.647461
C	1.973382	-0.703723	0.369211
C	2.493899	0.684980	0.763140
C	0.108496	0.771855	0.163191
H	-0.102718	-1.391625	0.128916
H	0.271757	-0.714522	1.718250
H	2.152871	-0.878764	-0.694146
H	2.482511	-1.485183	0.930806
H	2.696364	0.701346	1.837318
N	1.319159	1.592397	0.548963
H	1.497943	2.366523	-0.276957
N	1.002186	2.574198	1.790270
O	1.889606	2.656875	2.524486
N	1.415374	4.398680	-0.513071
O	1.467701	5.475478	-1.082194
O	1.636602	3.364147	-1.247131
C	3.731522	1.157445	0.018489
H	4.043733	2.147942	0.349910
H	4.548144	0.460196	0.208851
H	3.551847	1.191966	-1.056718
H	-0.766189	1.129155	0.665349
C	-0.093441	0.784154	-1.363462
H	-1.101887	0.509066	-1.592071
H	0.102879	1.765782	-1.741306
H	0.578379	0.086161	-1.817735

TS-18

Eopt -626.496683

C	0.441104	-0.621015	0.273998
C	1.949802	-0.543490	0.028364
C	2.335293	0.675208	0.852751
C	-0.039586	0.837502	0.227411

H	-0.087158	-1.235274	-0.453947
H	0.245671	-1.030742	1.269697
H	2.162269	-0.355958	-1.027317
H	2.491537	-1.436519	0.335974
H	2.285748	0.459812	1.924307
H	-0.325036	1.111259	-0.789598
N	1.247447	1.621090	0.508483
H	1.493377	2.207985	-0.533031
N	1.057823	2.831726	1.502486
O	2.027461	3.055850	2.143340
N	1.738236	4.131073	-1.027846
O	1.934491	5.010282	-1.819976
O	1.694955	2.914248	-1.612000
C	-1.162171	1.175503	1.189682
H	-1.482306	2.213412	1.098984
H	-2.019415	0.539241	0.959992
H	-0.870249	0.975759	2.223442
C	3.701992	1.307844	0.531027
H	3.844562	2.177024	1.138563
H	4.478896	0.600306	0.732793
H	3.732106	1.585761	-0.501812

TS-19

Eopt -587.158477

N	-0.476695	0.186675	-0.401956
O	0.089337	-1.985689	0.245032
C	-0.830724	1.332711	0.476592
C	-1.576208	-0.383950	-1.209360
H	-1.406574	-1.471282	-1.266103
N	0.298693	-0.884383	0.545534
H	0.403449	0.531424	-1.089292
O	1.568961	0.837670	-1.691959
N	2.305852	0.074922	-0.965334
O	3.493971	0.066840	-1.202327
C	-1.840819	2.226389	-0.240673
H	-2.017179	3.121766	0.373854
H	-1.384030	2.578372	-1.180158
C	-2.940002	-0.049736	-0.612367
H	-3.722735	-0.530247	-1.218229
H	-3.003991	-0.502989	0.390264
C	-3.161775	1.474653	-0.526924
H	-3.900702	1.687134	0.261387
H	-3.593072	1.845833	-1.469838
H	-1.474462	0.008983	-2.233204
H	-1.246502	0.951093	1.422145
H	0.102039	1.866602	0.704764

TS-20

Eopt -623.063530

N	-0.574589	0.400862	-0.337861
O	0.229248	-1.262439	1.130292
C	-1.087319	1.724761	0.071223
H	-1.163240	2.359320	-0.824712
C	-1.611407	-0.568043	-0.737519
H	-1.803255	-1.251610	0.107389
N	0.386305	-0.139360	0.903460
H	0.247583	0.536672	-1.173141
O	1.339225	0.601890	-1.926868
N	2.151761	0.156835	-1.036075
O	3.318027	0.065207	-1.344804
H	-0.346203	2.183128	0.743397
H	-1.236179	-1.171705	-1.576237
C	-2.435457	1.586184	0.762942
H	-2.307823	1.015533	1.702833
H	-2.813840	2.585118	1.031851
C	-2.894574	0.163935	-1.122254
H	-2.714392	0.783302	-2.021605
H	-3.663943	-0.578320	-1.382603
O	-3.407146	0.950089	-0.060384

TS-21

Eopt -626.490800

N	-0.590829	0.020514	-0.059592
O	0.466987	-2.002710	0.308115
C	-0.950951	1.075727	0.936882
C	-1.710185	-0.763822	-0.630482
H	-1.943221	-1.588680	0.042790
N	0.581995	-0.884043	0.573764
H	-0.024712	0.528038	-0.896693
O	0.789287	1.113630	-1.912021
N	1.901357	0.553062	-1.594182
O	2.866487	0.845053	-2.279754
C	-1.831904	2.135221	0.222918
H	-2.591583	2.463780	0.933650
H	-1.227221	3.007687	-0.023757
C	-2.933111	0.140790	-0.872351
H	-3.459198	-0.223477	-1.754315
H	-3.626448	0.059763	-0.033670
C	-2.511317	1.598866	-1.048572
H	-3.377863	2.215856	-1.287093
H	-1.828025	1.677766	-1.898295
H	-1.345456	-1.189138	-1.563709
C	0.395906	1.707674	1.334650
H	0.223653	2.516810	2.013272
H	1.010108	0.970120	1.807587
H	0.889759	2.075173	0.459462
H	-1.451346	0.656755	1.784801

TS-22

Eopt -665.823185

N	-0.516533	0.044926	-0.056606
O	0.546622	-1.937936	0.505553
C	-0.945634	1.117918	0.872627
H	-0.047912	1.558893	1.302264
C	-1.621286	-0.776237	-0.610781
H	-1.725729	-1.676738	-0.003350
N	0.640239	-0.802441	0.686982
H	0.072950	0.523194	-0.907303
O	0.875786	1.063170	-1.927940
N	2.002506	0.553863	-1.569089
O	2.963420	0.841859	-2.261058
C	-1.779494	2.154843	0.105202
H	-2.406717	2.670566	0.833424
H	-1.120407	2.901273	-0.338416
C	-2.926839	0.030785	-0.648609
H	-3.584622	-0.428012	-1.386946
H	-3.436118	-0.037239	0.315018
C	-2.645148	1.494002	-0.989460
H	-3.577867	2.043648	-1.114521
H	-2.122892	1.538315	-1.949056
C	-1.756081	0.468579	2.009788
H	-1.624856	-0.592931	1.980185
H	-1.413612	0.844177	2.951351
H	-2.792876	0.703328	1.887933
C	-1.194888	-1.206024	-2.026785
H	-0.417574	-1.938148	-1.958398
H	-2.034930	-1.624640	-2.540585
H	-0.835897	-0.353901	-2.565219

TS-23

Eopt -701.519211

N	-0.481392	0.273624	-0.297857
O	0.287512	-1.893845	0.071142
C	-0.763808	1.293444	0.749341
H	-1.414785	2.043212	0.273371
H	-1.342419	0.813224	1.552788
C	-1.659937	-0.388267	-0.858589
H	-2.306203	0.374169	-1.315041
H	-1.341359	-1.098220	-1.632458
H	-2.216890	-0.923844	-0.075660
N	0.582373	-0.800417	0.325153
H	0.156214	0.729500	-1.161157
O	1.074018	1.053874	-2.110964
N	1.980442	0.236902	-1.707944
O	3.031883	0.234711	-2.309293
C	0.484460	1.949371	1.294769
C	1.198123	2.877456	0.519875

C	0.942795	1.643140	2.584220
C	2.352031	3.482382	1.024826
H	0.858372	3.116644	-0.490018
C	2.094306	2.251901	3.093215
H	0.395044	0.920238	3.194686
C	2.802689	3.171632	2.313096
H	2.899921	4.202112	0.411506
H	2.439280	2.005052	4.100373
H	3.703765	3.647312	2.708438

TS-24

Eopt -776.764537

N	-0.437303	0.266415	-0.140383
O	0.896954	-1.493858	0.765382
C	-1.407925	-0.804983	-0.351949
H	-2.304279	-0.382654	-0.802487
H	-0.975998	-1.533215	-1.034977
H	-1.670238	-1.307488	0.579104
N	0.934844	-0.356344	0.657551
H	0.062743	0.592581	-1.232060
O	0.635093	0.856336	-2.323656
N	1.835770	0.394671	-2.102654
O	2.609896	0.521819	-3.023127
C	-0.817999	1.411585	0.630354
C	-1.845616	1.376709	1.564934
C	-0.082759	2.590359	0.463708
C	-2.163196	2.505157	2.315341
H	-2.421918	0.476095	1.721128
C	-0.383974	3.709311	1.212240
H	0.720052	2.626823	-0.260172
C	-1.431866	3.681552	2.142358
H	-2.970376	2.440279	3.026823
H	0.177528	4.625396	1.087462
O	-1.630268	4.846349	2.835150
C	-2.776507	4.999293	3.669989
H	-2.704262	4.363485	4.556686
H	-2.780653	6.042733	3.972743
H	-3.697160	4.772130	3.126370

TS-25

Eopt -662.187944

N	-0.437747	0.289421	-0.144092
O	0.765042	-1.500656	0.864361
C	-1.432800	-0.749016	-0.412170
H	-2.293501	-0.289779	-0.894576
H	-0.996089	-1.484638	-1.084067
H	-1.751804	-1.251762	0.500543
N	0.856142	-0.367124	0.734158
H	0.133994	0.589218	-1.200323

O	0.778997	0.820012	-2.267845
N	1.931254	0.270758	-1.998860
O	2.755798	0.352850	-2.880607
C	-0.833904	1.449955	0.598974
C	-1.814021	1.396282	1.584675
C	-0.166099	2.654121	0.358163
C	-2.148375	2.532478	2.311775
H	-2.335875	0.473565	1.795398
C	-0.486840	3.784433	1.084210
H	0.599783	2.702768	-0.403977
C	-1.482943	3.735649	2.066328
H	-2.920039	2.464029	3.063311
H	0.021606	4.721751	0.902419
H	-1.732727	4.613472	2.624839

TS-26

Eopt -507.202979

N	-0.319764	0.425219	-0.389194
O	0.469342	-1.980378	0.102148
C	-1.574164	-0.239683	-0.730611
H	-2.180868	0.412360	-1.378532
H	-1.342102	-1.156409	-1.294802
H	-2.152893	-0.501775	0.167833
N	0.909596	-0.950423	0.251592
H	0.436563	0.706418	-1.384590
O	1.313190	0.758455	-2.217639
N	2.058977	-0.208465	-1.795008
O	3.059617	-0.446986	-2.412405
C	-0.323810	1.363426	0.572571
C	-0.264293	2.205744	1.448119
H	-0.221707	2.960330	2.211833

TS-27

Eopt -754.470622

N	-0.504839	0.251993	-0.146900
O	1.224243	-1.426160	0.376501
C	-1.349896	-0.925716	-0.272349
H	-2.356532	-0.625192	-0.562878
H	-0.940217	-1.559254	-1.056913
H	-1.398421	-1.497471	0.655738
N	1.138907	-0.301165	0.395258
H	-0.164302	0.694154	-1.272136
O	0.294749	1.070479	-2.365056
N	1.557333	0.782226	-2.207801
O	2.268424	1.038008	-3.148645
C	-0.846120	1.274672	0.764984
C	-1.864769	1.136154	1.712445
C	-0.095146	2.456265	0.718588
C	-2.140126	2.171513	2.588402

H	-2.454126	0.233313	1.765695
C	-0.360752	3.486590	1.599506
H	0.693504	2.562001	-0.012950
C	-1.389881	3.351613	2.539731
H	-2.934737	2.066577	3.313859
H	0.219992	4.397405	1.559467
C	-1.673807	4.414293	3.443022
N	-1.903733	5.275706	4.174693

TS-28

Eopt -768.232994

N	-0.511942	0.303377	-0.288914
O	0.408826	-1.739877	0.353756
C	-0.843936	1.411364	0.616579
C	-1.630975	-0.493026	-0.789582
H	-2.298355	0.163365	-1.365411
H	-1.246050	-1.281278	-1.449356
H	-2.188114	-0.948432	0.042440
N	0.602008	-0.602390	0.485627
H	0.128326	0.713738	-1.170904
O	1.088796	1.043681	-2.074690
N	2.012165	0.321845	-1.554187
O	3.099751	0.336235	-2.088590
F	-1.533436	2.349027	-0.067436
F	0.306002	1.952064	1.072416
F	-1.586497	0.973688	1.655590

NO-3

Eopt -303.929585

N	-0.679606	0.077750	0.097564
O	0.541568	-1.686497	-0.031191
C	-0.835450	1.451235	0.545238
H	-1.014890	2.105379	-0.308997
H	-1.677526	1.527755	1.234536
C	-1.745643	-0.608142	-0.620837
H	-2.579083	0.078774	-0.731855
H	-1.389323	-0.927420	-1.600663
H	-2.059864	-1.493009	-0.066424
N	0.449607	-0.518618	0.364802
C	0.460520	1.875915	1.260576
H	0.367103	2.887265	1.597244
H	0.631016	1.234835	2.100127
H	1.283887	1.800717	0.581377

NO-4

Eopt -343.263477

N	-0.679606	0.077750	0.097564
O	0.541568	-1.686497	-0.031191
C	-0.835450	1.451235	0.545238

H	-1.677526	1.527755	1.234536
C	-1.745643	-0.608142	-0.620837
H	-2.579083	0.078774	-0.731855
H	-1.389323	-0.927420	-1.600663
H	-2.059864	-1.493009	-0.066424
N	0.449607	-0.518618	0.364802
C	0.460520	1.875915	1.260576
H	0.367103	2.887265	1.597244
H	0.631016	1.234835	2.100127
H	1.283887	1.800717	0.581377
C	-1.088787	2.374770	-0.660790
H	-2.080220	2.215125	-1.030215
H	-0.981217	3.395205	-0.357406
H	-0.380945	2.155657	-1.432703

NO-5

Eopt -382.594955

N	-0.550836	0.437739	-0.338838
O	1.528063	0.987279	-0.247283
C	-0.836139	1.564648	0.545157
H	-0.284089	1.449828	1.477971
H	-0.515217	2.493587	0.073923
H	-1.898855	1.604846	0.749322
C	-1.631104	-0.464427	-0.840185
N	0.679442	0.204125	-0.698342
C	-1.041011	-1.549374	-1.743783
H	-0.325935	-2.173788	-1.210346
H	-1.861242	-2.179841	-2.088578
H	-0.543551	-1.123112	-2.613693
C	-2.633247	0.378002	-1.643310
H	-3.103707	1.148857	-1.033185
H	-2.138546	0.857721	-2.488968
H	-3.423191	-0.268669	-2.026292
C	-2.314586	-1.123302	0.366946
H	-3.096008	-1.797225	0.014639
H	-1.593769	-1.702301	0.945906
H	-2.781425	-0.391035	1.025460

NO-6

Eopt -460.048278

N	-0.732948	0.572766	-0.556457
C	-0.814303	1.271681	0.721974
H	-0.004939	0.953617	1.379857
H	-0.719733	2.345322	0.560576
H	-1.773629	1.046028	1.176940
C	-1.794202	-0.366974	-0.960186
C	-1.812861	-0.647296	-2.462204
C	-1.694518	-1.671571	-0.156955
H	-2.732610	0.131367	-0.697858

C	-2.985293	-1.572979	-2.805287
H	-0.875682	-1.122073	-2.758624
H	-1.885296	0.292539	-3.013209
C	-2.848184	-2.615122	-0.508619
H	-0.735920	-2.144809	-0.393248
H	-1.693400	-1.455386	0.913627
C	-2.914963	-2.882105	-2.014192
H	-2.984222	-1.776314	-3.878441
H	-3.929593	-1.064170	-2.582089
H	-2.736801	-3.551656	0.042430
H	-3.791347	-2.166078	-0.178279
H	-3.776959	-3.511692	-2.247720
H	-2.022815	-3.439225	-2.321174
N	0.319290	0.696954	-1.311379
O	1.203041	1.451066	-0.877720

NO-7

Eopt -382.594693

N	-0.664621	-0.065620	0.169416
O	0.181827	-2.036946	0.276421
C	-0.714908	1.348330	0.581740
H	-1.578639	1.465809	1.246789
C	-1.721974	-0.618526	-0.663404
H	-2.415397	0.181602	-0.902427
N	0.264094	-0.849102	0.627290
C	0.548986	1.934303	1.208165
H	0.833193	1.300469	2.052896
H	-2.236501	-1.419256	-0.129361
H	-0.959812	1.917737	-0.321687
H	-1.298757	-1.039140	-1.577077
C	1.707309	1.957038	0.214169
H	2.567687	2.492750	0.622357
H	2.032134	0.951996	-0.053433
H	1.418992	2.467751	-0.712888
C	0.251382	3.337950	1.741991
H	-0.545405	3.317402	2.488172
H	1.138134	3.771580	2.210993
H	-0.057437	4.021476	0.942254

NO-8

Eopt -343.262189

N	-0.679606	0.077750	0.097564
O	0.541568	-1.686497	-0.031191
C	-0.835450	1.451235	0.545238
H	-1.660484	1.518357	1.223259
C	-1.745643	-0.608142	-0.620837
H	-2.575124	0.056430	-0.744150
N	0.449607	-0.518618	0.364802
C	0.460520	1.875915	1.260576

H	0.367103	2.887265	1.597244
H	0.631016	1.234835	2.100127
H	1.283887	1.800717	0.581377
C	-1.242401	-1.059069	-2.004677
H	-1.030276	-2.107603	-1.982784
H	-1.995165	-0.862727	-2.739317
H	-0.352107	-0.520182	-2.253428
H	-2.057388	-1.464566	-0.060253
H	-1.007894	2.087985	-0.297206

NO-9

Eopt -500.588874

N	-0.809989	0.793176	-1.037198
C	-0.874258	1.496597	0.252714
H	-1.691842	2.222151	0.198230
H	-1.156304	0.750829	0.997563
C	-1.792343	-0.250812	-1.346221
H	-2.184058	-0.045000	-2.342846
H	-2.604722	-0.142735	-0.626554
C	-1.222445	-1.676114	-1.296101
H	-0.397899	-1.720052	-2.011675
C	-2.304244	-2.662259	-1.740091
H	-1.916247	-3.682431	-1.744511
H	-3.159475	-2.633035	-1.058782
H	-2.665397	-2.434023	-2.745207
C	-0.683212	-2.030250	0.090417
H	0.120245	-1.358799	0.394685
H	-1.475314	-1.976795	0.842824
H	-0.284978	-3.046634	0.096473
C	0.415372	2.189449	0.697843
H	0.704466	2.906461	-0.072840
C	1.562632	1.197629	0.898835
H	1.791490	0.649373	-0.015183
H	2.467812	1.721967	1.210622
H	1.311913	0.472256	1.677799
C	0.128378	2.962953	1.988454
H	1.024212	3.488044	2.323856
H	-0.662433	3.702405	1.845713
H	-0.181574	2.286139	2.789642
N	0.017281	1.244634	-1.938792
O	-0.021895	0.688816	-3.044143

NO-10

Eopt -421.925200

N	-0.575707	0.034989	0.033761
O	0.700525	-1.693118	-0.169093
C	-0.756543	1.432980	0.478770
H	-1.679365	1.429767	1.067189
C	-1.709397	-0.680254	-0.599819

H	-2.508306	0.056300	-0.600497
N	0.577614	-0.530466	0.241633
C	0.382141	1.897488	1.374941
H	0.136034	2.895823	1.739197
H	0.518338	1.238149	2.232276
H	1.325348	1.949259	0.829166
C	-0.928700	2.362274	-0.729061
H	-1.800786	2.108998	-1.332318
H	-1.051525	3.389415	-0.382749
H	-0.042413	2.316720	-1.365925
C	-1.409205	-1.054487	-2.060587
H	-1.044143	-2.077692	-2.140664
H	-2.316429	-0.959252	-2.660005
H	-0.655634	-0.391348	-2.485819
C	-2.192271	-1.861625	0.253959
H	-3.244183	-2.056900	0.035876
H	-1.618517	-2.764162	0.051652
H	-2.107533	-1.630142	1.316922

NO-11

Eopt -655.498360

N	-0.716741	1.185671	-1.029157
C	-1.411233	0.081650	-1.717340
C	-0.834855	-1.280428	-1.311788
C	-2.927441	0.152296	-1.498172
H	-1.208685	0.239806	-2.775369
C	-1.551306	-2.408972	-2.060314
H	-0.956340	-1.431394	-0.234899
H	0.236907	-1.298056	-1.520553
C	-3.629777	-0.986053	-2.245235
H	-3.154295	0.073677	-0.430640
H	-3.298546	1.122367	-1.835572
C	-3.065672	-2.351384	-1.843959
H	-1.154707	-3.373389	-1.734769
H	-1.336023	-2.324066	-3.131066
H	-4.703845	-0.943680	-2.050425
H	-3.498436	-0.843889	-3.323464
H	-3.557880	-3.144250	-2.412311
H	-3.286031	-2.535858	-0.786408
C	-0.757713	1.318404	0.441361
C	0.633463	1.176524	1.067753
C	-1.445258	2.615374	0.880288
H	-1.367215	0.483069	0.786724
C	0.548775	1.260854	2.594203
H	1.272263	1.977027	0.685647
H	1.078672	0.228900	0.756368
C	-1.522837	2.695087	2.407394
H	-0.874230	3.462707	0.492070
H	-2.443111	2.666334	0.438756

C	-0.139040	2.551618	3.047026
H	1.551532	1.191536	3.022130
H	-0.014402	0.400032	2.972093
H	-1.984662	3.639977	2.702905
H	-2.175994	1.896668	2.777460
H	-0.223161	2.572032	4.136344
H	0.480376	3.408940	2.760596
N	-0.029557	2.103773	-1.655563
O	0.035110	2.034400	-2.889029

NO-12

Eopt -342.050468

C	0.593432	-0.264129	0.151333
C	1.985208	-0.214854	-0.390442
C	2.363020	1.126221	0.279042
C	0.070914	1.158235	-0.164041
H	-0.044275	-1.045009	-0.207075
H	0.700455	-0.372857	1.210400
H	2.018830	-0.153800	-1.458169
H	2.589916	-1.048258	-0.099468
H	2.279057	1.059713	1.343668
H	3.352049	1.462011	0.046737
H	-0.581572	1.437083	0.636837
H	-0.455947	1.252249	-1.090582
N	1.323005	1.980041	-0.305342
N	1.658893	2.085759	-1.660334
O	1.801926	3.164276	-2.159007

NO-13

Eopt -381.385286

C	0.514387	-0.239786	0.154849
C	2.011460	-0.447336	-0.124660
C	2.590718	0.961505	0.008133
C	0.193083	1.100828	-0.513172
H	-0.105703	-1.045974	-0.232814
H	0.341598	-0.168638	1.230374
H	2.158603	-0.813817	-1.142672
H	2.480229	-1.149704	0.562077
H	3.487558	1.137556	-0.581353
H	-0.558025	1.694233	0.006685
H	-0.125455	0.994428	-1.552786
N	1.488608	1.796750	-0.487701
N	1.693017	3.000902	-0.911003
O	0.688708	3.595302	-1.334545
C	2.880196	1.312315	1.479437
H	3.395891	0.498715	1.945284
H	3.487984	2.191835	1.523466
H	1.957845	1.490139	1.991829

NO-14

Eopt -420.718520

C	0.460512	-0.232887	0.128103
C	1.965467	-0.458689	-0.088868
C	2.579226	0.942557	0.050287
C	0.185267	1.110577	-0.551180
H	-0.148570	-1.031701	-0.290727
H	0.234937	-0.165693	1.193157
H	2.145146	-0.841093	-1.095377
H	2.397156	-1.160937	0.622406
H	3.447858	1.072562	-0.594275
H	-0.092170	1.007440	-1.603023
N	1.486678	1.788816	-0.473568
N	1.718853	2.992547	-0.882894
O	0.737413	3.603380	-1.335705
C	2.939210	1.322365	1.483852
H	3.762259	0.697328	1.833175
H	3.250420	2.366198	1.535024
H	2.089774	1.181981	2.154578
C	-0.895004	1.964505	0.138328
H	-1.383735	2.577466	-0.589903
H	-1.613305	1.322780	0.604303
H	-0.438549	2.586582	0.879657

NO-15

Eopt -420.718593

C	0.460512	-0.232887	0.128103
C	1.965467	-0.458689	-0.088868
C	2.579226	0.942557	0.050287
C	0.185267	1.110577	-0.551180
H	-0.148570	-1.031701	-0.290727
H	0.234937	-0.165693	1.193157
H	2.145146	-0.841093	-1.095377
H	2.397156	-1.160937	0.622406
H	3.447858	1.072562	-0.594275
N	1.486678	1.788816	-0.473568
N	1.718853	2.992547	-0.882894
O	0.737413	3.603380	-1.335705
C	2.939210	1.322365	1.483852
H	3.762259	0.697328	1.833175
H	3.250420	2.366198	1.535024
H	2.089774	1.181981	2.154578
H	-0.560530	1.659920	-0.015540
C	-0.234690	0.903508	-2.018272
H	-0.744186	-0.032447	-2.114716
H	-0.886793	1.697120	-2.318010
H	0.635119	0.901979	-2.641432

NO-16

Eopt -381.386677

C	-1.462834	-1.692638	-0.107709
C	-0.720969	-0.372271	0.073686
C	-2.694005	0.455753	1.334859
C	-3.339629	-0.903295	1.075217
H	0.346645	-0.531181	0.213302
H	-1.204450	-2.380897	0.707099
H	-1.187060	-2.149530	-1.056983
H	-2.948769	0.833688	2.321200
H	-3.013154	1.178537	0.579757
H	-3.130654	-1.577622	1.915056
H	-4.418085	-0.788026	0.976837
H	-0.879791	0.262757	-0.801995
N	-1.241178	0.311269	1.249758
N	-0.385217	0.734235	2.147325
O	-0.850563	1.316304	3.128568
C	-2.871249	-1.481046	-0.139425
H	-3.360793	-2.420672	-0.288927
H	-3.106031	-0.823557	-0.950280

NO-17

Eopt -417.293345

C	-1.369760	-1.612761	0.046869
C	-0.808346	-0.179064	0.015755
C	-2.770637	0.587255	1.117254
C	-3.306174	-0.856547	1.133843
H	0.260701	-0.214318	0.043981
H	-1.055129	-2.099250	0.946444
H	-1.004022	-2.155743	-0.799480
H	-3.155622	1.119833	1.961676
H	-3.082903	1.072968	0.216437
H	-2.991073	-1.343221	2.033154
H	-4.375250	-0.839202	1.092903
H	-1.125669	0.308624	-0.882224
O	-2.799480	-1.571049	0.002215
N	-1.303137	0.567279	1.180264
N	-0.894941	-0.075861	2.354890
O	-0.219518	0.507095	3.152572

NO-18

Eopt -420.713396

N	-0.454641	0.095638	-0.064196
O	0.592368	-1.893894	0.051500
C	-0.897575	1.077933	0.868202
C	-1.657092	-0.723262	-0.428583
H	-1.827536	-1.510025	0.276295
N	0.525049	-0.765452	0.444461
H	-1.457030	-1.138764	-1.394105

C	-1.694223	2.153389	0.065843
H	-2.306051	2.664328	0.779641
H	-1.056622	2.855696	-0.429263
C	-2.954483	0.157293	-0.447512
H	-3.708537	-0.348029	-1.014038
H	-3.329258	0.350048	0.535997
C	-2.540489	1.459620	-1.036647
H	-3.354310	2.099249	-1.307702
H	-1.965242	1.239636	-1.911631
H	-1.526599	0.579208	1.575665
C	0.258591	1.767896	1.615752
H	-0.138489	2.490633	2.297572
H	0.819504	1.035993	2.158517
H	0.898067	2.256452	0.910569

NO-19

Eopt -460.047674

N	-0.614734	-0.071725	0.252850
O	0.783591	-1.476076	-0.606220
C	-0.887335	1.177761	0.984026
C	-1.769789	-0.841127	-0.263462
N	0.618138	-0.426497	0.034280
H	-1.457235	-1.204201	-1.244004
C	-1.587900	2.170931	0.036052
H	-2.160648	2.865457	0.654028
H	-0.831693	2.758471	-0.489127
C	-2.964665	0.104355	-0.437855
H	-3.672153	-0.371258	-1.118899
H	-3.487591	0.234243	0.514191
C	-2.505572	1.458090	-0.976773
H	-3.363271	2.086411	-1.219234
H	-1.963686	1.293409	-1.912247
H	-1.593411	0.895146	1.769916
C	0.342288	1.772237	1.648700
H	0.032312	2.658414	2.204513
H	0.802853	1.070437	2.343566
H	1.088652	2.070513	0.913437
C	-2.071511	-2.032985	0.640822
H	-2.917488	-2.592862	0.238245
H	-1.212902	-2.699408	0.706198
H	-2.333374	-1.695339	1.645572

NO-20

Eopt -495.739031

N	-0.494391	0.244294	-0.308332
C	-0.852571	1.393147	0.535910
H	0.033937	1.929203	0.803582
H	-1.511634	2.040645	-0.003796
H	-1.340731	1.045834	1.422461

C	-1.712304	-0.492156	-0.676067
H	-2.371367	0.155341	-1.215773
H	-2.200464	-0.839470	0.210484
C	-1.337068	-1.695717	-1.560511
C	-1.285042	-1.552357	-2.953588
C	-1.047629	-2.934316	-0.972278
C	-0.943576	-2.647597	-3.758431
H	-1.506034	-0.606658	-3.402717
C	-0.706163	-4.029556	-1.777121
H	-1.087353	-3.043775	0.091367
C	-0.654136	-3.886196	-3.170198
H	-0.903852	-2.538138	-4.822076
H	-0.485170	-4.975254	-1.327992
H	-0.393418	-4.722435	-3.784714
N	0.144324	0.698724	-1.468305
O	0.788534	1.706974	-1.440817

NO-21

Eopt -570.986075

N	-1.157742	1.075697	-0.871726
C	-0.381420	0.991572	0.373724
H	0.317591	1.800701	0.413638
H	-1.044052	1.051024	1.211748
H	0.147279	0.061755	0.402339
C	-2.118065	-0.035911	-0.926561
C	-1.816100	-1.254145	-0.303148
C	-3.335539	0.122591	-1.602251
C	-2.731609	-2.313877	-0.355422
H	-0.886531	-1.375164	0.212757
C	-4.251047	-0.937143	-1.654528
H	-3.566097	1.052739	-2.078241
C	-3.949082	-2.155376	-1.031112
H	-2.501053	-3.244024	0.120571
H	-5.180614	-0.816124	-2.170434
N	-0.290747	0.997909	-1.968206
O	0.180857	1.996162	-2.430171
O	-4.883275	-3.236735	-1.084453
C	-5.768849	-3.157277	0.035522
H	-6.297548	-2.227460	0.006906
H	-6.467861	-3.966406	-0.004391
H	-5.203772	-3.218510	0.942075

NO-22

Eopt -456.410107

N	-0.489359	0.235821	-0.427952
C	-0.762275	1.169608	0.674073
H	0.137585	1.686581	0.934632
H	-1.503830	1.877087	0.366715
H	-1.119232	0.624851	1.523026

N	-0.022313	0.948587	-1.538732
O	1.150966	1.140240	-1.676636
C	-1.725616	-0.474413	-0.785917
C	-2.047762	-1.682740	-0.153392
C	-2.582033	0.056825	-1.759702
C	-3.226327	-2.359829	-0.494650
H	-1.393868	-2.088353	0.590114
C	-3.760599	-0.620263	-2.100960
H	-2.336066	0.979410	-2.242650
C	-4.082746	-1.828590	-1.468434
H	-3.472294	-3.282413	-0.011703
H	-4.414493	-0.214650	-2.844465
H	-4.982606	-2.345563	-1.728993

NO-23

Eopt -301.424719

N	-0.501122	0.216000	-0.289980
C	-0.844840	1.370586	0.552451
H	0.051032	1.874593	0.849580
H	-1.465906	2.043582	-0.000954
H	-1.369844	1.033996	1.421921
C	-1.731903	-0.476418	-0.698187
C	-2.713942	-1.080692	-1.034840
H	-3.588719	-1.618962	-1.334723
N	0.185794	0.656392	-1.427610
O	1.338301	0.371273	-1.578493

NO-24

Eopt -548.693289

N	-1.165572	1.080176	-0.871722
C	-0.372573	0.992539	0.361862
H	0.320844	1.807268	0.397048
H	-1.022766	1.040273	1.209307
H	0.164600	0.066882	0.375822
C	-2.121425	-0.037311	-0.922215
C	-1.798447	-1.259572	-0.310562
C	-3.348211	0.113477	-1.577599
C	-2.705505	-2.326760	-0.355997
H	-0.859922	-1.376868	0.190872
C	-4.255030	-0.953843	-1.623749
H	-3.593346	1.044657	-2.042944
C	-3.933996	-2.173760	-1.012985
H	-2.460402	-3.257998	0.110590
H	-5.192852	-0.836929	-2.125736
C	-4.931028	-3.346168	-1.063644
N	-5.673457	-4.219185	-1.101378
N	-0.303000	1.012785	-1.971389
O	0.201245	2.011734	-2.396857

NO-25

Eopt -562.453777

N	-0.514430	0.251514	-0.286694
C	-0.890991	1.396635	0.554614
H	-0.009568	1.923729	0.854889
H	-1.527427	2.053335	-0.000899
H	-1.410075	1.046365	1.422233
C	-1.725357	-0.472624	-0.699221
F	-2.380275	-0.914554	0.395438
F	-1.379535	-1.524266	-1.471851
F	-2.528336	0.355922	-1.400103
N	0.164745	0.709812	-1.421897
O	1.355402	0.828822	-1.399481

PABA

Eopt -476.404571

N	-0.444806	0.216876	-0.169634
C	-0.776524	1.297121	0.770544
C	-1.659745	1.055998	1.831535
C	-0.209540	2.568077	0.605855
C	-1.975984	2.085832	2.727837
H	-2.092648	0.085594	1.957279
C	-0.525779	3.597911	1.502158
H	0.464816	2.752180	-0.204236
C	-1.409001	3.356788	2.563149
H	-2.650344	1.901730	3.537926
H	-0.092876	4.568314	1.376414
C	-1.756514	4.488473	3.548097
O	-2.576650	4.264574	4.533302
O	-1.247384	5.629739	3.400216
H	-2.793281	4.970039	5.147296
H	0.193927	0.559165	-0.858734
H	-1.279482	-0.102578	-0.618260

TS-29

Eopt -811.526682

N	-0.557180	0.348323	-0.225857
O	0.959795	-1.552234	0.183708
N	1.002781	-0.418865	0.274568
H	-0.171712	0.767688	-1.357419
O	0.475911	1.132012	-2.335832
N	1.616472	0.596273	-2.028366
O	2.517327	0.751518	-2.809514
C	-0.876831	1.353078	0.705763
C	-1.804600	1.129870	1.739403
C	-0.211080	2.590577	0.617027
C	-2.073354	2.135873	2.663243
H	-2.316038	0.167056	1.811420
C	-0.475288	3.586385	1.551078

H	0.500814	2.760493	-0.191948
C	-1.407489	3.371049	2.579747
H	-2.797941	1.963836	3.459695
H	0.033317	4.550192	1.493233
H	-1.217153	-0.435141	-0.240536
C	-1.655956	4.473964	3.550746
O	-2.563728	4.155086	4.488729
O	-1.104532	5.554372	3.514047
H	-2.666670	4.922201	5.078780

NO-PABA

Eopt -605.751592

N	-0.444806	0.216876	-0.169634
C	-0.776524	1.297121	0.770544
C	-1.659745	1.055998	1.831535
C	-0.209540	2.568077	0.605855
C	-1.975984	2.085832	2.727837
H	-2.092648	0.085594	1.957279
C	-0.525779	3.597911	1.502158
H	0.464816	2.752180	-0.204236
C	-1.409001	3.356788	2.563149
H	-2.650344	1.901730	3.537926
H	-0.092876	4.568314	1.376414
C	-1.756514	4.488473	3.548097
O	-2.576650	4.264574	4.533302
O	-1.247384	5.629739	3.400216
H	-2.793281	4.970039	5.147296
H	0.480978	0.354140	-0.521886
N	-1.355181	0.227910	-1.233164
O	-1.632722	-0.792327	-1.793893

H₃O⁺

Eopt -76.861459

H	-1.658607	-0.617755	-0.077309
H	-1.658590	0.796458	0.739187
H	-1.658590	0.796458	-0.893806
O	-1.991929	0.325058	-0.077309

4-Carboxybenzenediazonium

Eopt -529.719191

N	-0.967238	0.453073	-0.432460
C	-1.086493	1.470607	0.621811
C	-1.906854	1.228725	1.731956
C	-0.383741	2.678772	0.519828
C	-2.020588	2.163152	2.706880
H	-2.443422	0.306265	1.809822
C	-0.497475	3.613199	1.494752
H	0.242625	2.863454	-0.327792
C	-1.317837	3.371317	2.604896

H	-2.646953	1.978469	3.554500
H	0.039094	4.535658	1.416886
C	-1.447079	4.433165	3.712766
O	-2.284183	4.186346	4.845567
O	-0.816036	5.518047	3.621189
H	-2.632860	5.018621	5.173199
N	-0.857147	-0.282066	-1.232495

Aniline

Eopt -287.732312

N	-0.465281	0.217443	-0.162052
H	-0.154678	0.609730	-1.027867
C	-0.787873	1.299994	0.778648
C	-1.778322	1.110666	1.751833
C	-0.104963	2.521354	0.702264
C	-2.085859	2.142698	2.648634
H	-2.299739	0.178131	1.810154
C	-0.412500	3.553386	1.599066
H	0.651266	2.665911	-0.040785
C	-1.402948	3.364058	2.572251
H	-2.842087	1.998142	3.391684
H	0.108919	4.485921	1.540746
H	-1.280451	-0.339328	-0.321757
H	-1.637758	4.152037	3.256980

TS-30

N	-0.507107	0.273812	-0.122759
O	1.066537	-1.583596	0.089928
N	1.041622	-0.488239	0.361145
H	-0.204808	0.645208	-1.253845
O	0.293447	1.025012	-2.366224
N	1.557085	0.845038	-2.120744
O	2.311854	1.123369	-3.023819
C	-0.825069	1.304716	0.782001
C	-1.830926	1.141095	1.737659
C	-0.091494	2.493656	0.729687
C	-2.115979	2.168510	2.620336
H	-2.390744	0.215572	1.780435
C	-0.373279	3.510868	1.623373
H	0.688282	2.613008	-0.009649
C	-1.388412	3.361245	2.571417
H	-2.900631	2.043558	3.351960
H	0.186488	4.435048	1.591797
H	-1.173811	-0.496240	-0.117076
H	-1.607583	4.154252	3.255525

NO-Aniline

Eopt -417.084471

N	-0.444806	0.216876	-0.169634
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C	-0.776524	1.297121	0.770544
C	-1.659745	1.055998	1.831535
C	-0.209540	2.568077	0.605855
C	-1.975984	2.085832	2.727837
H	-2.092648	0.085594	1.957279
C	-0.525779	3.597911	1.502158
H	0.464816	2.752180	-0.204236
C	-1.409001	3.356788	2.563149
H	-2.650344	1.901730	3.537926
H	-0.092876	4.568314	1.376414
H	0.480978	0.354140	-0.521886
N	-1.355181	0.227910	-1.233164
O	-1.632722	-0.792327	-1.793893
H	-1.650455	4.143089	3.247496

Benzenediazonium

Eopt -341.060717

N	-0.949382	0.534461	-0.324376
C	-1.082057	1.493707	0.660969
C	-1.933700	1.210231	1.731848
C	-0.360700	2.682553	0.516339
C	-2.062408	2.181616	2.705510
H	-2.464130	0.271349	1.786307
C	-0.514013	3.628810	1.508771
H	0.282513	2.843523	-0.335760
C	-1.358452	3.383978	2.594868
H	-2.710535	2.004895	3.549989
H	0.017628	4.567077	1.450406
N	-0.848161	-0.227754	-1.107395
H	-1.467976	4.129485	3.354555

Varenicline

Eopt -667.733562

N	-2.031966	-0.000308	1.515758
N	3.308419	-1.362902	0.089873
N	3.308449	1.362791	0.090467
C	-1.635801	-1.160227	-0.606294
C	-1.635775	1.160526	-0.605789
C	-2.179451	0.000332	-1.415897
C	-0.174462	-0.700237	-0.401891
C	-0.174447	0.700416	-0.401587
C	-2.344616	-1.233397	0.758249
C	-2.344589	1.233118	0.758786
C	0.949796	-1.420669	-0.242858
C	0.949826	1.420754	-0.242239
C	2.156014	-0.708104	-0.072578
C	2.156030	0.708089	-0.072269
C	4.450226	-0.680088	0.251103
C	4.450241	0.679883	0.251399

H	-2.549995	-0.000488	2.371121
H	-1.746775	-2.097195	-1.110947
H	-1.746730	2.097717	-1.110034
H	-1.748672	0.000541	-2.395351
H	-3.244136	0.000367	-1.522415
H	-3.398975	-1.331213	0.604432
H	-1.988216	-2.074649	1.315181
H	-1.988171	2.074120	1.316084
H	-3.398946	1.331024	0.605011
H	0.930627	-2.490494	-0.245309
H	0.930681	2.490581	-0.244225
H	5.370697	-1.209994	0.380849
H	5.370723	1.209712	0.381376

TS-31

Eopt	-1002.883364		
N	-2.181174	-0.337238	1.382531
N	3.432469	-1.087936	-0.191906
N	3.340757	1.608430	0.651963
C	-1.521612	-0.768069	-0.994161
C	-1.603796	1.481441	-0.246781
C	-2.169773	0.584597	-1.370605
C	-0.109819	-0.335064	-0.640047
C	-0.155883	1.027562	-0.208613
C	-2.229879	-1.304841	0.263595
C	-2.300239	1.100991	1.078229
C	1.065692	-1.047455	-0.629418
C	0.972047	1.678013	0.225750
C	2.258674	-0.398527	-0.197065
C	2.211775	0.974255	0.232180
C	4.503057	-0.445670	0.221296
C	4.456621	0.912412	0.646622
H	-2.999099	-0.662963	2.154999
H	-1.566722	-1.531036	-1.783506
H	-1.728081	2.559950	-0.415079
H	-1.818297	0.926319	-2.355458
H	-3.269453	0.548438	-1.385242
H	-3.287277	-1.522909	0.046623
H	-1.762236	-2.231166	0.629824
H	-1.866371	1.644931	1.932427
H	-3.371947	1.352394	1.039781
H	1.123108	-2.092340	-0.941762
H	0.957311	2.712738	0.574353
H	5.456715	-0.986169	0.233387
H	5.374887	1.407574	0.983373
N	-0.817495	-0.721340	2.276565
O	-0.376209	0.191726	2.829978
O	-3.752747	-1.201494	3.127758
N	-2.778040	-1.711545	3.791515

O	-3.054666	-2.329767	4.795486
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NO-Varenicline

Eopt	-797.103548		
N	-2.255857	-0.094829	1.450755
N	3.305547	-1.407886	0.088392
N	3.278575	1.406422	0.190363
C	-1.638535	-1.202568	-0.670452
C	-1.661532	1.163352	-0.586446
C	-2.247271	0.003405	-1.417454
C	-0.219251	-0.725592	-0.450231
C	-0.232663	0.697589	-0.399707
C	-2.364739	-1.339592	0.682234
C	-2.374653	1.208456	0.780547
C	0.936140	-1.430983	-0.282845
C	0.909062	1.410995	-0.180757
C	2.144485	-0.720154	-0.066670
C	2.130809	0.709604	-0.014929
C	4.394376	-0.702964	0.288146
C	4.380833	0.709865	0.339437
H	-1.710024	-2.146849	-1.207276
H	-1.747382	2.140992	-1.057723
H	-1.887633	0.044255	-2.446129
H	-3.337812	-0.006798	-1.429438
H	-3.420023	-1.562842	0.504016
H	-1.937623	-2.130386	1.295043
H	-1.931630	1.950633	1.438948
H	-3.432368	1.450843	0.648310
H	0.966285	-2.512894	-0.314268
H	0.918620	2.492771	-0.134747
H	5.328343	-1.239829	0.415703
H	5.304399	1.253909	0.506291
N	-2.022389	-0.227332	2.734534
O	-1.963936	0.807255	3.400534

TTP

Eopt	-751.698860		
F	6.692421	-0.906238	0.782707
F	7.743470	0.850220	-0.035920
F	6.960509	-0.698422	-1.395581
N	1.549387	-0.437702	0.433013
N	4.217094	0.247421	0.014154
N	3.866522	2.211719	-0.670020
N	5.248520	1.937149	-0.776222
C	2.582313	-1.086477	1.267510
C	3.901676	-1.108389	0.466857
C	1.882933	0.997168	0.340968
C	3.338968	1.161526	-0.121422
C	5.403566	0.727247	-0.335631

C	6.741251	-0.030160	-0.243257
H	0.644077	-0.530796	0.847436
H	2.301010	-2.092347	1.499879
H	2.698062	-0.533024	2.175911
H	4.696733	-1.497555	1.067967
H	3.767862	-1.730442	-0.393401
H	1.785457	1.429658	1.314801
H	1.219549	1.491572	-0.337550

TS-32

Eopt -1086.834079

N	-0.618890	0.502381	-0.672949
O	-0.637833	-1.166587	1.047547
C	-1.026573	1.909163	-0.549719
H	-0.976369	2.367954	-1.550312
C	-1.497725	-0.376728	-1.440449
H	-1.336430	-1.412831	-1.097510
N	-0.337492	-0.062777	0.922896
H	0.518883	0.463311	-1.075794
O	1.802303	0.398736	-1.213006
N	2.063348	0.055976	-0.000304
O	3.220121	-0.107283	0.298150
H	-0.292287	2.416879	0.090520
H	-1.202906	-0.347069	-2.502281
C	-2.423016	2.054850	0.047361
H	-2.423723	1.819230	1.122405
H	-2.788199	3.081556	-0.081809
N	-3.326514	1.130934	-0.639673
C	-2.940261	-0.004483	-1.288998
N	-3.988967	-0.652070	-1.748917
N	-5.098734	0.062381	-1.393655
C	-4.689448	1.116741	-0.731265
C	-5.561258	2.183483	-0.138087
F	-6.849562	1.927024	-0.345153
F	-5.276319	3.388978	-0.670112
F	-5.353198	2.287255	1.188645

NTTP

Eopt -881.057515

F	6.692421	-0.906238	0.782707
F	7.743470	0.850220	-0.035920
F	6.960509	-0.698422	-1.395581
N	1.549387	-0.437702	0.433013
N	4.217094	0.247421	0.014154
N	3.866522	2.211719	-0.670020
N	5.248520	1.937149	-0.776222
C	2.582313	-1.086477	1.267510
C	3.901676	-1.108389	0.466857
C	1.882933	0.997168	0.340968

C	3.338968	1.161526	-0.121422
C	5.403566	0.727247	-0.335631
C	6.741251	-0.030160	-0.243257
H	2.301010	-2.092347	1.499879
H	2.698062	-0.533024	2.175911
H	4.696733	-1.497555	1.067967
H	3.767862	-1.730442	-0.393401
H	1.785457	1.429658	1.314801
H	1.219549	1.491572	-0.337550
N	0.281953	-0.568033	1.013205
O	-0.590308	-1.137323	0.423797