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Electronic Supplementary Information

A fully diastereoselective oxidation of a mesoionic dipole with triplet molecular oxygen

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Contents:

Figures S1-S12 and Table S1.

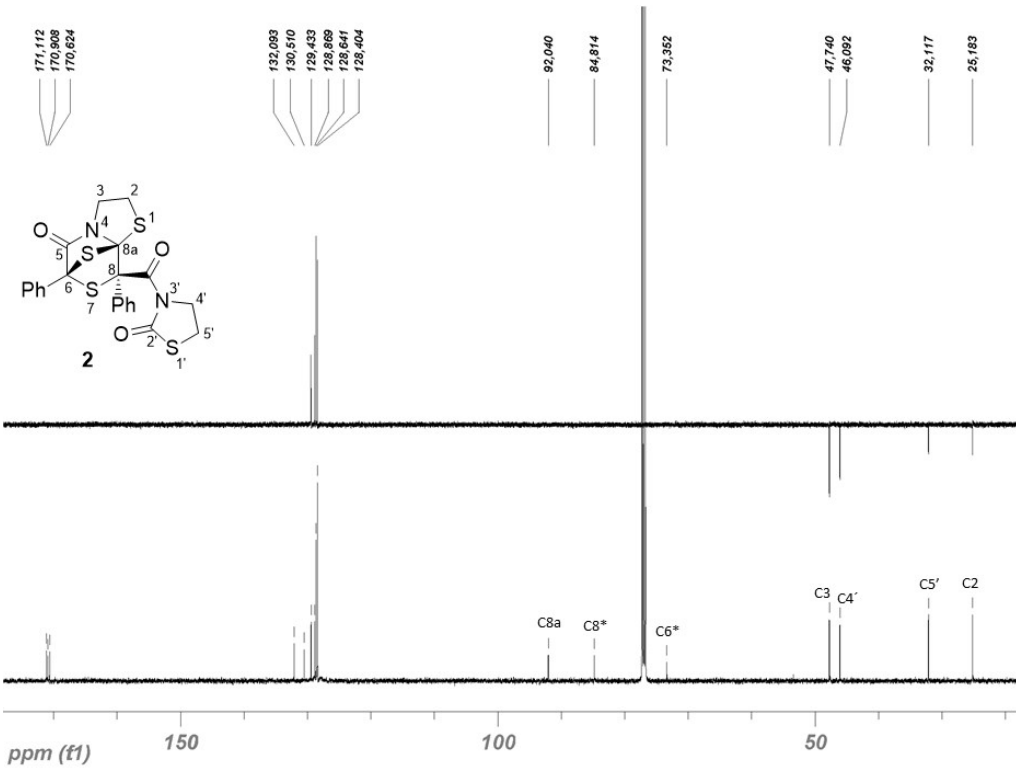


Figure S1 ^{13}C NMR and DEPT spectra of **2** recorded in $CDCl_3$ (125 MHz).
*The carbon resonances attributed to C6 and C8 may be interchanged.

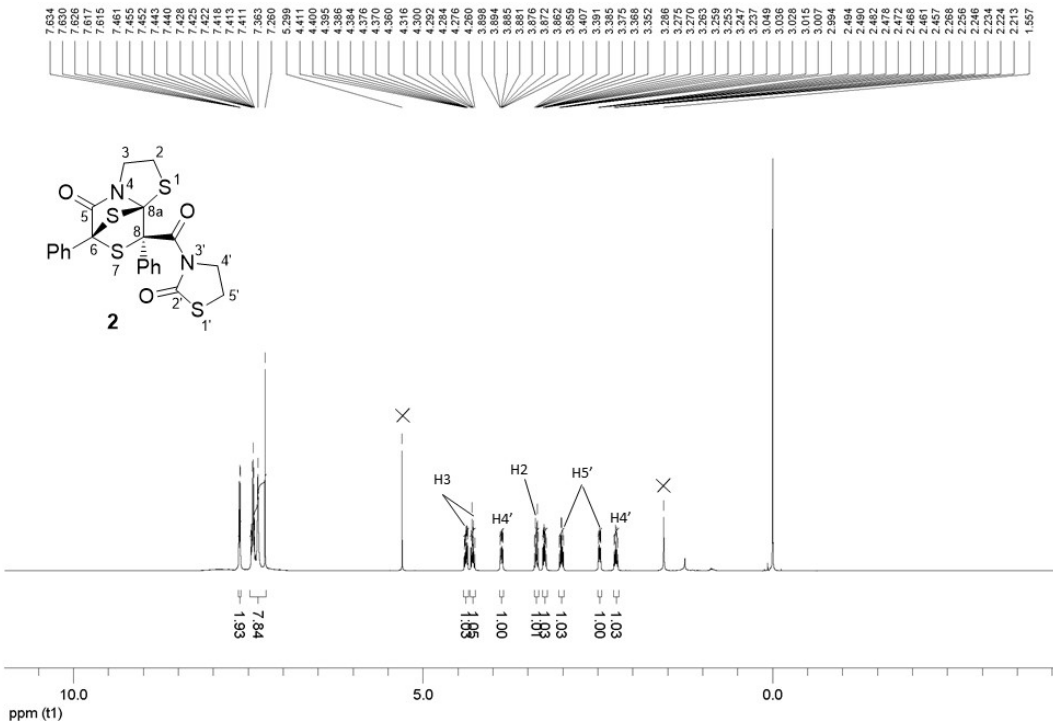


Figure S2 ^{1}H NMR spectrum of **2** recorded in $CDCl_3$ (500 MHz).

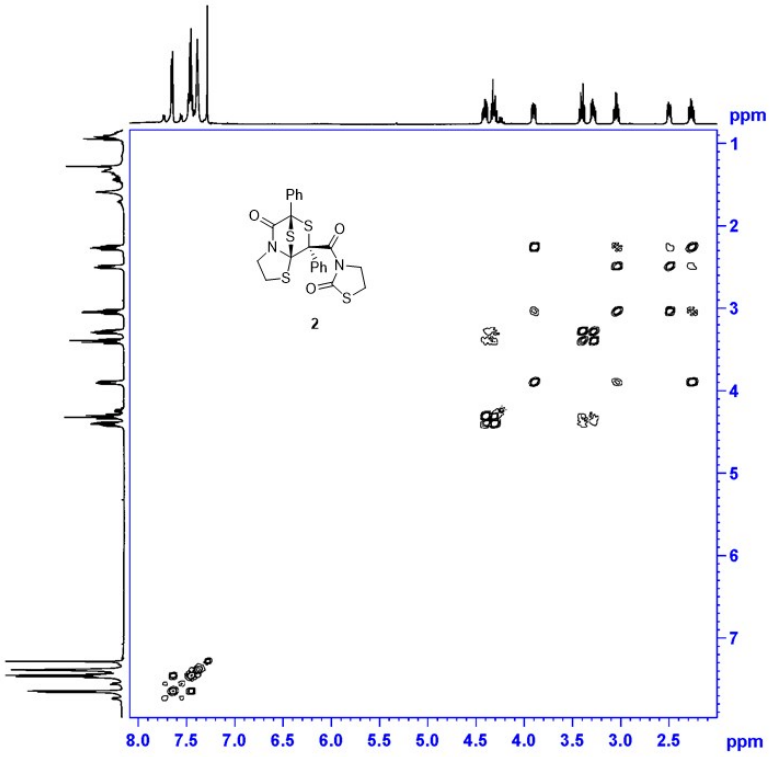


Figure S3 COSY spectrum of **2** recorded in $CDCl_3$.

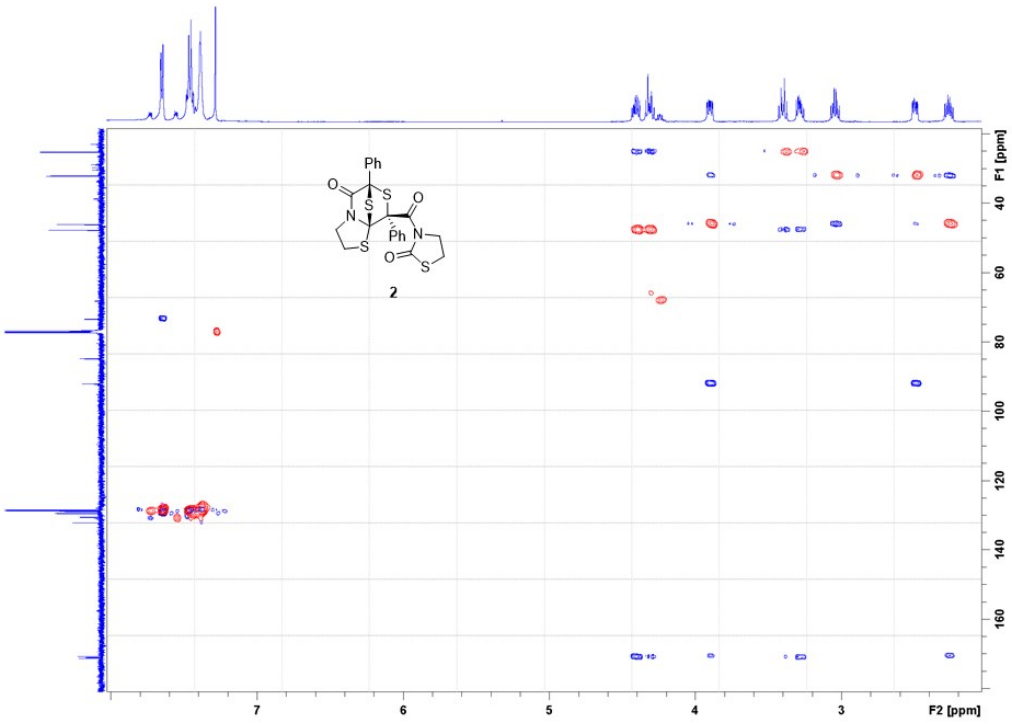


Figure S4 HMBC and HSQC spectra of **2** recorded in $CDCl_3$.

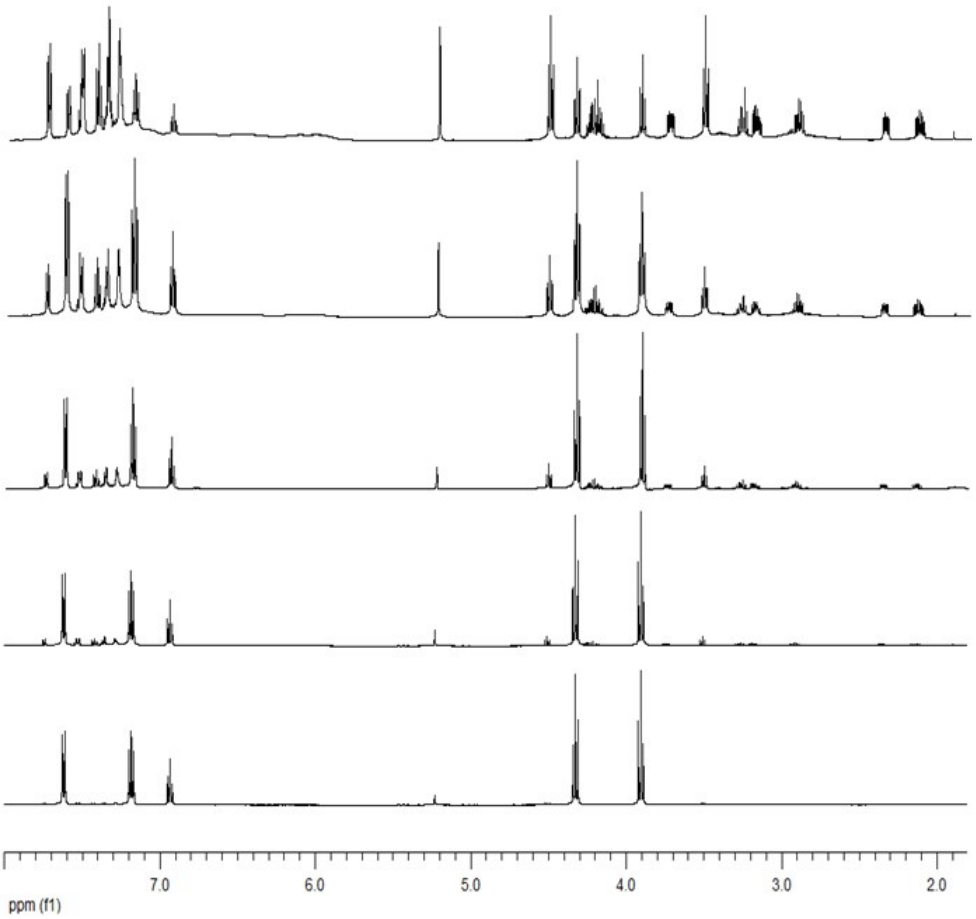


Figure S5 ^{1}H NMR monitoring showing the chemical transformation of **1**. Spectra were recorded in CD_2Cl_2 (500 MHz) every 24 h.

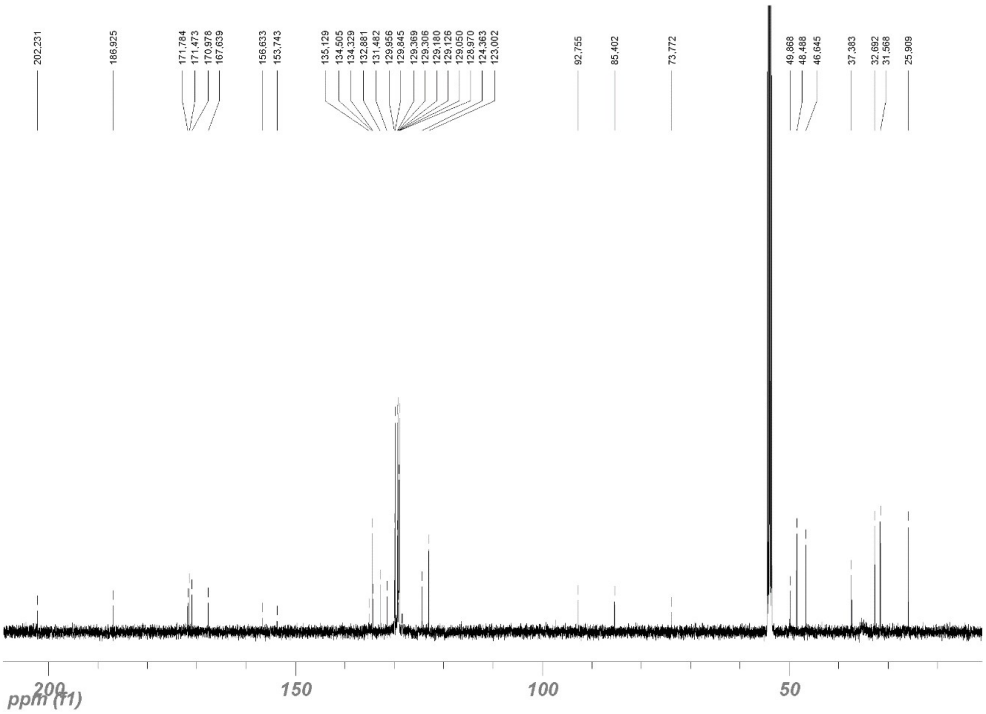


Figure S6 ^{13}C NMR spectrum of **1**, after 5-d reaction, recorded in CD_2Cl_2 (125 MHz).

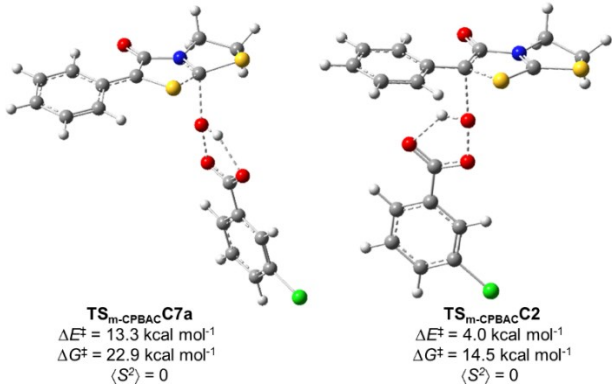


Figure S7 Optimized geometries of the saddle points corresponding to the attack of *m*-CPBA to mesoionic dipole **1** at C2 and C7a (**TS$_{m\text{-CPBA}}$C2** and **TS$_{m\text{-CPBA}}$C7a** respectively) at (U)B3LYP-D3BJ/def2-TZVP in CH_2Cl_2 (SMD). Relative electronic and free energies are given with respect to the reagents in kcal mol^{-1}. Eigenvalues of the total spin operator [$\langle S^2 \rangle$] are given without the spin annihilation diagnostic.

To understand the enhanced reactivity of the C2 atom of dipole **1** with *m*-CPBA, a frontier molecular orbital (FMO) analysis of both reagents was undertaken. HOMO and LUMO orbitals of the mesoionic ring are largely localized at C2 and C7a, respectively. As a result, the electronic demand of both reactions should be different. The only virtual orbital of the peroxoacid capable of reacting with the HOMO of **1** is the σ*(O-O) (LUMO+2), which turned to be the most favorable interaction found (LUMO+2$_{m\text{-CPBA}}$-HOMO$_{\mathbf{1}}$ = 0.17 eV) (**TS$_{m\text{-CPBA}}$C2**), *versus* the HOMO$_{m\text{-CPBA}}$-LUMO$_{\mathbf{1}}$ (0.20 eV) (**TS$_{m\text{-CPBA}}$C7a**) (Fig. S8).

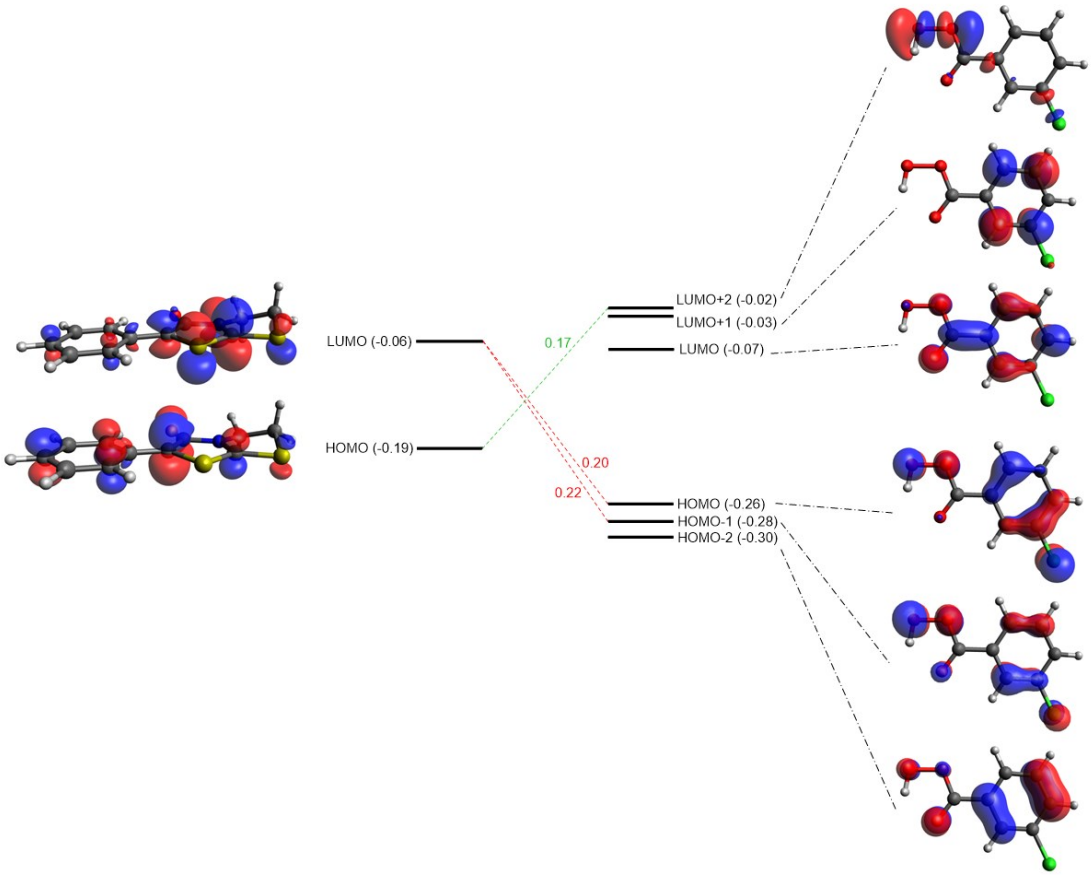
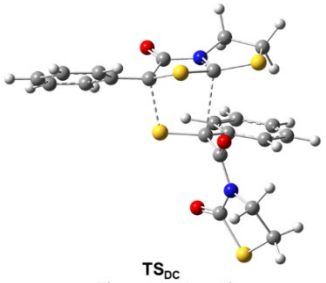


Figure S8 FMOs of **1** and *m*-CPBA, and energy gaps in eV. LUMO$_{\mathbf{1}}$-HOMO-1$_{m\text{-CPBA}}$ gap is also shown, because such orbitals should also be interacting as the reaction progresses.



TS_{DC}
$\Delta E^{\ddagger}$ = 5.8 kcal mol^{-1}
$\Delta G^{\ddagger}$ = 21.1 kcal mol^{-1}
$\langle S^2 \rangle$ = 0

Figure S9 Optimized geometry of concerted saddle point (**TS_{DC}**) corresponding to the 1,3-dipolar cycloaddition of **1** and **3** at (U)B3LYP-D3BJ/def2-TZVP level in CH_2Cl_2 (SMD). Relative electronic and free energies are given with respect to the reagents in kcal mol^{-1}. Eigenvalue of the total spin operator [$\langle S^2 \rangle$] is given without the spin annihilation diagnostic.

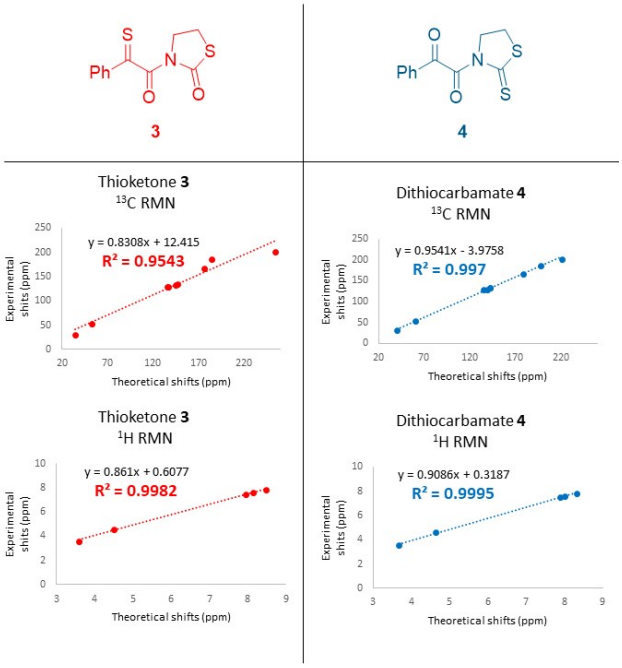


Figure S10 Plots of linear relationships between experimental and theoretical chemical shifts of **3** and **4** at the (U)B3LYP-D3BJ/def2TZVPP//def2-TZVP level in $CHCl_3$ (SMD).

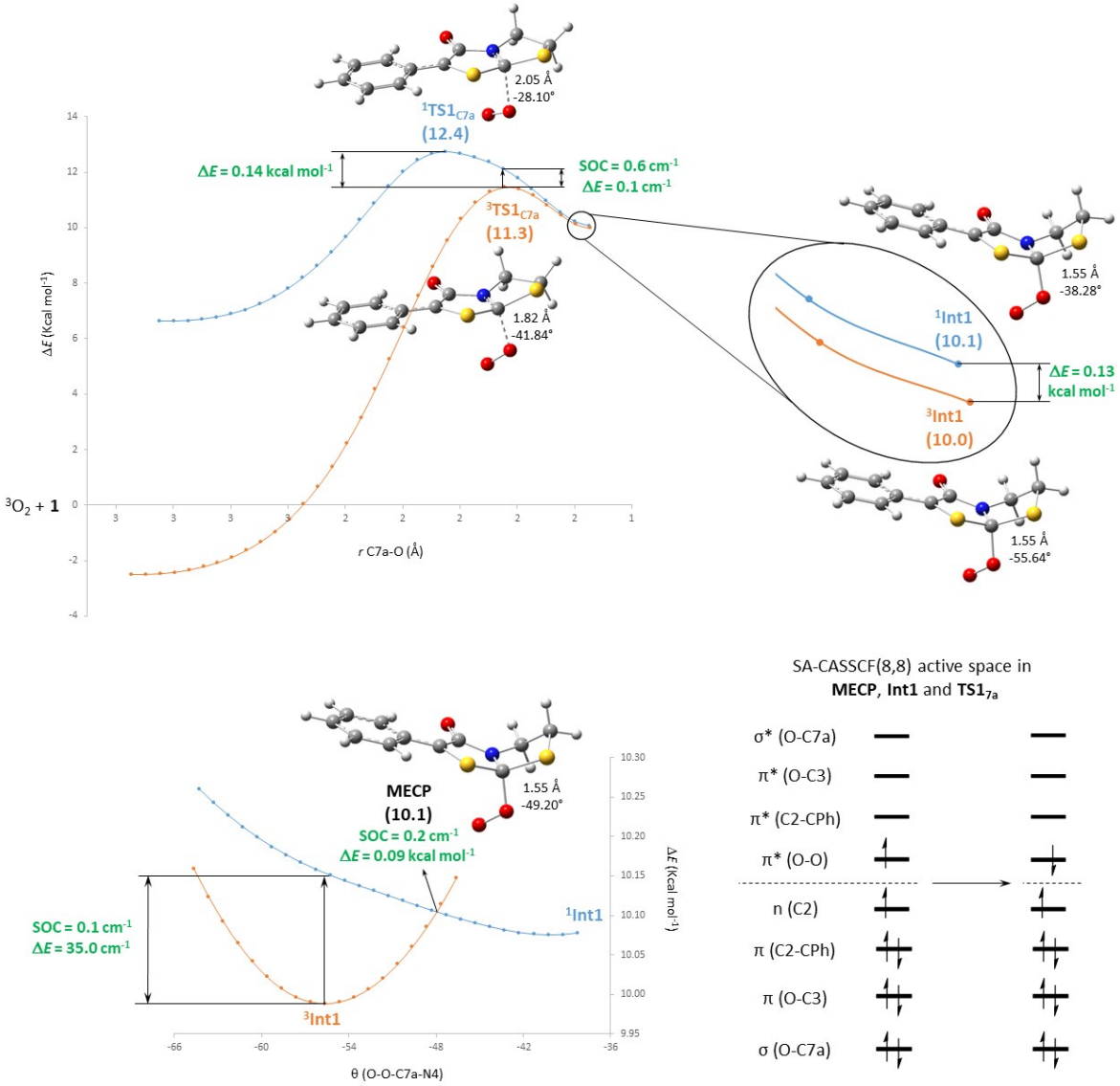


Figure S11 Optimized geometries of **^{3}TSC$_{7a}$**, **^{1}TSC$_{7a}$**, **^{3}Int1**, **^{1}Int1**, and **MECP**, their electronic energies (given in parentheses) and PES scan at (U)B3LYP-D3BJ/def2-TZVP-level of theory [all energy data are computed in CH_2Cl_2 (SMD)]. At the **MECP** only one energy value is given because the singlet and triplet electronic energies are almost identical at (U)DFT. Bond distances (O-C7a) are given in angstrom and dihedral angles in degrees (O-O-C7a-N4). Potential energies are given in kcal mol^{-1} with respect to $^3O_2$ and **1**. The singlet PESs (blue curves) are computed with the broken-symmetry (U)DFT. Green values given in cm^{-1} denote energy gaps and triplet-singlet spin-orbit coupling constants are given at the SA-CASSCF(8,8)/def2-TZVP//(U)B3LYP. Electronic energy differences between singlet and triplet states given in kcal mol^{-1} (green) are single point energies at CASSCF(8,8)/def2-TZVP//(U)B3LYP-D3BJ. Configurations of the CAS active space are identical for all the critical points computed and shown at the bottom right corner.

Table S1 Relative electronic and free energies of saddle points **$TS_{1\text{-}1}$a**, **$TS_{1\text{-}1}$b**, **TS6a**, **TS6b**, **TS6c** and **TS6d** with respect to **1** and $^3O_2$.

Saddle point	$\Delta E^{\ddagger}$ (kcal mol^{-1})	$\Delta G^{\ddagger}$ (kcal mol^{-1})
$TS_{1\text{-}1}$a	12.8	28.3
$TS_{1\text{-}1}$b	12.1	27.9
TS6a	-10.8	11.1
TS6b	-12.6	9.5
TS6c	-6.7	15.0
TS6d	-11.6	10.0

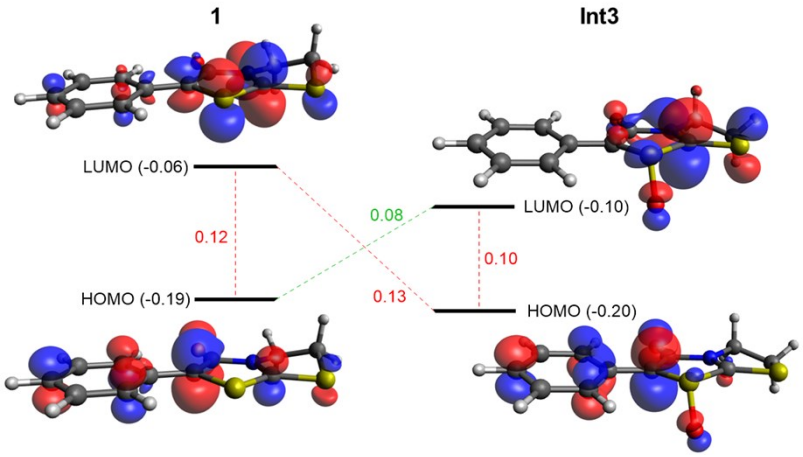


Figure S12 FMOs of **1** and **Int3** and their energy gaps in eV at (U)B3LYP-D3BJ/def2-TZVP in CH_2Cl_2 (SMD). Note that even though the wavefunctions of **1** and **Int3** are open-shells, for clarity, we do not differentiate between α and β orbitals as they are pure singlet states.

Additional Spectroscopic Data.

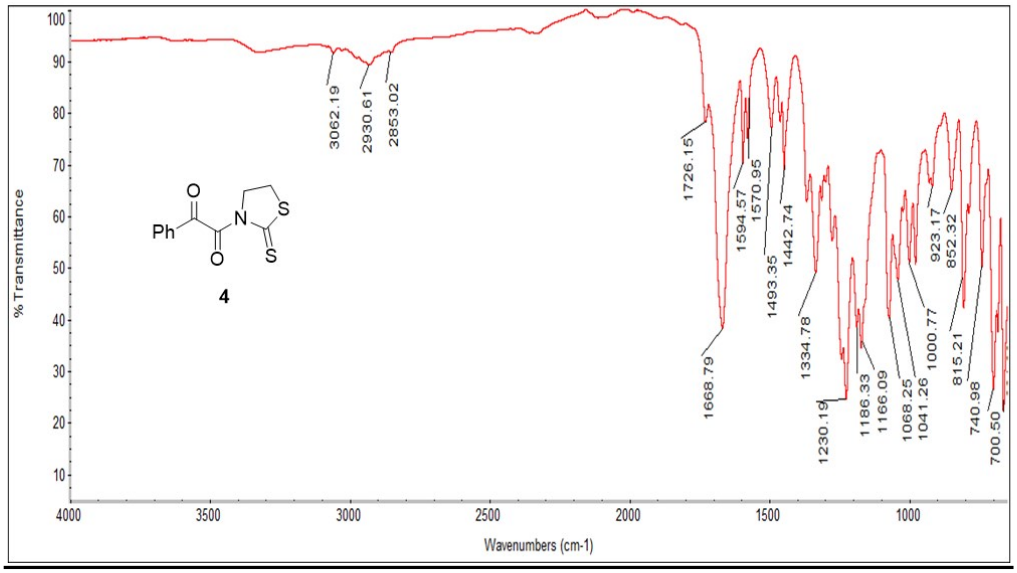


Figure S13 FT-IR spectrum (ATR mode) of compound **4**.

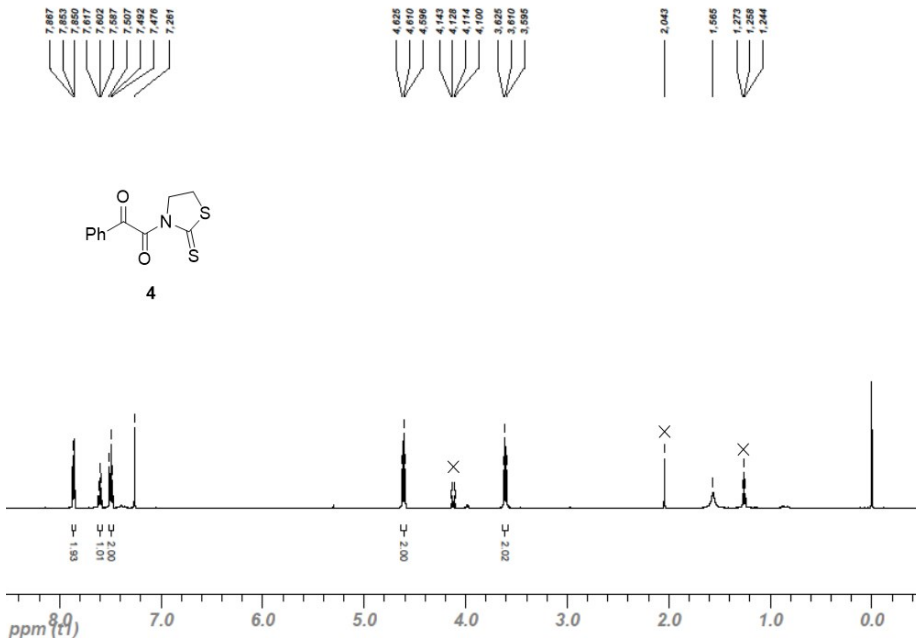


Figure S14 ^{1}H NMR spectrum of **4** recorded in $CDCl_3$ (125 MHz).

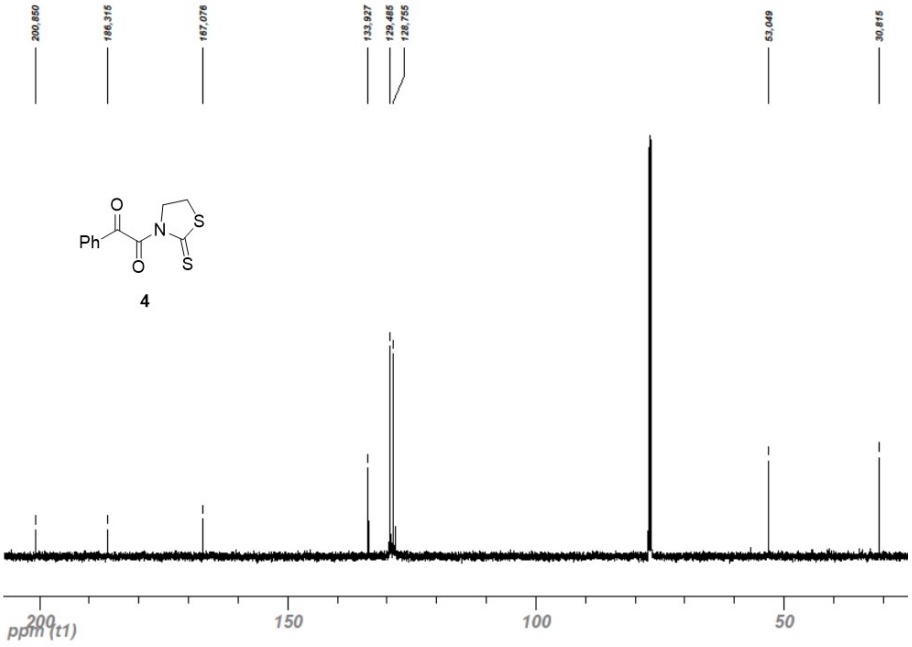


Figure S15 ^{13}C NMR spectrum of **4** recorded in $CDCl_3$ (125 MHz).

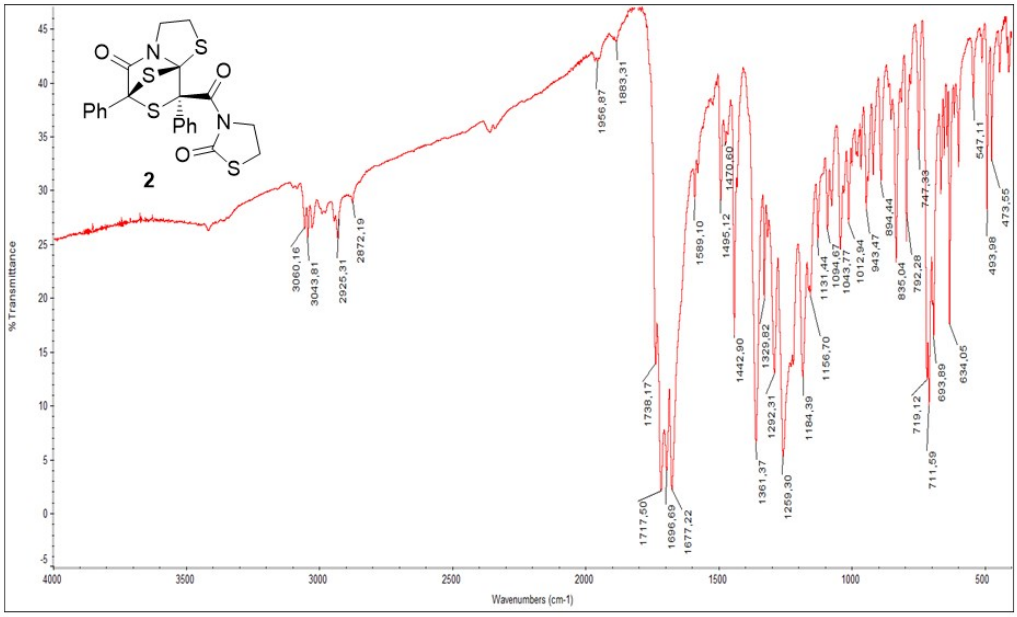


Figure S16 FT-IR spectrum (ATR mode) of compound **2**.

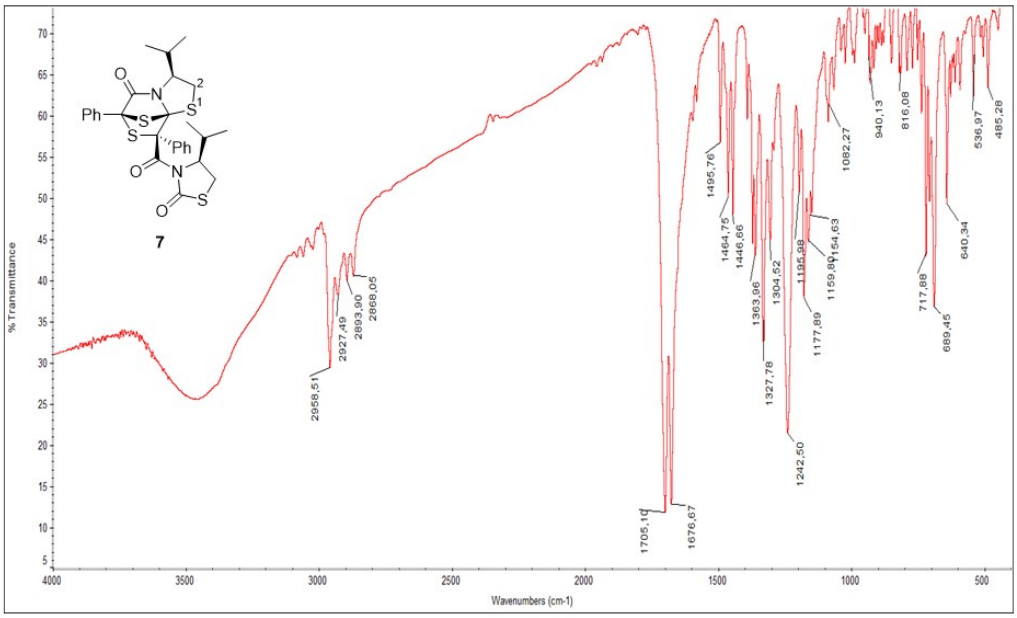


Figure S17 FT-IR spectrum (ATR mode) of compound **7**.

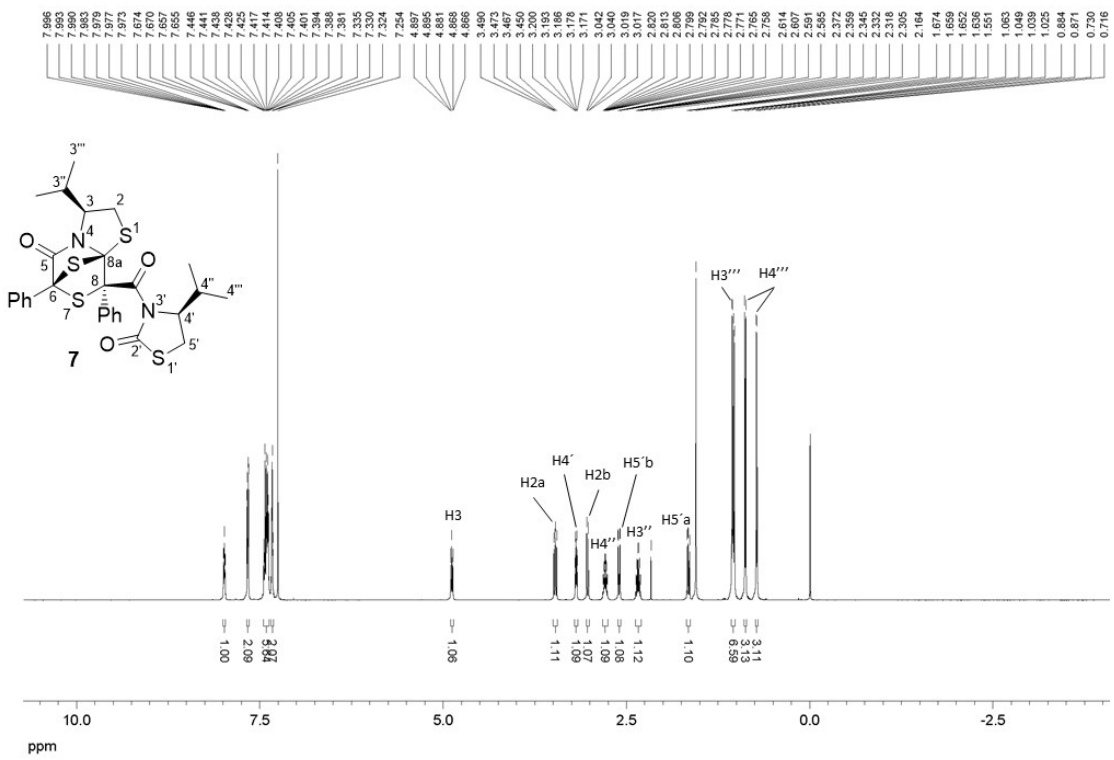


Figure S18 ^{1}H NMR spectrum of **7** recorded in $CDCl_3$ at 500 MHz.

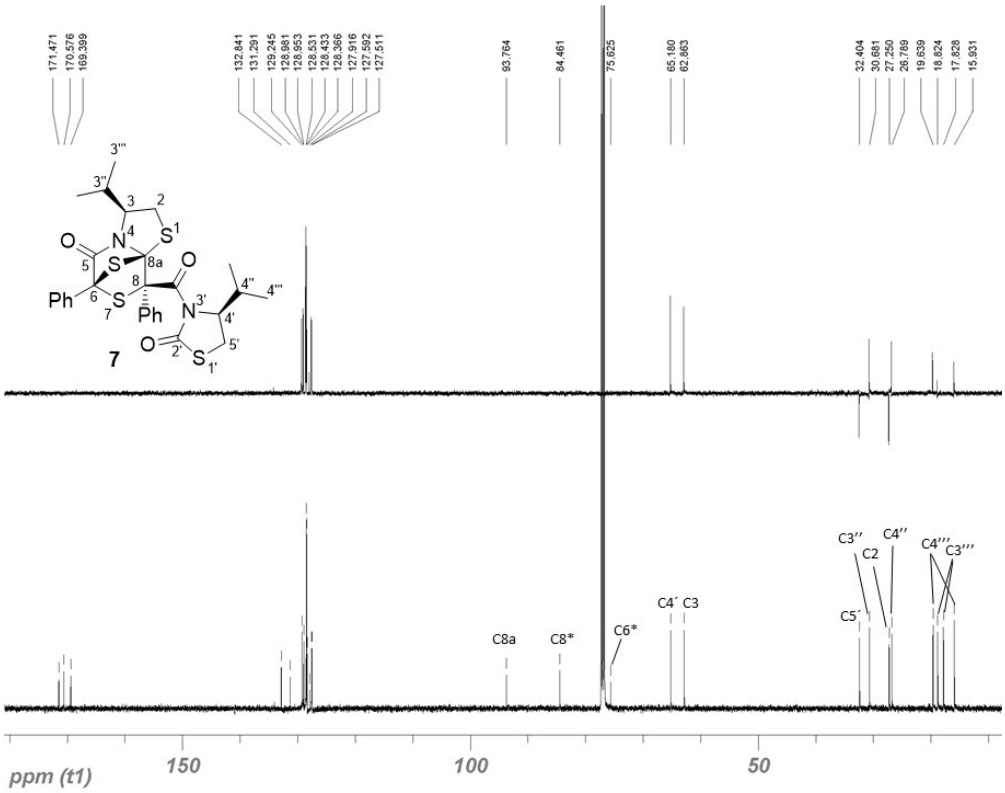


Figure S19 ^{13}C NMR spectrum of **7** recorded in $CDCl_3$ at 125 MHz.
*The carbon resonances attributed to C6 and C8 may be interchanged.

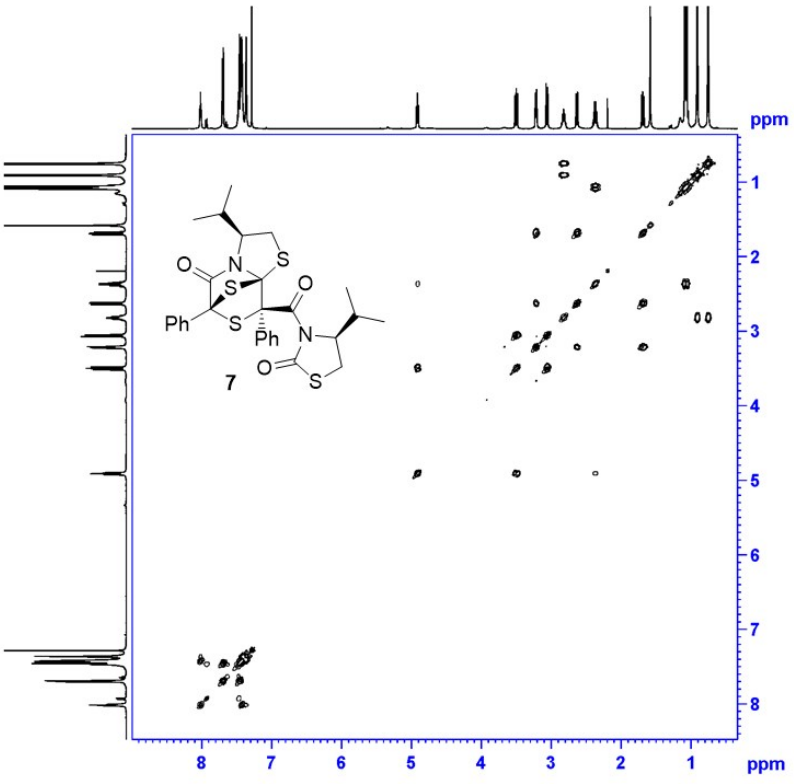


Figure S20 COSY spectrum of **7** recorded in $CDCl_3$.

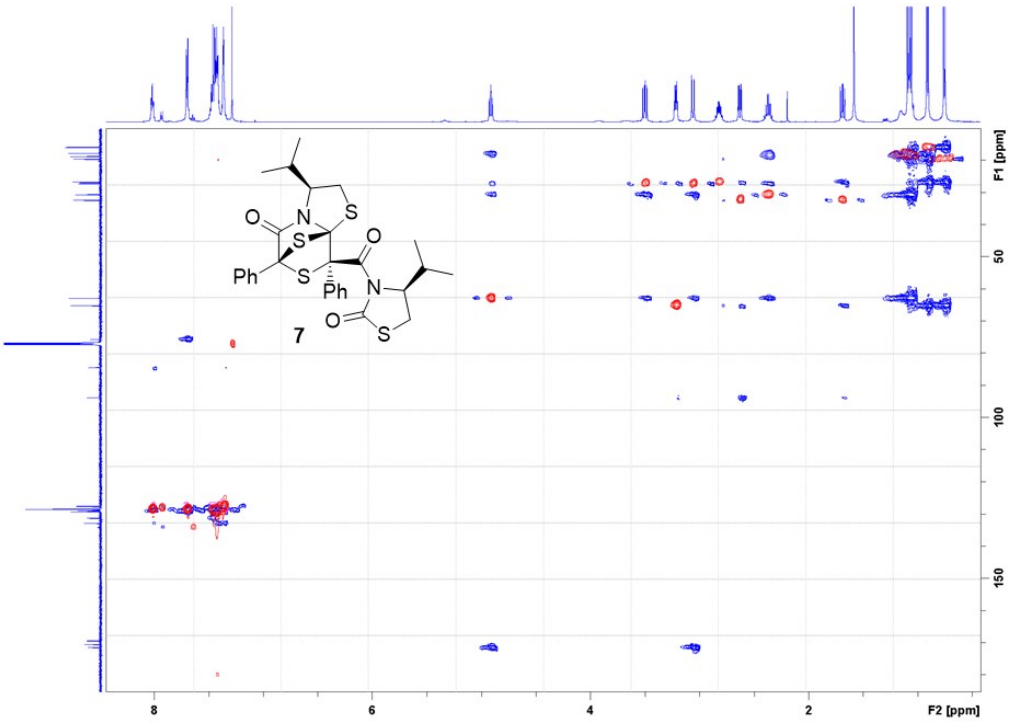


Figure S21 HMBC and HSQC spectrum of **7** recorded in $CDCl_3$.

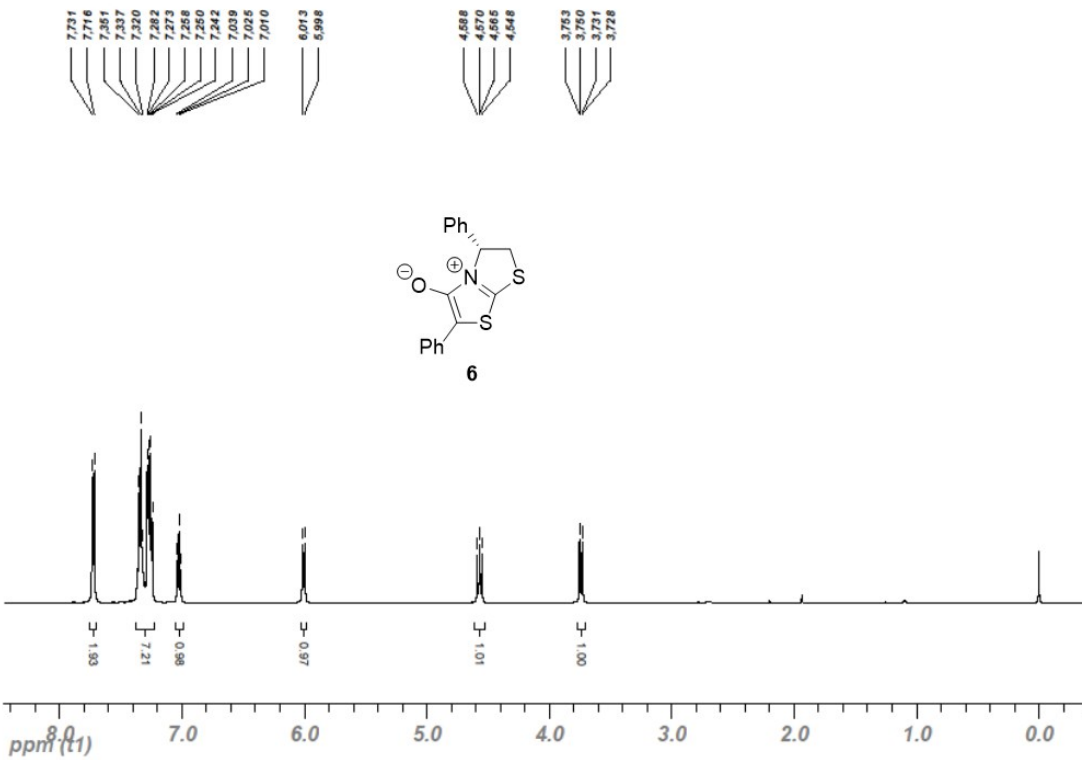


Figure S22 ^1H NMR spectrum of **6** recorded in $CDCl_3$ at 500 MHz.

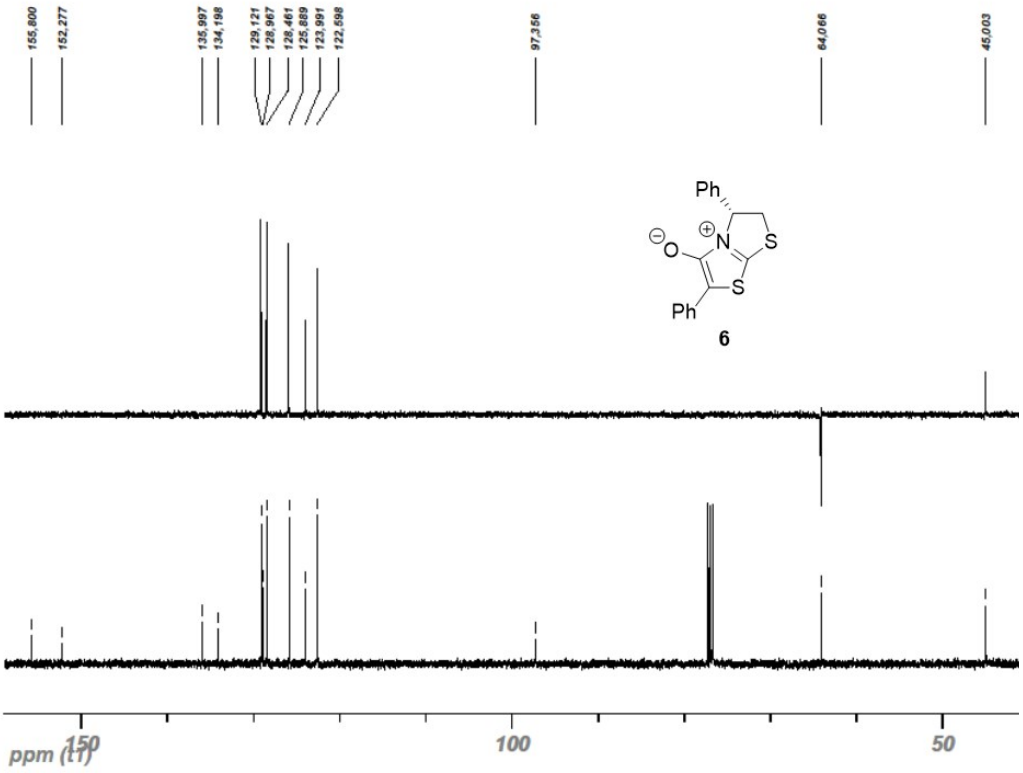


Figure S23 ^{13}C NMR spectrum of **6** recorded in $CDCl_3$ at 125 MHz.

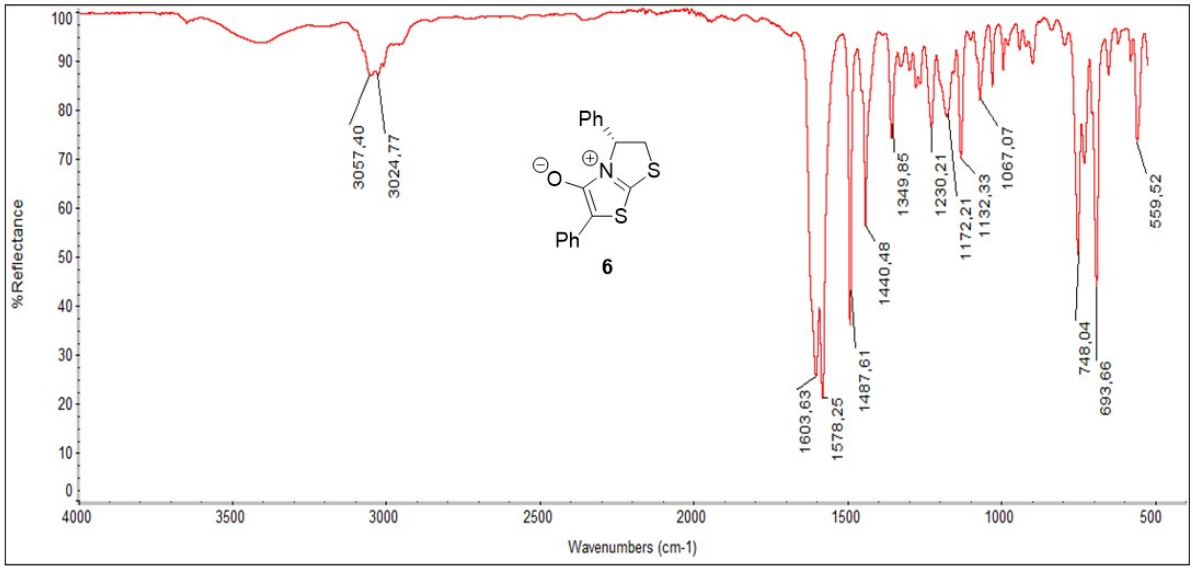


Figure S24 FT-IR spectrum (ATR mode) of compound **6**.

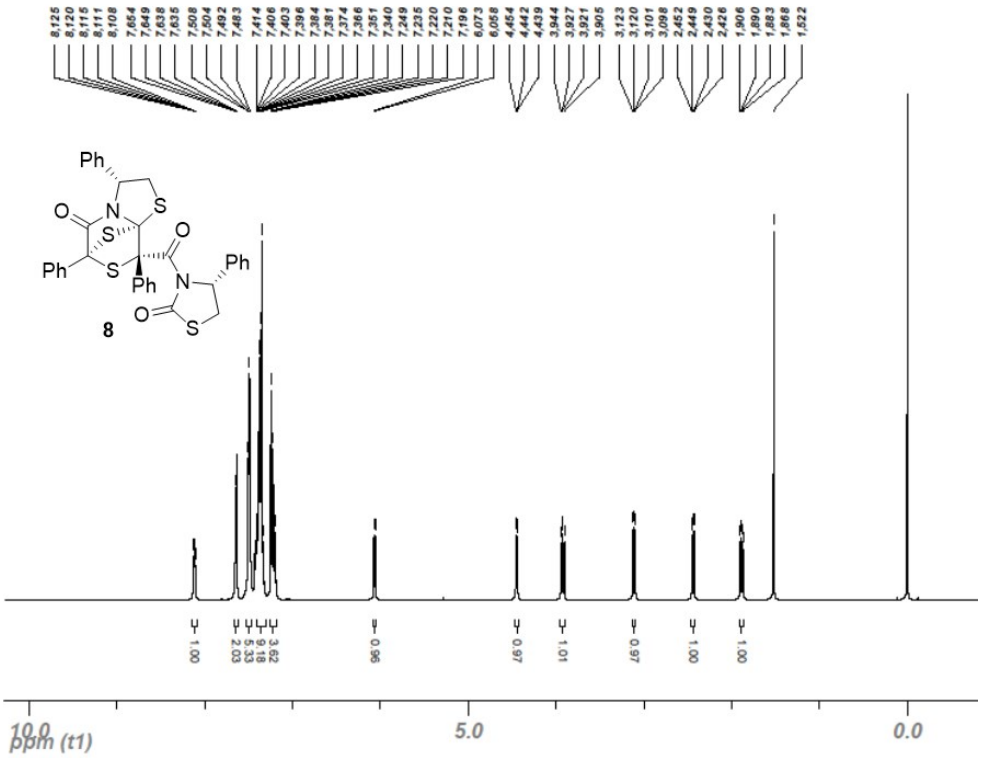


Figure S25 ^{1}H NMR spectrum of **8** recorded in $CDCl_3$ at 500 MHz.

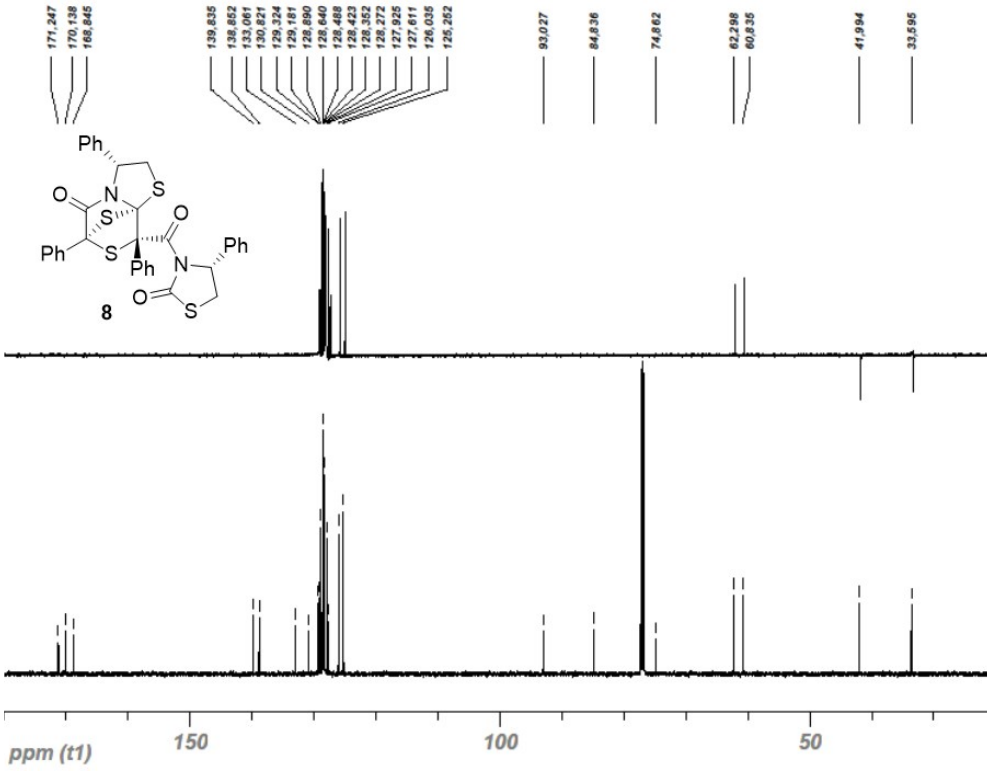


Figure S26 ^{13}C NMR spectrum of **8** recorded in $CDCl_3$ at 125 MHz.

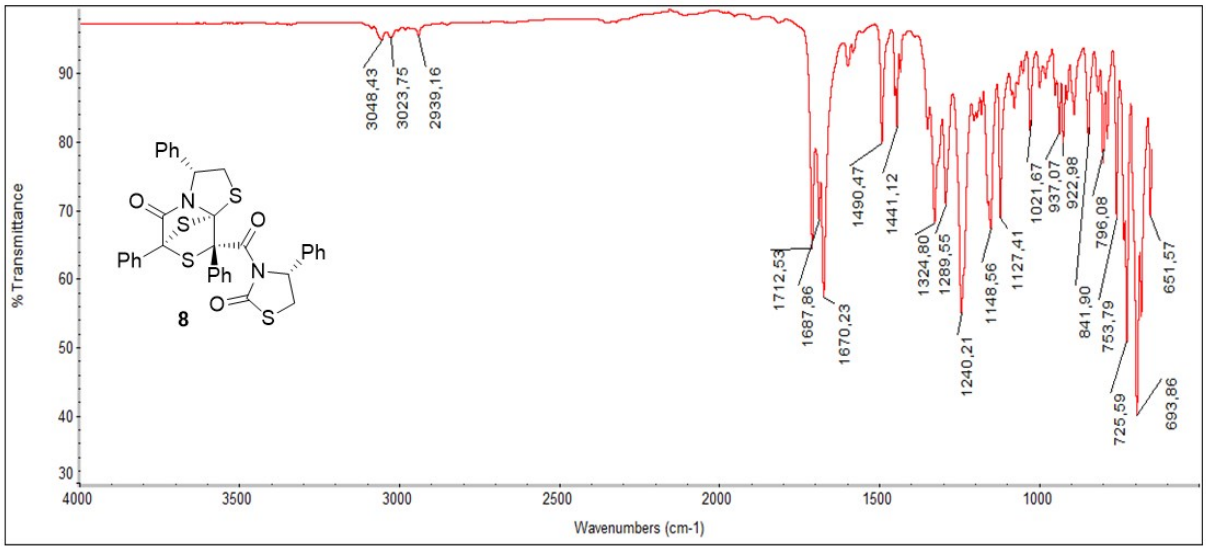


Figure S27 FT-IR spectrum (ATR mode) of compound **8**.

Crystal Data for Compounds 2, 7 and 8.

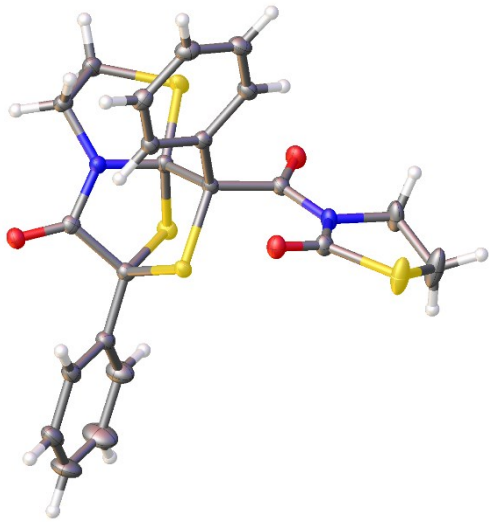


Figure S28 Thermal ellipsoids drawn at the 50% probability level.

Acquisition Data for 2. Single clear colorless prism-shaped crystals of **2** were recrystallized from a mixture of CH_2Cl_2 and ethyl acetate by slow evaporation. A suitable crystal (0.14×0.08×0.06) was selected and mounted on a MITIGEN holder in perfluoroether oil on a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using OLEX2,[1] the structure was solved with the SheLXT structure solution program,[2] using the Direct Methods solution method. The model was refined with SheLXL[3] using Least Squares minimization.

Crystal Data. $C_{22}H_{18}N_2O_3S_4$, M_r = 486.62, trigonal, R-3 (No. 148), a = 23.7837(4) Å, b = 23.7837(4) Å, c = 21.6038(4) Å, α = 90˚, β = 90˚, γ = 120˚, V = 10583.3(4) Å^3, T = 100(2) K, Z = 18, Z' = 1, μ(MoK $_\alpha$) = 0.430, 56521 reflections measured, 6068 unique (R_{int} = 0.0338) which were used in all calculations. The final wR_2 was 0.0996 (all data) and R_1 was 0.0342 (I > 2(I)).

Compound	**2**
Formula	$C_{22}H_{18}N_2O_3S_4$
$D_{calc.}$/ g cm^{-3}	1.374
μ/mm^{-1}	0.430
Formula Weight	486.62
Colour	clear colourless
Shape	prism
Max Size/mm	0.14
Mid Size/mm	0.08
Min Size/mm	0.06
T/K	100(2)
Crystal System	trigonal
Space Group	R-3
a/Å	23.7837(4)
b/Å	23.7837(4)
c/Å	21.6038(4)
α/°	90
β/°	90
γ/°	120
V/Å^3	10583.3(4)
Z	18
Z'	1
Θ_{min}/°	2.967
Θ_{max}/°	28.679
Measured Refl.	56521
Independent Refl.	6068
Reflections Used	5583
R_{int}	0.0338
Parameters	280
Restraints	0
Largest Peak	0.850
Deepest Hole	-0.639
GooF	1.074
wR_2 (all data)	0.0996
wR_2	0.0980
R_1 (all data)	0.0367
R_1	0.0342

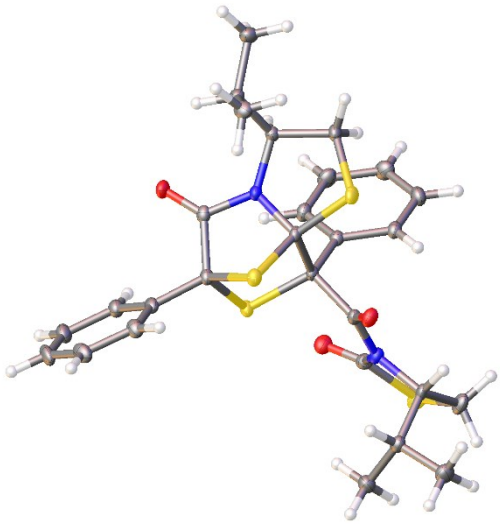


Figure S29 Thermal ellipsoids drawn at the 50% probability level.

Acquisition Data for 7. Single clear colorless prism-shaped crystals of **10** were recrystallized from acetone by slow evaporation. A suitable crystal (0.23×0.11×0.02) was selected and mounted on a MITIGEN holder in perfluoroether oil on a Rigaku AFC12 FRE-VHF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using OLEX2,[1] the structure was solved with the SheLXT structure solution program,[2] using the Direct Methods solution method. The model was refined with SheLXL[3] using Least Squares minimization.

Crystal Data. $C_{28}H_{30}N_2O_3S_4$, M_r = 570.78, orthorhombic, $P2_12_12_1$ (No. 19), a = 9.4421(2) Å, b = 14.8451(4) Å, c = 19.2118(4) Å, $\alpha = \beta = \gamma = 90^{\circ}$, V = 2692.89(11) Å^3, T = 100(2) K, Z = 4, Z' = 1, μ(MoK$_\alpha$) = 0.387, 23556 reflections measured, 6950 unique (R_{int} = 0.0688) which were used in all calculations. The final wR_2 was 0.1003 (all data) and R_1 was 0.0401 (I > 2(I)).

Compound	**7**
Formula	$C_{28}H_{30}N_2O_3S_4$
$D_{calc.}$/ g cm^{-3}	1.408
μ/mm^{-1}	0.387
Formula Weight	570.78
Colour	clear colourless
Shape	prism
Max Size/mm	0.23
Mid Size/mm	0.11
Min Size/mm	0.02
T/K	100(2)
Crystal System	orthorhombic
Flack Parameter	0.01(5)
Hooft Parameter	0.08(2)
Space Group	$P2_12_12_1$
a/Å	9.4421(2)
b/Å	14.8451(4)
c/Å	19.2118(4)
α/°	90
β/°	90
γ/°	90
V/Å^3	2692.89(11)
Z	4
Z'	1
Θ_{min}/°	2.942
Θ_{max}/°	28.698
Measured Refl.	23556
Independent Refl.	6950
Reflections Used	6514
R_{int}	0.0688
Parameters	338
Restraints	0
Largest Peak	0.432
Deepest Hole	-0.454
GooF	1.050
wR_2 (all data)	0.1003
wR_2	0.0987
R_1 (all data)	0.0433
R_1	0.0401

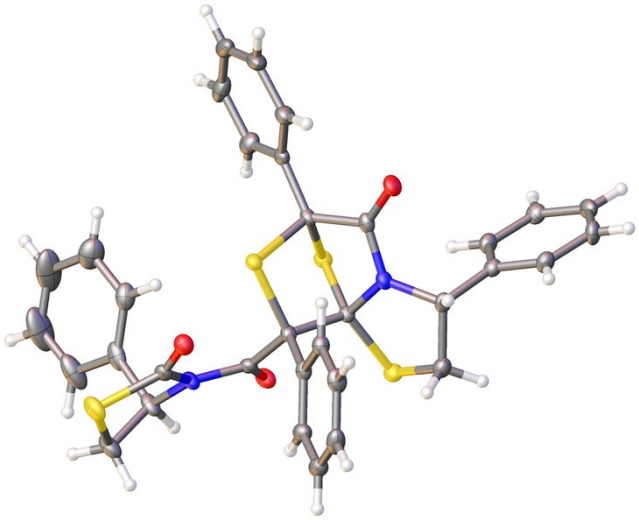


Figure S30 Thermal ellipsoids drawn at the 50% probability level.

Experimental. Single clear colourless prism-shaped crystals of **8** were recrystallised from a mixture of CH_2Cl_2 and ethanol by slow evaporation. A suitable crystal 0.03×0.02×0.01 mm^3 was selected and mounted on a MITIGEN holder with silicon oil on an Rigaku AFC12 FRE-VHF diffractometer. The crystal was kept at a steady T = 100(2) K during data collection. Using OLEX2,[1] the structure was solved with the SheLXT structure solution program,[2] using the Direct Methods solution method. The model was refined with SheLXL[3] using Least Squares minimization.

Crystal Data. $C_{34}H_{26}N_2O_3S_4$, M_r = 638.81, orthorhombic, $P2_12_12_1$ (No. 19), a = 12.4820(4) Å, b = 12.8583(5) Å, c = 19.5132(7) Å, $\alpha = \beta = \gamma$ 90°, V = 3131.82(19) $Å^3$, T = 100(2) K, Z = 4, Z' = 1, $\mu(MoK_\alpha)$ = 0.341, 50041 reflections measured, 7916 unique (R_{int} = 0.0888) which were used in all calculations. The final wR_2 was 0.0887 (all data) and R_1 was 0.0555 (I > 2(I)).

Compound	**8**
Formula	$C_{34}H_{26}N_2O_3S_4$
$D_{calc.}$/ g cm^{-3}	1.355
μ /mm^{-1}	0.341
Formula Weight	638.81
Colour	clear colourless
Shape	prism
Size/mm^3	0.03×0.02×0.01
T/K	100(2)
Crystal System	orthorhombic
Flack Parameter	-0.04(3)
Hooft Parameter	-0.03(3)
Space Group	$P2_12_12_1$
a/Å	12.4820(4)
b/Å	12.8583(5)
c/Å	19.5132(7)
α/°	90
β/°	90
γ/°	90
V/Å^3	3131.82(19)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK$_\alpha$
Θ_{min}/°	2.087
Θ_{max}/°	28.500
Measured Refl.	50041
Independent Refl.	7916
Reflections with I > 2(I)	6913
R_{int}	0.0888
Parameters	388
Restraints	0
Largest Peak	0.453
Deepest Hole	-0.283
GooF	1.113
wR_2 (all data)	0.0887
wR_2	0.0856
R_1 (all data)	0.0690
R_1	0.0555

References

[1] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.,* 2009, **42**, 339-341.

[2] G. M. Sheldrick, *Acta Cryst.,* 2008, **A64**, 112-122.

[3] G. M. Sheldrick, *Acta Cryst.,* 2014, **A71**, 3-8.

Additional Computational Data.

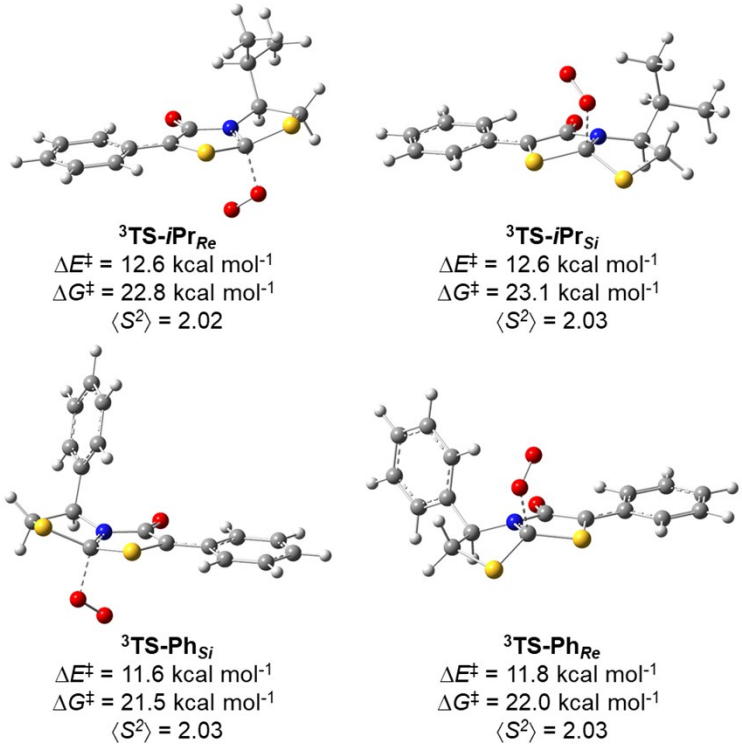


Figure S31 Optimized geometries of **^{3}TS-*i*Pr$_{Re}$**, **^{3}TS-*i*Pr$_{Si}$**, **^{3}TS-Ph$_{Re}$** and **^{3}TS-Ph$_{Si}$** at the (U)B3LYP/def2-TZVP in CH_2Cl_2 (SMD). Relative electronic and free energies are given with respect to **5** and **6** and $^3O_2$ in kcal mol^{-1}. Eigenvalues of the total spin operator [$\langle S^2 \rangle$] are given without spin annihilation diagnostic.

Cartesian Coordinates for All Optimized Geometries at (U)B3LYP-D3BJ/def2-TZVP

Structure of $TS_{m\text{-}CPBA}C2$

```
Zero-point correction=                           0.285028 (Hartree/Particle)
 Thermal correction to Energy=                    0.308774
 Thermal correction to Enthalpy=                  0.309718
 Thermal correction to Gibbs Free Energy=         0.226085
 Sum of electronic and zero-point Energies=          -2306.813327
 Sum of electronic and thermal Energies=             -2306.789580
 Sum of electronic and thermal Enthalpies=           -2306.788636
 Sum of electronic and thermal Free Energies=        -2306.872270
One imaginary frequency: 465.6154i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.525149	0.464585	-0.094064
2	6	0	-2.955302	-1.939540	-0.470100
3	6	0	-2.556517	-0.278119	1.131748
4	8	0	-2.450654	0.074609	2.299741
5	7	0	-2.738575	-1.659270	0.802842
6	16	0	-2.915141	-0.575699	-1.467117
7	16	0	-3.236910	-3.602019	-0.816421
8	6	0	-2.870995	-2.774984	1.738392
9	6	0	-2.671785	-4.032797	0.895229
10	1	0	-1.624042	-4.316518	0.827324
11	1	0	-3.262416	-4.871758	1.252021
12	1	0	-2.116904	-2.689695	2.516924
13	1	0	-3.863297	-2.736299	2.189944
14	6	0	-2.562250	1.910234	-0.243583
15	6	0	-2.659658	2.505534	-1.512018
16	6	0	-2.470850	2.755184	0.876390
17	6	0	-2.671227	3.883883	-1.656491
18	1	0	-2.719081	1.891358	-2.402679
19	6	0	-2.480581	4.133910	0.721909
20	1	0	-2.387076	2.319429	1.859978
21	6	0	-2.581177	4.709750	-0.540250
22	1	0	-2.747159	4.313718	-2.647351
23	1	0	-2.407619	4.763715	1.599911
24	1	0	-2.586819	5.786044	-0.653990
25	8	0	-0.311631	-0.038129	-0.116314
26	1	0	-0.182022	0.825552	0.337387
27	8	0	1.374630	-0.315739	-0.205115
28	6	0	1.990259	0.710831	0.324683
29	8	0	1.411512	1.680964	0.799807
30	6	0	3.483493	0.597079	0.302764
31	6	0	4.118033	-0.510467	-0.259952
32	6	0	4.237543	1.628248	0.860742
33	6	0	5.501855	-0.563944	-0.251815
34	1	0	3.541048	-1.312340	-0.695509
35	6	0	5.622948	1.552446	0.857268
36	1	0	3.730556	2.479526	1.291705
37	6	0	6.267745	0.454239	0.300327
38	1	0	6.210474	2.351376	1.290074
39	1	0	7.346946	0.389692	0.294693
40	17	0	6.304770	-1.952088	-0.956220

Structure of $TS_{m\text{-}CPBA}C7a$

```
Zero-point correction=                           0.284540 (Hartree/Particle)
 Thermal correction to Energy=                    0.308384
 Thermal correction to Enthalpy=                  0.309329
 Thermal correction to Gibbs Free Energy=         0.224715
 Sum of electronic and zero-point Energies=          -2306.799051
```

```
 Sum of electronic and thermal Energies=             -2306.775207
 Sum of electronic and thermal Enthalpies=           -2306.774263
 Sum of electronic and thermal Free Energies=        -2306.858876
One imaginary frequency: 475.1190i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.308586	-0.144218	-0.156417
2	6	0	1.767850	1.729489	-0.645211
3	6	0	3.291037	0.849417	0.903647
4	8	0	3.900870	0.873069	1.966829
5	7	0	2.401396	1.865449	0.531425
6	16	0	2.315319	0.328466	-1.461317
7	16	0	1.152087	3.238237	-1.272842
8	6	0	2.220058	3.149658	1.206330
9	6	0	1.071063	3.836636	0.469840
10	1	0	0.104887	3.546491	0.874928
11	1	0	1.166807	4.918705	0.468284
12	1	0	1.979313	2.987356	2.255028
13	1	0	3.152012	3.712376	1.134121
14	6	0	3.984285	-1.420992	-0.129653
15	6	0	3.722530	-2.404607	-1.102746
16	6	0	4.932731	-1.710224	0.869512
17	6	0	4.383343	-3.618928	-1.081300
18	1	0	2.983868	-2.227115	-1.874948
19	6	0	5.588565	-2.932034	0.882579
20	1	0	5.145182	-0.969071	1.623529
21	6	0	5.322341	-3.891292	-0.088006
22	1	0	4.161624	-4.360462	-1.837885
23	1	0	6.315606	-3.134117	1.658876
24	1	0	5.836937	-4.843230	-0.071836
25	8	0	0.020798	0.674782	-0.002203
26	1	0	-0.486527	0.673271	-0.847443
27	8	0	-1.506033	0.143638	0.842392
28	6	0	-2.422028	0.060041	-0.071743
29	8	0	-2.235561	0.296656	-1.265622
30	6	0	-3.769063	-0.359982	0.445739
31	6	0	-4.813685	-0.475579	-0.470294
32	6	0	-3.988421	-0.629281	1.796120
33	6	0	-6.064100	-0.859351	-0.016957
34	1	0	-4.637827	-0.266143	-1.514923
35	6	0	-5.250834	-1.013013	2.227491
36	1	0	-3.175074	-0.539312	2.501448
37	6	0	-6.300441	-1.131277	1.324183
38	1	0	-5.424553	-1.223272	3.274626
39	1	0	-7.285310	-1.429922	1.655273
40	17	0	-7.380512	-1.004876	-1.163668

Structure of TS_{DC}

```
Zero-point correction=                           0.360008 (Hartree/Particle)
 Thermal correction to Energy=                    0.387251
 Thermal correction to Enthalpy=                  0.388195
 Thermal correction to Gibbs Free Energy=         0.300264
 Sum of electronic and zero-point Energies=          -2777.478211
 Sum of electronic and thermal Energies=             -2777.450968
 Sum of electronic and thermal Enthalpies=           -2777.450024
 Sum of electronic and thermal Free Energies=        -2777.537954
One imaginary frequency: 255.4533i
```

Standard orientation:

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

1	6	0	-2.392463	-0.004025	0.169217
2	6	0	-0.744663	1.368136	1.305607
3	6	0	0.612565	-0.202897	-0.084097
4	6	0	-2.269354	1.356049	-0.450290
5	8	0	-2.868679	1.821008	-1.399115
6	7	0	-1.263771	2.026535	0.232063
7	16	0	-1.814586	0.122704	1.845692
8	16	0	0.326554	2.340253	2.244725
9	6	0	-0.904259	3.434472	0.080680
10	6	0	0.332522	3.657444	0.948968
11	1	0	1.252103	3.561543	0.381514
12	1	0	0.307128	4.621542	1.449451
13	1	0	-0.698631	3.658366	-0.962607
14	1	0	-1.747401	4.037845	0.420790
15	6	0	-3.567909	-0.854338	-0.113170
16	6	0	-4.016280	-0.995834	-1.431593
17	6	0	-4.213781	-1.569858	0.898415
18	6	0	-5.090722	-1.826114	-1.721180
19	1	0	-3.523866	-0.455827	-2.225852
20	6	0	-5.286825	-2.399403	0.604149
21	1	0	-3.889301	-1.481512	1.927853
22	6	0	-5.731025	-2.529669	-0.707151
23	1	0	-5.425978	-1.924027	-2.745847
24	1	0	-5.776456	-2.942005	1.402518
25	1	0	-6.568891	-3.175483	-0.936533
26	16	0	-0.744565	-0.958108	-0.782932
27	6	0	1.382388	0.837861	-0.764696
28	6	0	0.928729	1.442143	-1.946649
29	6	0	2.579849	1.319014	-0.204302
30	6	0	1.629689	2.482575	-2.534294
31	1	0	0.017654	1.081876	-2.403733
32	6	0	3.286883	2.352124	-0.802915
33	1	0	2.960023	0.891175	0.712534
34	6	0	2.814583	2.947393	-1.968069
35	1	0	1.252515	2.930650	-3.445337
36	1	0	4.206062	2.701240	-0.348844
37	1	0	3.364030	3.756164	-2.432390
38	6	0	1.322071	-1.025051	0.947580
39	8	0	0.979747	-1.124752	2.110329
40	6	0	3.364768	-2.256015	1.590653
41	6	0	4.763127	-2.336171	0.998919
42	1	0	3.339453	-1.613198	2.465843
43	1	0	3.000439	-3.245248	1.874128
44	1	0	5.353224	-3.119287	1.467920
45	1	0	5.291074	-1.387087	1.074749
46	7	0	2.496991	-1.689563	0.551596
47	16	0	4.499967	-2.730304	-0.759533
48	6	0	2.857177	-2.024706	-0.752154
49	8	0	2.193173	-1.907135	-1.750061

Structure of **1**

```
Zero-point correction=                           0.177417 (Hartree/Particle)
 Thermal correction to Energy=                    0.189926
 Thermal correction to Enthalpy=                  0.190870
 Thermal correction to Gibbs Free Energy=         0.137348
 Sum of electronic and zero-point Energies=          -1351.105166
 Sum of electronic and thermal Energies=             -1351.092657
 Sum of electronic and thermal Enthalpies=           -1351.091713
 Sum of electronic and thermal Free Energies=        -1351.145235
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.028031	0.602375	0.315404

2	6	0	2.877275	1.498206	-0.138335
3	1	0	4.183658	0.654824	1.390871
4	1	0	4.956716	0.821691	-0.203836
5	1	0	2.784858	2.383790	0.485661
6	1	0	2.982927	1.803748	-1.180819
7	6	0	1.866831	-0.631045	-0.020447
8	6	0	0.313180	1.134836	-0.018090
9	7	0	1.675221	0.678350	-0.010475
10	16	0	3.520797	-1.131501	-0.093095
11	8	0	0.067476	2.347613	-0.032666
12	16	0	0.414961	-1.486620	-0.000339
13	6	0	-0.523513	-0.003502	-0.007326
14	6	0	-1.970354	-0.041084	0.002499
15	6	0	-2.679013	-1.257006	0.021448
16	6	0	-2.723066	1.149971	-0.006122
17	6	0	-4.064830	-1.282986	0.031708
18	1	0	-2.144744	-2.200025	0.028983
19	6	0	-4.110109	1.113367	0.004791
20	1	0	-2.201721	2.095013	-0.021710
21	6	0	-4.795047	-0.097804	0.023555
22	1	0	-4.577448	-2.236987	0.046535
23	1	0	-4.661864	2.045758	-0.002198
24	1	0	-5.877176	-0.119195	0.031604

Structure of $^3O_2$

Zero-point correction= 0.003730 (Hartree/Particle)
Thermal correction to Energy= 0.006093
Thermal correction to Enthalpy= 0.007037
Thermal correction to Gibbs Free Energy= -0.016233
Sum of electronic and zero-point Energies= -150.386720
Sum of electronic and thermal Energies= -150.384357
Sum of electronic and thermal Enthalpies= -150.383413
Sum of electronic and thermal Free Energies= -150.406683
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.602014
2	8	0	0.000000	0.000000	-0.602014

Structure of O_2^{2-}

Zero-point correction= 0.002713 (Hartree/Particle)
Thermal correction to Energy= 0.005090
Thermal correction to Enthalpy= 0.006035
Thermal correction to Gibbs Free Energy= -0.017078
Sum of electronic and zero-point Energies= -150.492563
Sum of electronic and thermal Energies= -150.490186
Sum of electronic and thermal Enthalpies= -150.489241
Sum of electronic and thermal Free Energies= -150.512354
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.672324
2	8	0	0.000000	0.000000	-0.672324

Structure of **1**

```
Zero-point correction=                           0.177417 (Hartree/Particle)
 Thermal correction to Energy=                    0.189926
 Thermal correction to Enthalpy=                  0.190870
 Thermal correction to Gibbs Free Energy=         0.137348
 Sum of electronic and zero-point Energies=          -1351.105166
 Sum of electronic and thermal Energies=             -1351.092657
 Sum of electronic and thermal Enthalpies=           -1351.091713
 Sum of electronic and thermal Free Energies=        -1351.145235
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.028031	0.602375	0.315404
2	6	0	2.877275	1.498206	-0.138335
3	1	0	4.183658	0.654824	1.390871
4	1	0	4.956716	0.821691	-0.203836
5	1	0	2.784858	2.383790	0.485661
6	1	0	2.982927	1.803748	-1.180819
7	6	0	1.866831	-0.631045	-0.020447
8	6	0	0.313180	1.134836	-0.018090
9	7	0	1.675221	0.678350	-0.010475
10	16	0	3.520797	-1.131501	-0.093095
11	8	0	0.067476	2.347613	-0.032666
12	16	0	0.414961	-1.486620	-0.000339
13	6	0	-0.523513	-0.003502	-0.007326
14	6	0	-1.970354	-0.041084	0.002499
15	6	0	-2.679013	-1.257006	0.021448
16	6	0	-2.723066	1.149971	-0.006122
17	6	0	-4.064830	-1.282986	0.031708
18	1	0	-2.144744	-2.200025	0.028983
19	6	0	-4.110109	1.113367	0.004791
20	1	0	-2.201721	2.095013	-0.021710
21	6	0	-4.795047	-0.097804	0.023555
22	1	0	-4.577448	-2.236987	0.046535
23	1	0	-4.661864	2.045758	-0.002198
24	1	0	-5.877176	-0.119195	0.031604

Structure of **1 cation**

```
Zero-point correction=                           0.178051 (Hartree/Particle)
 Thermal correction to Energy=                    0.190558
 Thermal correction to Enthalpy=                  0.191503
 Thermal correction to Gibbs Free Energy=         0.137389
 Sum of electronic and zero-point Energies=          -1350.923502
 Sum of electronic and thermal Energies=             -1350.910994
 Sum of electronic and thermal Enthalpies=           -1350.910050
 Sum of electronic and thermal Free Energies=        -1350.964164
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.048218	0.592123	0.249948
2	6	0	2.894426	1.510038	-0.154374
3	1	0	4.285987	0.665820	1.308445
4	1	0	4.940987	0.758616	-0.345793
5	1	0	2.833273	2.382150	0.491425
6	1	0	2.963188	1.827349	-1.194812

7	6	0	1.857371	-0.611241	-0.005896
8	6	0	0.334032	1.149277	-0.029832
9	7	0	1.680129	0.698049	-0.003373
10	16	0	3.470315	-1.145936	-0.045198
11	8	0	0.057978	2.329929	-0.075651
12	16	0	0.395960	-1.498039	0.010755
13	6	0	-0.539733	-0.018056	-0.006972
14	6	0	-1.960075	-0.036093	0.001540
15	6	0	-2.666335	-1.263680	-0.036380
16	6	0	-2.704188	1.168797	0.052715
17	6	0	-4.043105	-1.283983	-0.024369
18	1	0	-2.131556	-2.204335	-0.079504
19	6	0	-4.083655	1.131698	0.065221
20	1	0	-2.184849	2.112806	0.084416
21	6	0	-4.760590	-0.086680	0.026514
22	1	0	-4.566974	-2.229657	-0.055331
23	1	0	-4.640955	2.057986	0.106099
24	1	0	-5.842435	-0.106105	0.036277

Structure of ^{3}**INT1**

```
Zero-point correction=                           0.182729 (Hartree/Particle)
 Thermal correction to Energy=                    0.198189
 Thermal correction to Enthalpy=                  0.199133
 Thermal correction to Gibbs Free Energy=         0.136430
 Sum of electronic and zero-point Energies=          -1501.440738
 Sum of electronic and thermal Energies=             -1501.425278
 Sum of electronic and thermal Enthalpies=           -1501.424334
 Sum of electronic and thermal Free Energies=        -1501.487036
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.957837	-0.380576	0.051946
2	6	0	-2.256004	0.513425	0.214595
3	6	0	-0.000937	0.281116	-0.765481
4	8	0	0.116623	1.110305	-1.644651
5	7	0	-1.378648	-0.230798	-0.470969
6	16	0	0.270514	-1.560217	1.082928
7	16	0	-3.903450	0.041126	0.134372
8	6	0	-2.055718	-1.091466	-1.465299
9	6	0	-3.409870	-1.430686	-0.861364
10	1	0	-4.161980	-1.614221	-1.623822
11	1	0	-3.351134	-2.283305	-0.187559
12	1	0	-2.159450	-0.523723	-2.391822
13	1	0	-1.452272	-1.977650	-1.644339
14	6	0	2.386185	-0.105128	0.009745
15	6	0	2.886850	1.091599	-0.533353
16	6	0	3.301587	-1.030494	0.541227
17	6	0	4.249880	1.343413	-0.540533
18	1	0	2.204467	1.822870	-0.937159
19	6	0	4.661533	-0.772627	0.528138
20	1	0	2.939195	-1.964159	0.952019
21	6	0	5.143669	0.416197	-0.013369
22	1	0	4.616231	2.273082	-0.956869
23	1	0	5.348923	-1.502102	0.936804
24	1	0	6.207122	0.617660	-0.023783
25	8	0	-2.947814	2.130082	1.576213
26	8	0	-1.869267	1.517607	0.905813

Structure of ^{1}**INT1**

```
Zero-point correction=                           0.184438 (Hartree/Particle)
 Thermal correction to Energy=                    0.199803
 Thermal correction to Enthalpy=                  0.200747
 Thermal correction to Gibbs Free Energy=         0.139336
 Sum of electronic and zero-point Energies=          -1501.490599
 Sum of electronic and thermal Energies=             -1501.475233
 Sum of electronic and thermal Enthalpies=           -1501.474289
 Sum of electronic and thermal Free Energies=        -1501.535700
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.814639	0.991322	0.482314
2	6	0	1.649912	-0.634763	0.143087
3	6	0	0.271559	1.297613	-0.521266
4	8	0	0.153604	2.225912	-1.290257
5	7	0	1.448615	0.557722	-0.483393
6	16	0	-0.558628	1.627498	1.969081
7	16	0	3.254407	-1.225827	0.138812
8	6	0	2.612522	0.967734	-1.298188
9	6	0	3.830755	0.344955	-0.633443
10	1	0	4.612329	0.118801	-1.353538
11	1	0	4.232518	0.976794	0.156272
12	1	0	2.474063	0.598522	-2.314745
13	1	0	2.666142	2.051964	-1.313823
14	6	0	-1.986222	0.278224	0.005667
15	6	0	-2.013753	-0.239160	-1.300313
16	6	0	-3.093507	0.068596	0.843467
17	6	0	-3.116779	-0.943287	-1.753451
18	1	0	-1.172596	-0.092855	-1.964434
19	6	0	-4.192465	-0.632085	0.385765
20	1	0	-3.073545	0.460028	1.850989
21	6	0	-4.207673	-1.139929	-0.913325
22	1	0	-3.126574	-1.338937	-2.760290
23	1	0	-5.041492	-0.788603	1.037986
24	1	0	-5.070103	-1.689831	-1.267630
25	8	0	1.207372	-2.520901	1.242737
26	8	0	0.712553	-1.302762	0.665620

Structure of $TS_{1\text{-}1}a$

```
Zero-point correction=                           0.355585 (Hartree/Particle)
 Thermal correction to Energy=                    0.381203
 Thermal correction to Enthalpy=                  0.382147
 Thermal correction to Gibbs Free Energy=         0.299383
 Sum of electronic and zero-point Energies=          -2702.189201
 Sum of electronic and thermal Energies=             -2702.163583
 Sum of electronic and thermal Enthalpies=           -2702.162639
 Sum of electronic and thermal Free Energies=        -2702.245403
One imaginary frequency: 347.2307i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.271573	0.714325	-0.390018
2	6	0	-0.790853	2.075198	-0.674178
3	6	0	-1.467201	-1.395488	0.570502
4	6	0	1.363386	2.078285	0.210686
5	8	0	2.281663	2.567807	0.841965
6	7	0	0.134566	2.713538	0.070226
7	16	0	-0.203013	0.699914	-1.455009
8	16	0	-2.279368	2.919581	-0.825675
9	6	0	-0.318935	3.934677	0.733354
10	6	0	-1.494030	4.432798	-0.103269

11	1	0	-2.237988	4.953263	0.493077
12	1	0	-1.169518	5.062632	-0.928614
13	1	0	-0.618586	3.689660	1.753523
14	1	0	0.492894	4.657322	0.758350
15	6	0	2.456880	0.079191	-1.021356
16	6	0	3.758168	0.429405	-0.648813
17	6	0	2.279351	-0.959914	-1.941422
18	6	0	4.847300	-0.241930	-1.190714
19	1	0	3.912189	1.218483	0.068737
20	6	0	3.369159	-1.630733	-2.475896
21	1	0	1.286332	-1.272676	-2.237853
22	6	0	4.660410	-1.276086	-2.100048
23	1	0	5.847874	0.043956	-0.891748
24	1	0	3.206234	-2.434660	-3.181908
25	1	0	5.512010	-1.800371	-2.514398
26	16	0	-0.904262	-0.034627	1.530654
27	6	0	-2.842488	-1.503169	0.170746
28	6	0	-3.762509	-0.463298	0.427152
29	6	0	-3.332633	-2.638333	-0.515300
30	6	0	-5.085312	-0.548965	0.021244
31	1	0	-3.431029	0.430635	0.940031
32	6	0	-4.655999	-2.711020	-0.919462
33	1	0	-2.653175	-3.451623	-0.719611
34	6	0	-5.548301	-1.672172	-0.658201
35	1	0	-5.759027	0.272499	0.234336
36	1	0	-4.997834	-3.594946	-1.445239
37	1	0	-6.580726	-1.737795	-0.976582
38	6	0	-0.403787	-2.287485	0.271179
39	8	0	-0.432688	-3.411245	-0.247613
40	6	0	2.000207	-2.485461	1.049808
41	6	0	2.363185	-1.973493	2.437917
42	1	0	1.718255	-3.536542	1.054769
43	1	0	2.828304	-2.346280	0.356279
44	1	0	3.407754	-2.146349	2.689764
45	1	0	1.721649	-2.402217	3.206668
46	7	0	0.836993	-1.707041	0.644321
47	16	0	2.081583	-0.165608	2.345923
48	6	0	0.799533	-0.391522	1.087670

Structure of **$TS_{1\text{-}1}$b**

```
Zero-point correction=                           0.355729 (Hartree/Particle)
 Thermal correction to Energy=                    0.381345
 Thermal correction to Enthalpy=                  0.382289
 Thermal correction to Gibbs Free Energy=         0.299782
 Sum of electronic and zero-point Energies=          -2702.190117
 Sum of electronic and thermal Energies=             -2702.164501
 Sum of electronic and thermal Enthalpies=           -2702.163557
 Sum of electronic and thermal Free Energies=        -2702.246063
One imaginary frequency: 414.3625i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.381725	0.793776	0.204620
2	6	0	-0.501345	2.360703	-0.246271
3	6	0	-1.457082	-1.306871	-0.345802
4	6	0	0.304075	0.765125	1.241608
5	8	0	0.267145	0.158997	2.292428
6	7	0	-0.743239	1.599089	0.819489
7	16	0	1.108946	2.266922	-0.804602
8	16	0	-1.772784	3.421340	-0.680294
9	6	0	-2.014995	1.829065	1.506819
10	6	0	-2.903469	2.557167	0.497438
11	1	0	-3.539939	3.300698	0.968263
12	1	0	-3.505572	1.862538	-0.082330

13	1	0	-1.822381	2.431782	2.394698
14	1	0	-2.448003	0.875673	1.798492
15	6	0	2.783298	0.581147	0.646962
16	6	0	3.848404	1.223010	0.005329
17	6	0	3.076136	-0.318936	1.677506
18	6	0	5.160875	0.980573	0.379611
19	1	0	3.665300	1.920499	-0.802350
20	6	0	4.393424	-0.564260	2.046680
21	1	0	2.273810	-0.829033	2.183846
22	6	0	5.441522	0.081061	1.403130
23	1	0	5.964736	1.493118	-0.132976
24	1	0	4.595756	-1.266757	2.845341
25	1	0	6.465895	-0.110655	1.695853
26	16	0	-0.745204	-0.342811	-1.630073
27	6	0	-2.865513	-1.257922	-0.069544
28	6	0	-3.749898	-0.521464	-0.887247
29	6	0	-3.427173	-1.924410	1.044192
30	6	0	-5.107795	-0.454269	-0.611285
31	1	0	-3.368477	-0.000081	-1.757180
32	6	0	-4.783295	-1.843992	1.314235
33	1	0	-2.776749	-2.500536	1.684378
34	6	0	-5.640424	-1.110881	0.493480
35	1	0	-5.753643	0.118430	-1.266266
36	1	0	-5.179420	-2.362456	2.179539
37	1	0	-6.699749	-1.057579	0.709038
38	6	0	-0.492002	-2.165890	0.253688
39	8	0	-0.647519	-3.090030	1.059828
40	6	0	1.912496	-2.766344	-0.317435
41	6	0	2.431734	-2.632074	-1.745448
42	1	0	1.528147	-3.764800	-0.116607
43	1	0	2.695910	-2.541166	0.402811
44	1	0	3.484638	-2.891784	-1.831450
45	1	0	1.846829	-3.227323	-2.444518
46	7	0	0.804792	-1.823660	-0.206390
47	16	0	2.228578	-0.855754	-2.172478
48	6	0	0.888047	-0.681891	-0.982127

Structure of $^{1}TS_{C7a}$

```
Zero-point correction=                           0.181827 (Hartree/Particle)
 Thermal correction to Energy=                    0.196878
 Thermal correction to Enthalpy=                  0.197822
 Thermal correction to Gibbs Free Energy=         0.138089
 Sum of electronic and zero-point Energies=          -1501.471488
 Sum of electronic and thermal Energies=             -1501.456436
 Sum of electronic and thermal Enthalpies=           -1501.455492
 Sum of electronic and thermal Free Energies=        -1501.515225
One imaginary frequency: 240.1465i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.723675	0.002425	-0.231252
2	6	0	-1.693782	-0.567373	-0.186957
3	6	0	-0.137777	1.178782	-0.214348
4	8	0	0.167796	2.361380	-0.220220
5	7	0	-1.473074	0.755501	-0.237984
6	16	0	-0.212430	-1.459365	-0.385325
7	16	0	-3.291195	-1.019002	-0.715741
8	6	0	-2.648679	1.598676	-0.448969
9	6	0	-3.854680	0.678201	-0.257113
10	1	0	-4.179729	0.651526	0.779860
11	1	0	-4.688838	0.949418	-0.898308
12	1	0	-2.658088	2.414071	0.271445
13	1	0	-2.604660	2.010643	-1.458041
14	6	0	2.154857	-0.024929	-0.159235

15	6	0	2.906154	1.166480	-0.058585
16	6	0	2.856783	-1.249544	-0.185426
17	6	0	4.288015	1.121451	0.011073
18	1	0	2.390022	2.112975	-0.036791
19	6	0	4.236731	-1.281109	-0.116752
20	1	0	2.317056	-2.186077	-0.253747
21	6	0	4.963523	-0.095796	-0.017984
22	1	0	4.844670	2.046721	0.089242
23	1	0	4.750777	-2.233383	-0.137379
24	1	0	6.044021	-0.122748	0.037234
25	8	0	-1.148110	0.123711	2.380636
26	8	0	-1.846517	-0.790262	1.849923

Structure of $^{3}TS_{C7a}$

```
Zero-point correction=                           0.181942 (Hartree/Particle)
 Thermal correction to Energy=                    0.196853
 Thermal correction to Enthalpy=                  0.197797
 Thermal correction to Gibbs Free Energy=         0.137355
 Sum of electronic and zero-point Energies=          -1501.473098
 Sum of electronic and thermal Energies=             -1501.458187
 Sum of electronic and thermal Enthalpies=           -1501.457243
 Sum of electronic and thermal Free Energies=        -1501.517685
One imaginary frequency: 277.3650i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745871	0.028030	-0.151354
2	6	0	-1.702033	-0.537294	-0.085155
3	6	0	-0.115105	1.202757	-0.039094
4	8	0	0.206586	2.380248	0.012202
5	7	0	-1.449219	0.801308	-0.044788
6	16	0	-0.199149	-1.421206	-0.379241
7	16	0	-3.210809	-0.872754	-0.940345
8	6	0	-2.585520	1.682903	-0.314278
9	6	0	-3.815112	0.776671	-0.387255
10	1	0	-4.286674	0.658946	0.585198
11	1	0	-4.547203	1.134795	-1.106218
12	1	0	-2.693150	2.418004	0.481495
13	1	0	-2.405315	2.201847	-1.256516
14	6	0	2.175235	-0.003848	-0.124150
15	6	0	2.936302	1.176376	0.036577
16	6	0	2.871256	-1.226219	-0.258144
17	6	0	4.318751	1.122579	0.058124
18	1	0	2.426041	2.120456	0.140579
19	6	0	4.252200	-1.265723	-0.237356
20	1	0	2.324816	-2.154021	-0.373536
21	6	0	4.987159	-0.091763	-0.079490
22	1	0	4.882460	2.038337	0.183377
23	1	0	4.760973	-2.215291	-0.342003
24	1	0	6.068765	-0.124996	-0.062277
25	8	0	-1.356818	-0.410368	2.451147
26	8	0	-2.129878	-0.991218	1.619932

Structure of $^{3}TS_{C2}$

```
Zero-point correction=                           0.181632 (Hartree/Particle)
 Thermal correction to Energy=                    0.196644
 Thermal correction to Enthalpy=                  0.197588
 Thermal correction to Gibbs Free Energy=         0.136877
 Sum of electronic and zero-point Energies=          -1501.452096
```

```
 Sum of electronic and thermal Energies=             -1501.437084
 Sum of electronic and thermal Enthalpies=           -1501.436140
 Sum of electronic and thermal Free Energies=        -1501.496851
One imaginary frequency: 278.7418i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.511168	-0.148726	0.285465
2	6	0	-1.797323	-0.396286	-0.739127
3	6	0	-0.376117	1.075002	0.417408
4	8	0	-0.058581	2.121053	0.968931
5	7	0	-1.608918	0.798385	-0.098469
6	16	0	-0.340958	-1.331636	-0.752150
7	16	0	-3.465889	-0.814768	-0.953185
8	6	0	-2.817030	1.609894	0.035117
9	6	0	-3.961919	0.603581	0.124128
10	1	0	-4.087357	0.228226	1.137813
11	1	0	-4.900563	1.010586	-0.241741
12	1	0	-2.740715	2.221223	0.931185
13	1	0	-2.916838	2.254807	-0.838822
14	6	0	1.959520	0.010853	-0.016286
15	6	0	2.818444	-1.075613	0.172037
16	6	0	2.467365	1.207695	-0.521568
17	6	0	4.165357	-0.965062	-0.142610
18	1	0	2.434724	-2.006791	0.568397
19	6	0	3.816438	1.312752	-0.836237
20	1	0	1.813190	2.054592	-0.665187
21	6	0	4.667656	0.230055	-0.647429
22	1	0	4.822497	-1.811694	0.008208
23	1	0	4.201666	2.245072	-1.228576
24	1	0	5.718750	0.316606	-0.891503
25	8	0	0.534821	-0.713962	1.858128
26	8	0	-0.588081	-1.225057	2.224124

Structure of **MECP singlet**

```
Zero-point correction= 0.182806 (Hartree/Particle)
Thermal correction to Energy= 0.197960
Thermal correction to Enthalpy= 0.198904
Thermal correction to Gibbs Free Energy= 0.137714
Sum of electronic and zero-point Energies= -1501.474086
Sum of electronic and thermal Energies= -1501.458932
Sum of electronic and thermal Enthalpies= -1501.457988
Sum of electronic and thermal Free Energies= -1501.519178
No imaginary frequencies

Standard orientation:
---------------------------------------------------------------------
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---------------------------------------------------------------------
1 6 0 0.725379 0.028329 -0.061499
2 6 0 -1.756323 -0.562663 0.088037
3 6 0 -0.135538 1.183012 0.198135
4 8 0 0.200222 2.350476 0.317718
5 7 0 -1.465336 0.783916 0.268129
6 16 0 -0.214858 -1.401806 -0.376280
7 16 0 -3.194858 -0.711824 -1.008483
8 6 0 -2.612582 1.666252 0.109750
9 6 0 -3.388234 1.118196 -1.085879
10 1 0 -4.448312 1.356799 -1.033822
11 1 0 -2.974704 1.471950 -2.027902
12 1 0 -3.222780 1.650463 1.013402
13 1 0 -2.251385 2.677290 -0.061795
14 6 0 2.154433 0.012863 -0.108827
```

```
15 6 0 2.922085 1.173361 0.144690
16 6 0 2.846318 -1.184258 -0.402744
17 6 0 4.304200 1.123086 0.105293
18 1 0 2.418087 2.099145 0.370207
19 6 0 4.226675 -1.219171 -0.444360
20 1 0 2.294915 -2.096562 -0.593856
21 6 0 4.967113 -0.066076 -0.189760
22 1 0 4.872645 2.022089 0.309152
23 1 0 4.730813 -2.150095 -0.671856
24 1 0 6.048714 -0.095853 -0.219326
25 8 0 -1.468579 -0.926667 2.409316
26 8 0 -2.253684 -1.204077 1.407725
```

Structure of **MECP triplet**

```
Zero-point correction= 0.182973 (Hartree/Particle)
Thermal correction to Energy= 0.197989
Thermal correction to Enthalpy= 0.198933
Thermal correction to Gibbs Free Energy= 0.138150
Sum of electronic and zero-point Energies= -1501.473930
Sum of electronic and thermal Energies= -1501.458914
Sum of electronic and thermal Enthalpies= -1501.457970
Sum of electronic and thermal Free Energies= -1501.518753
No imaginary frequencies

Standard orientation:
---------------------------------------------------------------------
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---------------------------------------------------------------------
1 6 0 0.725379 0.028329 -0.061499
2 6 0 -1.756323 -0.562663 0.088037
3 6 0 -0.135538 1.183012 0.198135
4 8 0 0.200222 2.350476 0.317718
5 7 0 -1.465336 0.783916 0.268129
6 16 0 -0.214858 -1.401806 -0.376280
7 16 0 -3.194858 -0.711824 -1.008483
8 6 0 -2.612582 1.666252 0.109750
9 6 0 -3.388234 1.118196 -1.085879
10 1 0 -4.448312 1.356799 -1.033822
11 1 0 -2.974704 1.471950 -2.027902
12 1 0 -3.222780 1.650463 1.013402
13 1 0 -2.251385 2.677290 -0.061795
14 6 0 2.154433 0.012863 -0.108827
15 6 0 2.922085 1.173361 0.144690
16 6 0 2.846318 -1.184258 -0.402744
17 6 0 4.304200 1.123086 0.105293
18 1 0 2.418087 2.099145 0.370207
19 6 0 4.226675 -1.219171 -0.444360
20 1 0 2.294915 -2.096562 -0.593856
21 6 0 4.967113 -0.066076 -0.189760
22 1 0 4.872645 2.022089 0.309152
23 1 0 4.730813 -2.150095 -0.671856
24 1 0 6.048714 -0.095853 -0.219326
25 8 0 -1.468579 -0.926667 2.409316
26 8 0 -2.253684 -1.204077 1.407725
```

Structure of **Int2**

```
Zero-point correction=                           0.185798 (Hartree/Particle)
 Thermal correction to Energy=                    0.199631
 Thermal correction to Enthalpy=                  0.200575
 Thermal correction to Gibbs Free Energy=         0.143904
 Sum of electronic and zero-point Energies=          -1501.507947
 Sum of electronic and thermal Energies=             -1501.494114
 Sum of electronic and thermal Enthalpies=           -1501.493170
 Sum of electronic and thermal Free Energies=        -1501.549840
```

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.533247	-0.103904	-0.145797
2	6	0	1.685463	-0.577357	0.043688
3	6	0	0.283416	1.220708	-0.294001
4	8	0	-0.130743	2.314388	-0.604950
5	7	0	1.577421	0.847522	-0.116733
6	16	0	0.334075	-0.997827	1.230903
7	16	0	3.401778	-0.974486	0.357945
8	6	0	2.811098	1.533820	-0.458884
9	6	0	3.884587	0.807494	0.341784
10	1	0	4.867527	0.888720	-0.115630
11	1	0	3.924445	1.159359	1.370201
12	1	0	3.003141	1.464538	-1.532095
13	1	0	2.739020	2.581374	-0.173373
14	6	0	-2.017797	-0.034271	-0.051996
15	6	0	-2.625864	1.036143	0.604636
16	6	0	-2.801741	-1.068442	-0.565242
17	6	0	-4.007430	1.071604	0.738727
18	1	0	-2.024313	1.836455	1.009244
19	6	0	-4.183423	-1.021943	-0.435136
20	1	0	-2.332216	-1.905964	-1.061150
21	6	0	-4.789106	0.047032	0.215937
22	1	0	-4.473101	1.903978	1.250354
23	1	0	-4.785933	-1.824956	-0.839645
24	1	0	-5.866260	0.080353	0.318432
25	8	0	-0.154083	-0.859861	-1.319286
26	8	0	1.271872	-1.207626	-1.174898

Structure of **Int3a**

```
Zero-point correction=                           0.184516 (Hartree/Particle)
 Thermal correction to Energy=                    0.199671
 Thermal correction to Enthalpy=                  0.200615
 Thermal correction to Gibbs Free Energy=         0.140697
 Sum of electronic and zero-point Energies=          -1501.495299
 Sum of electronic and thermal Energies=             -1501.480145
 Sum of electronic and thermal Enthalpies=           -1501.479201
 Sum of electronic and thermal Free Energies=        -1501.539119
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.812362	1.008972	0.093549
2	6	0	1.694231	-0.326687	-0.711239
3	6	0	0.380478	0.793548	1.009460
4	8	0	0.256364	1.162887	2.156103
5	7	0	1.509127	0.141809	0.566934
6	16	0	0.623651	-0.188427	-1.951523
7	16	0	3.242655	-1.101560	-0.860896
8	6	0	2.676503	0.056033	1.463342
9	6	0	3.536751	-1.081513	0.943380
10	1	0	4.592908	-0.914052	1.137451
11	1	0	3.236727	-2.045360	1.350042
12	1	0	3.203155	1.010584	1.426632
13	1	0	2.336410	-0.124201	2.478923
14	6	0	-1.968190	0.138856	0.129980
15	6	0	-1.885901	-1.087508	0.801746
16	6	0	-3.159954	0.500992	-0.514586
17	6	0	-2.981401	-1.935239	0.833552

18	1	0	-0.967582	-1.380926	1.293234
19	6	0	-4.248245	-0.351741	-0.475898
20	1	0	-3.223448	1.442374	-1.042021
21	6	0	-4.162682	-1.569855	0.196714
22	1	0	-2.913417	-2.881438	1.353586
23	1	0	-5.167391	-0.070759	-0.972878
24	1	0	-5.017149	-2.233755	0.220798
25	8	0	-0.905968	2.172181	-0.401811
26	8	0	0.284559	2.911120	-0.358742

Structure of **Int4**

```
Zero-point correction=                           0.180632 (Hartree/Particle)
 Thermal correction to Energy=                    0.194523
 Thermal correction to Enthalpy=                  0.195467
 Thermal correction to Gibbs Free Energy=         0.138432
 Sum of electronic and zero-point Energies=          -1426.305851
 Sum of electronic and thermal Energies=             -1426.291960
 Sum of electronic and thermal Enthalpies=           -1426.291016
 Sum of electronic and thermal Free Energies=        -1426.348051
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.545591	0.124695	0.053374
2	6	0	-1.886179	-0.411250	-0.191000
3	6	0	-0.259863	1.265334	0.132761
4	8	0	-0.041018	2.461581	0.253364
5	7	0	-1.689842	0.843749	-0.003653
6	16	0	-0.332529	-1.364504	-0.264598
7	16	0	-3.493211	-0.942196	-0.288629
8	6	0	-2.878898	1.700047	-0.024327
9	6	0	-4.063975	0.756501	0.213778
10	1	0	-4.340510	0.694054	1.263539
11	1	0	-4.932119	1.018504	-0.383668
12	1	0	-2.800329	2.455852	0.752495
13	1	0	-2.925936	2.187573	-0.998722
14	6	0	2.001146	0.100652	0.008953
15	6	0	2.708078	-1.115770	0.006416
16	6	0	2.755096	1.288367	-0.036655
17	6	0	4.093601	-1.144069	-0.063093
18	1	0	2.175402	-2.056026	0.078081
19	6	0	4.141026	1.250893	-0.093711
20	1	0	2.242131	2.238102	-0.028538
21	6	0	4.823994	0.038484	-0.112246
22	1	0	4.604205	-2.099263	-0.067182
23	1	0	4.692831	2.182636	-0.128286
24	1	0	5.905198	0.015718	-0.158104
25	8	0	-0.391212	-2.306515	0.894398

Structure of **4**

```
Zero-point correction=                           0.181275 (Hartree/Particle)
 Thermal correction to Energy=                    0.195435
 Thermal correction to Enthalpy=                  0.196379
 Thermal correction to Gibbs Free Energy=         0.137972
 Sum of electronic and zero-point Energies=          -1426.376546
 Sum of electronic and thermal Energies=             -1426.362385
 Sum of electronic and thermal Enthalpies=           -1426.361441
 Sum of electronic and thermal Free Energies=        -1426.419848
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.754643	0.502672	0.958919
2	6	0	0.336801	1.224776	0.154216
3	6	0	-2.045297	0.227604	0.301725
4	6	0	-2.193699	0.352369	-1.081232
5	6	0	-3.128945	-0.181397	1.082904
6	6	0	-3.414109	0.071211	-1.676725
7	1	0	-1.356719	0.658629	-1.694981
8	6	0	-4.347563	-0.460384	0.485553
9	1	0	-3.000709	-0.277622	2.152541
10	6	0	-4.491280	-0.334305	-0.894371
11	1	0	-3.526601	0.166246	-2.748773
12	1	0	-5.187021	-0.776311	1.091252
13	1	0	-5.443689	-0.553505	-1.360186
14	8	0	0.158886	2.394601	-0.116090
15	6	0	2.699341	1.440512	-0.499075
16	6	0	3.945833	0.681474	-0.082751
17	1	0	2.635096	2.412664	-0.019363
18	1	0	2.654362	1.572495	-1.581276
19	1	0	4.792795	0.903352	-0.726839
20	1	0	4.212925	0.867900	0.955877
21	6	0	1.780012	-0.748466	-0.074997
22	7	0	1.555912	0.612521	-0.071557
23	16	0	3.481387	-1.076148	-0.261452
24	8	0	-0.544898	0.396236	2.151395
25	16	0	0.649711	-1.939138	0.018028

Structure of **3**

```
Zero-point correction=                           0.181499 (Hartree/Particle)
 Thermal correction to Energy=                    0.195682
 Thermal correction to Enthalpy=                  0.196627
 Thermal correction to Gibbs Free Energy=         0.137788
 Sum of electronic and zero-point Energies=          -1426.382375
 Sum of electronic and thermal Energies=             -1426.368191
 Sum of electronic and thermal Enthalpies=           -1426.367247
 Sum of electronic and thermal Free Energies=        -1426.426086
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.768329	1.112705	0.107940
2	6	0	-0.441055	0.844970	0.974191
3	6	0	1.828427	0.114799	0.109404
4	6	0	1.673978	-1.077696	0.834096
5	6	0	3.011054	0.316776	-0.618408
6	6	0	2.673961	-2.036959	0.832167
7	1	0	0.772343	-1.258920	1.403831
8	6	0	4.005631	-0.642923	-0.618746
9	1	0	3.131051	1.231296	-1.182360
10	6	0	3.840850	-1.822522	0.106662
11	1	0	2.543399	-2.951672	1.395178
12	1	0	4.912875	-0.477964	-1.185153
13	1	0	4.621577	-2.572442	0.103679
14	8	0	-0.443979	1.231381	2.126354
15	16	0	0.788681	2.585430	-0.606943
16	6	0	-2.789445	0.143178	1.197486
17	6	0	-3.618239	-0.990651	0.611995
18	1	0	-3.304507	1.100578	1.104077
19	1	0	-2.562482	-0.033850	2.244720
20	1	0	-3.373978	-1.949078	1.065845

21	1	0	-4.683170	-0.801053	0.716163
22	6	0	-1.593635	-0.303318	-0.868812
23	7	0	-1.538949	0.205183	0.430742
24	16	0	-3.177583	-1.056269	-1.156952
25	8	0	-0.708668	-0.248868	-1.684692

Structure of **Int3b**

```
Zero-point correction=                           0.185255 (Hartree/Particle)
 Thermal correction to Energy=                    0.199634
 Thermal correction to Enthalpy=                  0.200579
 Thermal correction to Gibbs Free Energy=         0.143113
 Sum of electronic and zero-point Energies=          -1501.493286
 Sum of electronic and thermal Energies=             -1501.478906
 Sum of electronic and thermal Enthalpies=           -1501.477962
 Sum of electronic and thermal Free Energies=        -1501.535428
Noimaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.174857	1.898843	1.142937
2	6	0	0.588273	0.466754	0.189810
3	6	0	-0.267641	-0.623404	0.783761
4	7	0	-1.615515	-0.593617	0.280536
5	6	0	-2.699038	-1.395659	0.879634
6	6	0	-3.986303	-0.629881	0.603376
7	16	0	-3.704024	0.255017	-0.989136
8	6	0	-2.008295	0.190580	-0.704348
9	8	0	-1.220938	0.894292	-1.448807
10	8	0	0.194677	0.528799	-1.281303
11	8	0	0.026786	-1.440955	1.614614
12	1	0	-2.698552	-2.380387	0.413638
13	1	0	-2.513815	-1.496973	1.944715
14	1	0	-4.840917	-1.289428	0.481473
15	1	0	-4.194567	0.120514	1.362079
16	6	0	2.036941	0.066954	-0.012671
17	6	0	3.072024	0.942136	0.301350
18	6	0	4.391909	0.572532	0.077865
19	6	0	4.687837	-0.674681	-0.462659
20	6	0	3.657033	-1.552453	-0.781995
21	6	0	2.337387	-1.182842	-0.560382
22	1	0	2.828098	1.902707	0.733324
23	1	0	5.190958	1.257733	0.330924
24	1	0	5.717703	-0.963159	-0.631427
25	1	0	3.880034	-2.524667	-1.202584
26	1	0	1.541370	-1.870089	-0.815194

Structure of **Int4b**

```
Zero-point correction=                           0.184633 (Hartree/Particle)
 Thermal correction to Energy=                    0.199569
 Thermal correction to Enthalpy=                  0.200513
 Thermal correction to Gibbs Free Energy=         0.141285
 Sum of electronic and zero-point Energies=          -1501.490881
 Sum of electronic and thermal Energies=             -1501.475945
 Sum of electronic and thermal Enthalpies=           -1501.475001
 Sum of electronic and thermal Free Energies=        -1501.534229
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.095354	-1.802034	-1.156468
2	6	0	0.641633	-0.390355	-0.440980
3	6	0	-0.269744	0.776098	-0.692410
4	7	0	-1.603592	0.640557	-0.207276
5	6	0	-2.718845	1.355879	-0.860155
6	6	0	-3.929950	0.445473	-0.722085
7	16	0	-3.704947	-0.410613	0.889311
8	6	0	-1.997970	-0.176716	0.768667
9	8	0	0.003175	1.726118	-1.380229
10	1	0	-2.868591	2.310418	-0.356403
11	1	0	-2.465894	1.530378	-1.901597
12	1	0	-4.862096	1.002413	-0.691316
13	1	0	-3.969433	-0.312244	-1.501468
14	6	0	2.057205	-0.083022	-0.140932
15	6	0	3.064030	-1.005689	-0.436077
16	6	0	4.387430	-0.727178	-0.130712
17	6	0	4.726395	0.477499	0.478129
18	6	0	3.732158	1.402357	0.779370
19	6	0	2.407989	1.127306	0.471214
20	1	0	2.795859	-1.938986	-0.911082
21	1	0	5.156887	-1.450127	-0.369592
22	1	0	5.760184	0.694673	0.715378
23	1	0	3.987868	2.340299	1.255378
24	1	0	1.645790	1.852702	0.716412
25	8	0	0.128821	-0.296159	1.531720
26	8	0	-1.232488	-0.720083	1.639202

Structure of **Int3**

```
Zero-point correction=                           0.184199 (Hartree/Particle)
 Thermal correction to Energy=                    0.199181
 Thermal correction to Enthalpy=                  0.200125
 Thermal correction to Gibbs Free Energy=         0.139999
 Sum of electronic and zero-point Energies=          -1501.493369
 Sum of electronic and thermal Energies=             -1501.478387
 Sum of electronic and thermal Enthalpies=           -1501.477443
 Sum of electronic and thermal Free Energies=        -1501.537569
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.752086	1.105627	-0.006617
2	6	0	-0.363494	0.851727	0.983906
3	6	0	1.937674	0.268454	0.086918
4	6	0	1.992309	-0.777497	1.022788
5	6	0	3.035235	0.473575	-0.764584
6	6	0	3.112497	-1.588605	1.106469
7	1	0	1.161533	-0.956110	1.691008
8	6	0	4.148936	-0.339597	-0.679748
9	1	0	2.993761	1.272865	-1.491345
10	6	0	4.191566	-1.372781	0.256496
11	1	0	3.143367	-2.390048	1.832735
12	1	0	4.987918	-0.175190	-1.343143
13	1	0	5.065503	-2.008456	0.319745
14	8	0	-0.292462	1.376861	2.080367
15	16	0	0.532167	2.413120	-0.970972
16	6	0	-2.674640	0.124116	1.432204
17	6	0	-3.835818	0.099652	0.452718
18	1	0	-2.677634	1.021523	2.043639
19	1	0	-2.687451	-0.752106	2.082673
20	1	0	-4.742089	-0.294674	0.905635
21	1	0	-4.029387	1.084639	0.032375

22	6	0	-1.561565	-0.727202	-0.521720
23	7	0	-1.462383	0.122224	0.604228
24	16	0	-3.296115	-1.036515	-0.872818
25	8	0	-0.698740	-1.822984	-0.659238
26	8	0	-0.654346	-0.602440	-1.548035

Structure of **TS2**

```
Zero-point correction=                           0.182921 (Hartree/Particle)
 Thermal correction to Energy=                    0.197002
 Thermal correction to Enthalpy=                  0.197946
 Thermal correction to Gibbs Free Energy=         0.141050
 Sum of electronic and zero-point Energies=          -1501.472007
 Sum of electronic and thermal Energies=             -1501.457926
 Sum of electronic and thermal Enthalpies=           -1501.456981
 Sum of electronic and thermal Free Energies=        -1501.513877
One imaginary frequency: 158.3440i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.660410	-0.016114	-0.226185
2	6	0	-1.722395	-0.554980	0.193878
3	6	0	-0.214263	1.201531	-0.178329
4	8	0	0.138372	2.363635	-0.248471
5	7	0	-1.521744	0.798815	-0.093611
6	16	0	-0.279680	-1.416417	-0.552161
7	16	0	-3.385482	-1.008886	-0.315245
8	6	0	-2.728544	1.604140	-0.111580
9	6	0	-3.761581	0.728936	-0.816569
10	1	0	-4.779112	0.960222	-0.510900
11	1	0	-3.673203	0.800538	-1.898281
12	1	0	-3.042926	1.844334	0.906343
13	1	0	-2.537237	2.526359	-0.655785
14	6	0	2.092503	-0.025783	-0.174231
15	6	0	2.828886	1.157936	0.048064
16	6	0	2.806286	-1.233413	-0.336381
17	6	0	4.211558	1.123612	0.099296
18	1	0	2.303525	2.090059	0.177212
19	6	0	4.185792	-1.254521	-0.286719
20	1	0	2.271369	-2.161357	-0.492995
21	6	0	4.898102	-0.075471	-0.069012
22	1	0	4.759271	2.040779	0.273625
23	1	0	4.711929	-2.191604	-0.413804
24	1	0	5.979470	-0.094584	-0.027986
25	8	0	-0.606316	-0.070934	2.158709
26	8	0	-1.561906	-0.859806	1.630130

Structure of **TS3a**

```
Zero-point correction=                           0.183974 (Hartree/Particle)
 Thermal correction to Energy=                    0.197969
 Thermal correction to Enthalpy=                  0.198913
 Thermal correction to Gibbs Free Energy=         0.142552
 Sum of electronic and zero-point Energies=          -1501.481566
 Sum of electronic and thermal Energies=             -1501.467571
 Sum of electronic and thermal Enthalpies=           -1501.466627
 Sum of electronic and thermal Free Energies=        -1501.522988
One imaginary frequency: 164.9254i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.561955	-0.213819	0.363940
2	6	0	-1.751371	-0.461825	-0.437032
3	6	0	-0.293414	1.085662	0.420103
4	8	0	0.063488	2.116644	0.923046
5	7	0	-1.567566	0.843628	-0.069964
6	16	0	-0.360390	-1.218650	-1.069138
7	16	0	-3.399379	-0.892476	-0.614083
8	6	0	-2.770696	1.515530	0.429247
9	6	0	-3.935023	0.844897	-0.289506
10	1	0	-4.836127	0.824811	0.316928
11	1	0	-4.146096	1.305076	-1.252300
12	1	0	-2.826688	1.370468	1.509113
13	1	0	-2.723388	2.577579	0.202332
14	6	0	2.015207	-0.054957	0.080013
15	6	0	2.434859	0.866248	-0.879922
16	6	0	2.956812	-0.838304	0.745415
17	6	0	3.784958	1.006888	-1.166999
18	1	0	1.707969	1.472515	-1.404998
19	6	0	4.307995	-0.692573	0.456031
20	1	0	2.634399	-1.555814	1.486191
21	6	0	4.724788	0.228164	-0.498551
22	1	0	4.103615	1.725141	-1.911221
23	1	0	5.035231	-1.300916	0.978160
24	1	0	5.778181	0.339201	-0.722029
25	8	0	0.311331	-0.950168	1.481923
26	8	0	-1.101600	-0.991591	1.705366

Structure of **TS4a**

```
Zero-point correction=                           0.183273 (Hartree/Particle)
 Thermal correction to Energy=                    0.198019
 Thermal correction to Enthalpy=                  0.198964
 Thermal correction to Gibbs Free Energy=         0.139323
 Sum of electronic and zero-point Energies=          -1501.457931
 Sum of electronic and thermal Energies=             -1501.443185
 Sum of electronic and thermal Enthalpies=           -1501.442241
 Sum of electronic and thermal Free Energies=        -1501.501881
One imaginary frequency: 296.9104i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.079628	1.910018	0.411179
2	6	0	1.002156	-0.227502	0.582448
3	6	0	-0.154891	0.638623	0.112531
4	7	0	-1.315754	-0.070831	-0.239126
5	6	0	-1.216284	-1.366040	-0.948155
6	6	0	-2.510881	-2.106772	-0.689728
7	16	0	-3.758315	-0.778125	-0.619163
8	6	0	-2.588750	0.435639	-0.126567
9	8	0	-0.028182	1.832585	0.021519
10	1	0	-1.089696	-1.159615	-2.013062
11	1	0	-0.362282	-1.934041	-0.593838
12	1	0	-2.746739	-2.798707	-1.494502
13	1	0	-2.500621	-2.634262	0.262569
14	6	0	2.336942	-0.043661	0.118324
15	6	0	3.386317	-0.707886	0.787899
16	6	0	4.680296	-0.593669	0.322379
17	6	0	4.944897	0.179443	-0.807603
18	6	0	3.916309	0.843140	-1.476142
19	6	0	2.618323	0.744569	-1.017663
20	1	0	3.166075	-1.285583	1.674001
21	1	0	5.488202	-1.094362	0.838302

22	1	0	5.961904	0.270791	-1.166941
23	1	0	4.135931	1.438930	-2.351563
24	1	0	1.821231	1.257864	-1.533493
25	8	0	0.736680	-1.180887	1.428287
26	8	0	0.073594	-0.208046	2.329419

Structure of **TS5a**

```
Zero-point correction=                           0.362561 (Hartree/Particle)
 Thermal correction to Energy=                    0.391016
 Thermal correction to Enthalpy=                  0.391960
 Thermal correction to Gibbs Free Energy=         0.301885
 Sum of electronic and zero-point Energies=          -2852.617338
 Sum of electronic and thermal Energies=             -2852.588883
 Sum of electronic and thermal Enthalpies=           -2852.587939
 Sum of electronic and thermal Free Energies=        -2852.678013
One imaginary frequency: 167.5204i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.620636	1.214914	-1.479074
2	6	0	-1.187278	1.959721	-0.004293
3	6	0	-2.010569	1.533298	1.081979
4	7	0	-2.984175	0.602822	0.564335
5	6	0	-4.120069	0.020664	1.278489
6	6	0	-4.658893	-1.081128	0.362701
7	16	0	-4.135657	-0.646885	-1.361909
8	6	0	-2.932425	0.377104	-0.725761
9	8	0	-2.036290	1.859915	2.257984
10	1	0	-3.783273	-0.380863	2.230489
11	1	0	-4.853896	0.807886	1.454258
12	1	0	-4.220684	-2.049592	0.588335
13	1	0	-5.742805	-1.146511	0.385745
14	6	0	-0.033491	2.844413	0.097345
15	6	0	0.427814	3.573261	-1.008213
16	6	0	1.555859	4.371923	-0.913139
17	6	0	2.249130	4.471091	0.290409
18	6	0	1.795722	3.762720	1.397826
19	6	0	0.669693	2.955309	1.306553
20	1	0	-0.095197	3.510780	-1.954255
21	1	0	1.895420	4.920327	-1.782640
22	1	0	3.130229	5.095609	0.362844
23	1	0	2.324925	3.831696	2.340133
24	1	0	0.328488	2.406660	2.171274
25	16	0	4.340498	-1.601907	0.915299
26	6	0	2.996799	-1.828289	-0.184686
27	7	0	2.571404	-0.617534	-0.671383
28	6	0	3.519983	0.496405	-0.450483
29	6	0	4.201685	0.216427	0.874585
30	16	0	2.459447	-3.339974	-0.549891
31	1	0	5.192001	0.661901	0.924870
32	1	0	3.605716	0.548321	1.723180
33	1	0	4.238056	0.518392	-1.271761
34	1	0	2.971297	1.432476	-0.436408
35	6	0	1.385137	-0.316478	-1.363418
36	6	0	0.170235	-1.288359	-1.290843
37	8	0	1.329441	0.727752	-1.973291
38	6	0	-0.282026	-1.601008	0.135882
39	6	0	0.077569	-0.831563	1.236926
40	6	0	-0.414672	-1.134763	2.504013
41	6	0	-1.281638	-2.204401	2.676627
42	6	0	-1.652914	-2.973885	1.574440
43	6	0	-1.154358	-2.673993	0.315824
44	1	0	0.740864	0.014342	1.123550
45	1	0	-0.125353	-0.526945	3.351338

46	1	0	-1.665560	-2.441272	3.660949
47	1	0	-2.327262	-3.811890	1.701764
48	1	0	-1.424786	-3.272780	-0.543033
49	8	0	-0.884404	-0.741545	-2.034290
50	8	0	0.350629	-2.336715	-2.103989

Structure of **TS3b**

```
Zero-point correction=                           0.184675 (Hartree/Particle)
 Thermal correction to Energy=                    0.198314
 Thermal correction to Enthalpy=                  0.199258
 Thermal correction to Gibbs Free Energy=         0.143680
 Sum of electronic and zero-point Energies=          -1501.488617
 Sum of electronic and thermal Energies=             -1501.474978
 Sum of electronic and thermal Enthalpies=           -1501.474034
 Sum of electronic and thermal Free Energies=        -1501.529612
One imaginary frequency: 153.1431i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.258387	-1.465578	-1.101413
2	6	0	0.509470	-0.241132	-0.057916
3	6	0	-0.251984	1.054362	-0.350917
4	7	0	-1.576674	0.892719	0.098203
5	6	0	-2.727190	1.625454	-0.453995
6	6	0	-3.782738	0.574465	-0.777611
7	16	0	-3.566636	-0.745401	0.487932
8	6	0	-1.899805	-0.325683	0.618137
9	8	0	-1.180362	-0.879394	1.568704
10	8	0	0.219955	-0.512955	1.403424
11	8	0	0.129820	2.042772	-0.917129
12	1	0	-3.084392	2.332516	0.293809
13	1	0	-2.411944	2.164445	-1.343723
14	1	0	-4.794058	0.963492	-0.696396
15	1	0	-3.630797	0.120358	-1.754400
16	6	0	2.009047	-0.092691	-0.024135
17	6	0	2.842803	-1.014095	-0.652180
18	6	0	4.222458	-0.872411	-0.578694
19	6	0	4.780315	0.187250	0.128263
20	6	0	3.952301	1.107740	0.761838
21	6	0	2.572914	0.970373	0.685793
22	1	0	2.403119	-1.834709	-1.201307
23	1	0	4.861670	-1.590650	-1.076068
24	1	0	5.855970	0.297560	0.182891
25	1	0	4.379623	1.935570	1.312951
26	1	0	1.937049	1.692869	1.179029

Structure of **TS4b**

```
Zero-point correction=                           0.184181 (Hartree/Particle)
 Thermal correction to Energy=                    0.198407
 Thermal correction to Enthalpy=                  0.199351
 Thermal correction to Gibbs Free Energy=         0.141805
 Sum of electronic and zero-point Energies=          -1501.491108
 Sum of electronic and thermal Energies=             -1501.476882
 Sum of electronic and thermal Enthalpies=           -1501.475938
 Sum of electronic and thermal Free Energies=        -1501.533485
One imaginary frequency: 215.9352i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.116737	-1.748954	-1.271143
2	6	0	0.624319	-0.387505	-0.388271
3	6	0	-0.275970	0.778159	-0.684847
4	7	0	-1.607627	0.648331	-0.180063
5	6	0	-2.720369	1.430112	-0.755954
6	6	0	-3.957024	0.552112	-0.628380
7	16	0	-3.698434	-0.430988	0.905085
8	6	0	-1.994426	-0.231570	0.737168
9	8	0	-0.008028	1.723027	-1.380066
10	1	0	-2.820661	2.359316	-0.195994
11	1	0	-2.494011	1.654123	-1.793839
12	1	0	-4.866336	1.135623	-0.514663
13	1	0	-4.058335	-0.144801	-1.457022
14	6	0	2.050950	-0.067209	-0.101875
15	6	0	3.060699	-0.979411	-0.409909
16	6	0	4.383772	-0.693848	-0.106232
17	6	0	4.716287	0.507996	0.511434
18	6	0	3.716684	1.422427	0.825428
19	6	0	2.392608	1.137998	0.521826
20	1	0	2.794627	-1.908703	-0.894055
21	1	0	5.157676	-1.409153	-0.353843
22	1	0	5.749562	0.731326	0.745335
23	1	0	3.967416	2.358948	1.306951
24	1	0	1.625130	1.856255	0.773962
25	8	0	0.160603	-0.477536	1.406744
26	8	0	-1.212537	-0.883959	1.520597

Structure of **TS5b**

```
Zero-point correction=                           0.183206 (Hartree/Particle)
 Thermal correction to Energy=                    0.198055
 Thermal correction to Enthalpy=                  0.198999
 Thermal correction to Gibbs Free Energy=         0.139055
 Sum of electronic and zero-point Energies=          -1501.466047
 Sum of electronic and thermal Energies=             -1501.451198
 Sum of electronic and thermal Enthalpies=           -1501.450254
 Sum of electronic and thermal Free Energies=        -1501.510198
One imaginary frequency: 194.1151i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.304821	2.329326	0.618923
2	6	0	-0.727492	0.924044	-0.115277
3	6	0	0.319587	0.401327	-1.072102
4	7	0	1.589415	0.064828	-0.567255
5	6	0	2.754400	0.021787	-1.464844
6	6	0	3.971719	0.160064	-0.559278
7	16	0	3.489910	-0.668816	1.002771
8	6	0	1.820132	-0.462616	0.652477
9	8	0	0.139148	0.433659	-2.265112
10	1	0	2.755912	-0.928235	-2.000819
11	1	0	2.690995	0.839335	-2.176691
12	1	0	4.847000	-0.334240	-0.971326
13	1	0	4.202374	1.198625	-0.331350
14	6	0	-2.021942	0.268644	-0.079536
15	6	0	-3.091261	0.841636	0.629111
16	6	0	-4.321349	0.214075	0.672441
17	6	0	-4.509978	-0.997796	0.008779
18	6	0	-3.460178	-1.578573	-0.695511
19	6	0	-2.224609	-0.955581	-0.739555
20	1	0	-2.940057	1.781803	1.140784
21	1	0	-5.137565	0.664844	1.221528

22	1	0	-5.474349	-1.488462	0.043995
23	1	0	-3.603909	-2.522278	-1.204942
24	1	0	-1.410716	-1.425520	-1.268463
25	8	0	0.305332	-1.917303	0.759024
26	8	0	0.921623	-0.745095	1.524930

Structure of **TS6b**

```
Zero-point correction=                           0.361426 (Hartree/Particle)
 Thermal correction to Energy=                    0.390583
 Thermal correction to Enthalpy=                  0.391527
 Thermal correction to Gibbs Free Energy=         0.298166
 Sum of electronic and zero-point Energies=          -2852.607767
 Sum of electronic and thermal Energies=             -2852.578610
 Sum of electronic and thermal Enthalpies=           -2852.577666
 Sum of electronic and thermal Free Energies=        -2852.671027
One imaginary frequency: 521.0122i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.649085	0.862936	0.340164
2	6	0	-0.546267	2.128458	0.591369
3	6	0	-2.567122	1.940998	-0.587552
4	8	0	-3.349634	2.333613	-1.453527
5	7	0	-1.325110	2.608052	-0.369045
6	16	0	-1.230684	0.764119	1.330616
7	16	0	0.830879	3.097823	0.967801
8	6	0	-0.886731	3.861743	-0.979014
9	6	0	0.598923	3.973177	-0.644696
10	1	0	1.217673	3.467098	-1.382209
11	1	0	0.924335	5.003403	-0.530127
12	1	0	-1.055967	3.825449	-2.052539
13	1	0	-1.468453	4.679363	-0.550130
14	6	0	-3.695671	-0.131081	0.438449
15	6	0	-3.774753	-1.004260	1.538931
16	6	0	-4.644303	-0.280722	-0.589665
17	6	0	-4.744673	-1.991762	1.600933
18	1	0	-3.074233	-0.909753	2.360257
19	6	0	-5.615240	-1.268528	-0.516234
20	1	0	-4.600428	0.379282	-1.442410
21	6	0	-5.672713	-2.133113	0.572829
22	1	0	-4.779000	-2.650693	2.459455
23	1	0	-6.331412	-1.366960	-1.322802
24	1	0	-6.431897	-2.902887	0.623076
25	8	0	0.867047	0.432067	-0.733947
26	6	0	0.557840	-0.813626	-1.203989
27	7	0	0.672052	-1.918476	-0.286648
28	16	0	-0.990625	-1.039830	-2.129490
29	8	0	1.631234	-0.451188	-1.963463
30	6	0	1.626418	-2.059758	0.679822
31	6	0	-0.205959	-3.052101	-0.593314
32	6	0	-1.502135	-2.456920	-1.112354
33	6	0	2.479577	-0.882493	1.107226
34	8	0	1.802274	-3.120076	1.260865
35	1	0	-0.364823	-3.628444	0.313775
36	1	0	0.261218	-3.695378	-1.342194
37	1	0	-2.050763	-3.161227	-1.732988
38	1	0	-2.142232	-2.117371	-0.301832
39	6	0	3.735245	-0.677978	0.399250
40	16	0	1.986648	-0.072040	2.444635
41	6	0	4.189935	-1.627598	-0.529739
42	6	0	4.506187	0.473322	0.623402
43	6	0	5.388139	-1.438994	-1.198540
44	1	0	3.613380	-2.522144	-0.720148
45	6	0	5.693916	0.665029	-0.057621

46	1	0	4.150788	1.213368	1.326450
47	6	0	6.140999	-0.292386	-0.967292
48	1	0	5.733217	-2.183111	-1.904225
49	1	0	6.274995	1.561633	0.114771
50	1	0	7.072972	-0.141192	-1.496938

Structure of **Int6a**

```
Zero-point correction=                           0.361694 (Hartree/Particle)
 Thermal correction to Energy=                    0.388291
 Thermal correction to Enthalpy=                  0.389235
 Thermal correction to Gibbs Free Energy=         0.303284
 Sum of electronic and zero-point Energies=          -2777.433895
 Sum of electronic and thermal Energies=             -2777.407298
 Sum of electronic and thermal Enthalpies=           -2777.406353
 Sum of electronic and thermal Free Energies=        -2777.492304
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.312840	-0.084170	0.111830
2	6	0	1.331209	2.292637	-0.788873
3	6	0	-2.347724	-0.537857	-0.097051
4	6	0	1.583315	1.025807	1.133969
5	8	0	1.750007	0.885002	2.313408
6	7	0	1.755034	2.255069	0.472213
7	16	0	0.810343	0.823982	-1.443685
8	16	0	1.305417	3.843836	-1.486396
9	6	0	1.930801	3.556456	1.125963
10	6	0	2.176525	4.543158	-0.010828
11	1	0	1.762020	5.525556	0.196244
12	1	0	3.229112	4.627314	-0.270616
13	1	0	1.017081	3.782078	1.676683
14	1	0	2.773885	3.514560	1.810502
15	6	0	2.611734	-0.849373	-0.172279
16	6	0	3.540980	-1.068935	0.845206
17	6	0	2.865197	-1.380277	-1.437871
18	6	0	4.698857	-1.795636	0.597228
19	1	0	3.365460	-0.685427	1.837984
20	6	0	4.018993	-2.112963	-1.681330
21	1	0	2.158851	-1.243476	-2.243838
22	6	0	4.943382	-2.320959	-0.665058
23	1	0	5.407568	-1.952090	1.400118
24	1	0	4.190679	-2.519375	-2.669523
25	1	0	5.845817	-2.887298	-0.855967
26	16	0	-1.314646	0.063279	1.157514
27	6	0	-3.748331	-0.146959	-0.091910
28	6	0	-4.201732	0.917080	0.716303
29	6	0	-4.718318	-0.808212	-0.874818
30	6	0	-5.541722	1.275120	0.763256
31	1	0	-3.493426	1.489992	1.300531
32	6	0	-6.053305	-0.432778	-0.833126
33	1	0	-4.404093	-1.622153	-1.509150
34	6	0	-6.483473	0.606195	-0.011798
35	1	0	-5.847649	2.095323	1.401947
36	1	0	-6.769281	-0.965799	-1.448121
37	1	0	-7.526962	0.893092	0.016878
38	6	0	-1.755039	-1.508409	-0.935540
39	8	0	-2.277318	-2.180792	-1.828044
40	6	0	0.094852	-3.115556	-0.686050
41	6	0	-0.002906	-3.651882	0.736907
42	1	0	-0.551452	-3.655835	-1.373700
43	1	0	1.120314	-3.174243	-1.039854
44	1	0	0.663951	-4.495439	0.905405
45	1	0	-1.022330	-3.933533	0.995711

46	7	0	-0.351329	-1.718868	-0.658641
47	16	0	0.527862	-2.259615	1.798070
48	6	0	0.114948	-1.019147	0.500737
49	8	0	-0.877137	1.496990	0.926702

Structure of **Int6b**

```
Zero-point correction=                           0.361340 (Hartree/Particle)
 Thermal correction to Energy=                    0.388225
 Thermal correction to Enthalpy=                  0.389169
 Thermal correction to Gibbs Free Energy=         0.302817
 Sum of electronic and zero-point Energies=          -2777.433577
 Sum of electronic and thermal Energies=             -2777.406693
 Sum of electronic and thermal Enthalpies=           -2777.405749
 Sum of electronic and thermal Free Energies=        -2777.492101
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.234592	0.243719	0.060001
2	6	0	0.035494	2.431601	-0.480825
3	6	0	-1.811088	-1.215144	0.069672
4	6	0	1.355445	1.364698	1.103251
5	8	0	1.888731	1.268947	2.176853
6	7	0	0.769520	2.536465	0.643210
7	16	0	-0.029151	0.905551	-1.174082
8	16	0	-0.779131	3.864341	-0.922580
9	6	0	0.616589	3.790365	1.389869
10	6	0	0.164261	4.814440	0.354932
11	1	0	-0.495613	5.566904	0.776716
12	1	0	1.000540	5.290551	-0.151261
13	1	0	-0.130579	3.637795	2.169348
14	1	0	1.566426	4.067176	1.840071
15	6	0	2.545930	0.007301	-0.678043
16	6	0	3.768813	0.345732	-0.099711
17	6	0	2.536384	-0.609381	-1.930956
18	6	0	4.958670	0.068105	-0.762207
19	1	0	3.807862	0.807596	0.874986
20	6	0	3.726673	-0.891220	-2.586116
21	1	0	1.602763	-0.889416	-2.397460
22	6	0	4.943275	-0.552947	-2.004296
23	1	0	5.898805	0.335512	-0.297444
24	1	0	3.699202	-1.374811	-3.553832
25	1	0	5.871349	-0.770027	-2.517252
26	16	0	-1.033329	-0.552736	1.474305
27	6	0	-3.185023	-0.863230	-0.229422
28	6	0	-3.982485	-0.156543	0.693921
29	6	0	-3.770355	-1.168068	-1.475893
30	6	0	-5.276110	0.236595	0.384196
31	1	0	-3.590631	0.074703	1.676448
32	6	0	-5.066796	-0.776750	-1.775877
33	1	0	-3.191688	-1.719142	-2.201728
34	6	0	-5.833570	-0.068095	-0.854156
35	1	0	-5.856531	0.777038	1.122508
36	1	0	-5.482831	-1.027220	-2.744810
37	1	0	-6.845853	0.232351	-1.092560
38	6	0	-1.009446	-2.158290	-0.639035
39	8	0	-1.351159	-2.966831	-1.505529
40	6	0	1.191997	-3.251475	-0.189973
41	6	0	1.471614	-3.461857	1.290556
42	1	0	0.644047	-4.080081	-0.633929
43	1	0	2.123715	-3.108108	-0.737424
44	1	0	2.361035	-4.063134	1.472068
45	1	0	0.617335	-3.901941	1.802729
46	7	0	0.360150	-2.055077	-0.276216

47	16	0	1.771679	-1.780459	1.937208
48	6	0	0.644758	-1.055147	0.703120
49	8	0	-1.280805	-1.384503	2.694702

Structure of **Int6c**

```
Zero-point correction=                           0.361133 (Hartree/Particle)
 Thermal correction to Energy=                    0.387934
 Thermal correction to Enthalpy=                  0.388878
 Thermal correction to Gibbs Free Energy=         0.303763
 Sum of electronic and zero-point Energies=          -2777.433252
 Sum of electronic and thermal Energies=             -2777.406451
 Sum of electronic and thermal Enthalpies=           -2777.405507
 Sum of electronic and thermal Free Energies=        -2777.490622
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.266341	0.653932	-0.118075
2	6	0	0.479353	2.464514	0.336018
3	6	0	1.283804	-1.396087	0.230517
4	6	0	-0.098011	0.753227	-1.133218
5	8	0	-0.009151	0.240822	-2.212418
6	7	0	0.855594	1.683020	-0.663167
7	16	0	-1.095740	2.193576	0.927807
8	16	0	1.634745	3.610342	0.828078
9	6	0	2.134031	2.016467	-1.303730
10	6	0	2.906997	2.809934	-0.254833
11	1	0	3.524393	3.588354	-0.693000
12	1	0	3.505929	2.167907	0.386400
13	1	0	1.926703	2.603059	-2.198693
14	1	0	2.651860	1.099560	-1.571539
15	6	0	-2.622396	0.585863	-0.794208
16	6	0	-3.695356	1.361901	-0.356437
17	6	0	-2.833383	-0.326091	-1.831444
18	6	0	-4.949073	1.238029	-0.940252
19	1	0	-3.577687	2.070416	0.452282
20	6	0	-4.089056	-0.448835	-2.412919
21	1	0	-2.024460	-0.945772	-2.178835
22	6	0	-5.151366	0.330702	-1.972414
23	1	0	-5.765729	1.850789	-0.581403
24	1	0	-4.232048	-1.162168	-3.214425
25	1	0	-6.128132	0.231679	-2.428281
26	16	0	0.745981	-0.465099	1.584396
27	6	0	2.668463	-1.350679	-0.189398
28	6	0	3.660545	-0.731122	0.598561
29	6	0	3.072192	-1.858977	-1.441775
30	6	0	4.966782	-0.601366	0.150346
31	1	0	3.405969	-0.352496	1.580759
32	6	0	4.381414	-1.729123	-1.880836
33	1	0	2.340406	-2.351006	-2.064670
34	6	0	5.341842	-1.094337	-1.096329
35	1	0	5.699728	-0.118571	0.785896
36	1	0	4.654505	-2.126387	-2.851448
37	1	0	6.362608	-0.997863	-1.443365
38	6	0	0.263270	-2.247359	-0.304459
39	8	0	0.378620	-3.224226	-1.044574
40	6	0	-2.099604	-2.735804	0.419052
41	6	0	-2.417656	-2.529437	1.893864
42	1	0	-1.757016	-3.747741	0.209810
43	1	0	-2.976428	-2.526367	-0.194310
44	1	0	-3.428053	-2.837036	2.156895
45	1	0	-1.695690	-3.029255	2.536414
46	7	0	-1.017251	-1.810820	0.107128
47	16	0	-2.277732	-0.721555	2.139498

48	6	0	-1.014844	-0.596561	0.843607
49	8	0	0.755410	-1.243026	2.866677

Structure of **Int6d**

Zero-point correction= 0.361524 (Hartree/Particle)
Thermal correction to Energy= 0.388237
Thermal correction to Enthalpy= 0.389181
Thermal correction to Gibbs Free Energy= 0.303279
Sum of electronic and zero-point Energies= -2777.434128
Sum of electronic and thermal Energies= -2777.407415
Sum of electronic and thermal Enthalpies= -2777.406471
Sum of electronic and thermal Free Energies= -2777.492373
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.318904	-0.158554	-0.089272
2	6	0	2.215831	2.207050	-0.474457
3	6	0	-2.463891	-0.317678	0.119061
4	6	0	1.157731	0.840034	1.087689
5	8	0	0.751797	0.603757	2.187699
6	7	0	1.826399	2.050996	0.773568
7	16	0	1.948766	0.887663	-1.509392
8	16	0	2.894309	3.726906	-0.840055
9	6	0	2.073304	3.169241	1.688195
10	6	0	2.329274	4.385305	0.797101
11	1	0	3.107202	5.032523	1.191207
12	1	0	1.425162	4.958613	0.609177
13	1	0	2.935172	2.922338	2.307729
14	1	0	1.199566	3.313823	2.318511
15	6	0	2.370573	-1.210488	0.281783
16	6	0	3.189968	-1.775218	-0.697849
17	6	0	2.469882	-1.683187	1.591489
18	6	0	4.082127	-2.789705	-0.377933
19	1	0	3.137381	-1.438561	-1.721802
20	6	0	3.366840	-2.695437	1.909017
21	1	0	1.829667	-1.286852	2.362435
22	6	0	4.174666	-3.255361	0.927766
23	1	0	4.704342	-3.213529	-1.155443
24	1	0	3.423813	-3.049220	2.930261
25	1	0	4.870302	-4.046124	1.177376
26	16	0	-1.300471	0.585144	-0.771789
27	6	0	-3.843464	0.140512	0.149741
28	6	0	-4.189797	1.437103	-0.283552
29	6	0	-4.897709	-0.685156	0.592106
30	6	0	-5.508272	1.869435	-0.303929
31	1	0	-3.414656	2.127564	-0.591664
32	6	0	-6.211620	-0.239244	0.583586
33	1	0	-4.665820	-1.679938	0.939571
34	6	0	-6.534956	1.037213	0.130819
35	1	0	-5.731222	2.872163	-0.648982
36	1	0	-6.995152	-0.902980	0.930574
37	1	0	-7.562246	1.378693	0.125898
38	6	0	-1.959544	-1.507269	0.698302
39	8	0	-2.561678	-2.358549	1.354763
40	6	0	-0.179834	-3.097861	0.120857
41	6	0	-0.311795	-3.309000	-1.391316
42	1	0	-0.847437	-3.751246	0.677039
43	1	0	0.841577	-3.283891	0.435464
44	1	0	0.375142	-4.070582	-1.754745
45	1	0	-1.329520	-3.567182	-1.677751
46	7	0	-0.558018	-1.716126	0.418796
47	16	0	0.111484	-1.701839	-2.152084
48	6	0	-0.037695	-0.802562	-0.535711

49	8	0	-0.728929	1.757200	0.011385

Structure of **Int7**

```
Zero-point correction=                           0.361529 (Hartree/Particle)
 Thermal correction to Energy=                    0.388090
 Thermal correction to Enthalpy=                  0.389034
 Thermal correction to Gibbs Free Energy=         0.304038
 Sum of electronic and zero-point Energies=          -2777.436742
 Sum of electronic and thermal Energies=             -2777.410182
 Sum of electronic and thermal Enthalpies=           -2777.409237
 Sum of electronic and thermal Free Energies=        -2777.494233
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.449811	0.116535	-0.033089
2	6	0	-0.158211	2.391309	-0.359110
3	6	0	2.158860	-0.818013	0.054561
4	6	0	-1.824275	1.243290	0.977563
5	8	0	-2.565840	1.084580	1.935433
6	7	0	-1.193711	2.388387	0.681166
7	16	0	-0.745305	1.003334	-1.483322
8	16	0	-0.360506	4.081074	-1.165702
9	6	0	-1.459827	3.691180	1.255206
10	6	0	-1.626414	4.614431	0.050713
11	1	0	-1.454617	5.657693	0.308327
12	1	0	-2.618362	4.504266	-0.385593
13	1	0	-0.621026	4.008447	1.877606
14	1	0	-2.359812	3.638514	1.863961
15	6	0	-2.635797	-0.736012	-0.481965
16	6	0	-3.670552	-1.091506	0.385656
17	6	0	-2.658173	-1.245732	-1.782974
18	6	0	-4.701296	-1.920288	-0.045528
19	1	0	-3.673115	-0.715354	1.393601
20	6	0	-3.682916	-2.078339	-2.210028
21	1	0	-1.861376	-1.012044	-2.475094
22	6	0	-4.712703	-2.420101	-1.340789
23	1	0	-5.496791	-2.175990	0.643020
24	1	0	-3.672270	-2.459266	-3.223134
25	1	0	-5.514629	-3.067991	-1.671333
26	16	0	1.228554	0.113558	1.029274
27	6	0	3.586271	-0.592836	-0.080436
28	6	0	4.106775	0.697086	0.125721
29	6	0	4.468114	-1.640541	-0.393059
30	6	0	5.469183	0.926672	0.033944
31	1	0	3.433820	1.523154	0.315834
32	6	0	5.829681	-1.398765	-0.481776
33	1	0	4.082296	-2.634969	-0.550800
34	6	0	6.335613	-0.119770	-0.268494
35	1	0	5.854535	1.926529	0.185081
36	1	0	6.500961	-2.214941	-0.715618
37	1	0	7.399951	0.062232	-0.343997
38	6	0	1.398598	-1.904162	-0.616750
39	8	0	1.886278	-2.759939	-1.324511
40	6	0	-0.587964	-3.164643	0.041191
41	6	0	-0.520290	-3.298303	1.558625
42	1	0	-0.032977	-3.947287	-0.469819
43	1	0	-1.614098	-3.162382	-0.310503
44	1	0	-1.266567	-3.987077	1.950158
45	1	0	0.471531	-3.603644	1.888845
46	7	0	0.057670	-1.879307	-0.261529
47	16	0	-0.904004	-1.626171	2.190923
48	6	0	-0.354378	-0.824423	0.616646
49	8	0	1.058573	2.223538	0.090110

Structure of **2**

```
Zero-point correction=                           0.363079 (Hartree/Particle)
 Thermal correction to Energy=                    0.389574
 Thermal correction to Enthalpy=                  0.390519
 Thermal correction to Gibbs Free Energy=         0.306081
 Sum of electronic and zero-point Energies=         -2777.510606
 Sum of electronic and thermal Energies=            -2777.484110
 Sum of electronic and thermal Enthalpies=          -2777.483166
 Sum of electronic and thermal Free Energies=       -2777.567604
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.178945	-0.012282	-0.101030
2	6	0	0.334926	1.195911	-1.036017
3	6	0	-0.551674	0.180979	-0.194226
4	6	0	2.165421	1.446568	0.415765
5	8	0	2.975014	1.971154	1.151457
6	7	0	1.059721	2.040677	-0.105008
7	16	0	1.675016	0.207661	-1.847093
8	16	0	-0.559341	2.320172	-2.139046
9	6	0	0.838993	3.480664	-0.155909
10	6	0	-0.454887	3.688002	-0.926254
11	1	0	-1.323257	3.652163	-0.272992
12	1	0	-0.452795	4.628481	-1.472753
13	1	0	0.761594	3.881737	0.854295
14	1	0	1.681400	3.957444	-0.661240
15	6	0	3.421332	-0.798965	0.165006
16	6	0	3.864227	-0.953317	1.481705
17	6	0	4.140714	-1.398349	-0.866448
18	6	0	5.006005	-1.694029	1.754494
19	1	0	3.318536	-0.490437	2.291818
20	6	0	5.285411	-2.137705	-0.591803
21	1	0	3.812969	-1.294781	-1.893000
22	6	0	5.720818	-2.287913	0.719043
23	1	0	5.338562	-1.805488	2.778597
24	1	0	5.833717	-2.595827	-1.404869
25	1	0	6.611595	-2.864383	0.933848
26	16	0	0.713787	-0.836537	0.718262
27	6	0	-1.500295	0.962786	0.701111
28	6	0	-1.102022	1.444190	1.946441
29	6	0	-2.769845	1.295811	0.227460
30	6	0	-1.948411	2.247679	2.697593
31	1	0	-0.130741	1.178668	2.336508
32	6	0	-3.620556	2.096068	0.981139
33	1	0	-3.103382	0.948930	-0.740623
34	6	0	-3.211699	2.578328	2.218066
35	1	0	-1.620597	2.610884	3.663289
36	1	0	-4.601401	2.343471	0.595712
37	1	0	-3.873033	3.201167	2.806799
38	6	0	-1.311699	-0.743716	-1.158875
39	8	0	-1.196908	-0.631993	-2.360371
40	6	0	-3.005816	-2.452831	-1.630405
41	6	0	-4.265023	-2.906130	-0.910824
42	1	0	-3.242500	-1.815432	-2.476332
43	1	0	-2.421953	-3.304127	-1.983844
44	1	0	-4.663294	-3.821643	-1.340094
45	1	0	-5.034886	-2.136565	-0.914978
46	7	0	-2.204725	-1.690878	-0.658671
47	16	0	-3.743451	-3.206578	0.807658
48	6	0	-2.371900	-2.086973	0.667186
49	8	0	-1.691788	-1.757536	1.607639

Structure of **TS6a**

```
Zero-point correction=                           0.359538 (Hartree/Particle)
 Thermal correction to Energy=                    0.386315
 Thermal correction to Enthalpy=                  0.387259
 Thermal correction to Gibbs Free Energy=         0.301473
 Sum of electronic and zero-point Energies=          -2777.418101
 Sum of electronic and thermal Energies=             -2777.391324
 Sum of electronic and thermal Enthalpies=           -2777.390380
 Sum of electronic and thermal Free Energies=        -2777.476166
One imaginary frequency: 267.58i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.128284	0.779727	-0.258164
2	6	0	-0.794501	2.319917	-0.764299
3	6	0	-1.330234	-1.576212	0.358824
4	6	0	1.104809	2.023253	0.545259
5	8	0	1.883465	2.370954	1.409350
6	7	0	0.011905	2.827487	0.164442
7	16	0	-0.320900	0.819004	-1.354944
8	16	0	-2.222882	3.222118	-1.048305
9	6	0	-0.498659	3.993984	0.883869
10	6	0	-1.533384	4.617940	-0.048050
11	1	0	-2.349707	5.088672	0.492264
12	1	0	-1.087588	5.327884	-0.740823
13	1	0	-0.942495	3.647037	1.817479
14	1	0	0.313872	4.683469	1.098292
15	6	0	2.370116	0.358370	-0.946301
16	6	0	3.630548	0.758977	-0.486527
17	6	0	2.306402	-0.534059	-2.024442
18	6	0	4.785210	0.278382	-1.090302
19	1	0	3.702210	1.440654	0.346186
20	6	0	3.462586	-1.017004	-2.618796
21	1	0	1.351555	-0.877038	-2.400728
22	6	0	4.709743	-0.615856	-2.151917
23	1	0	5.749890	0.602891	-0.721093
24	1	0	3.385685	-1.711721	-3.445218
25	1	0	5.612661	-0.992986	-2.614699
26	16	0	-0.775808	-0.611211	1.736670
27	6	0	-2.734736	-1.676939	0.031701
28	6	0	-3.694161	-0.833330	0.631041
29	6	0	-3.203874	-2.602352	-0.925975
30	6	0	-5.039705	-0.924670	0.305615
31	1	0	-3.381194	-0.083503	1.343769
32	6	0	-4.550273	-2.677806	-1.249695
33	1	0	-2.494252	-3.260684	-1.403018
34	6	0	-5.484341	-1.845385	-0.638017
35	1	0	-5.745991	-0.261032	0.790344
36	1	0	-4.874373	-3.401105	-1.988903
37	1	0	-6.534106	-1.910584	-0.894070
38	6	0	-0.282190	-2.392069	-0.130209
39	8	0	-0.296552	-3.364609	-0.887277
40	6	0	2.193173	-2.756346	0.499350
41	6	0	2.796793	-2.430953	1.862038
42	1	0	1.920173	-3.805830	0.413018
43	1	0	2.881457	-2.504595	-0.305830
44	1	0	3.881793	-2.503682	1.862235
45	1	0	2.386056	-3.059996	2.649857
46	7	0	0.977283	-1.950687	0.411007
47	16	0	2.323137	-0.684229	2.209028
48	6	0	0.950791	-0.785093	1.100524
49	8	0	-1.150801	0.836005	1.687981

Structure of **TS6b**

```
Zero-point correction=                           0.359446 (Hartree/Particle)
 Thermal correction to Energy=                    0.386327
 Thermal correction to Enthalpy=                  0.387271
 Thermal correction to Gibbs Free Energy=         0.301671
 Sum of electronic and zero-point Energies=          -2777.420947
 Sum of electronic and thermal Energies=             -2777.394065
 Sum of electronic and thermal Enthalpies=           -2777.393121
 Sum of electronic and thermal Free Energies=        -2777.478721
One imaginary frequency: 379.1393i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.129699	0.898358	-0.129361
2	6	0	-1.186998	1.772071	-0.569210
3	6	0	-1.180788	-1.670959	0.164205
4	6	0	0.605614	1.786489	0.925654
5	8	0	1.130108	2.110806	1.967473
6	7	0	-0.717919	2.182658	0.604628
7	16	0	-0.088712	0.863087	-1.474848
8	16	0	-2.807295	2.180775	-0.891868
9	6	0	-1.688059	2.825521	1.493738
10	6	0	-2.820341	3.300564	0.583768
11	1	0	-3.793623	3.220489	1.059526
12	1	0	-2.663983	4.314485	0.223477
13	1	0	-2.027682	2.085055	2.218664
14	1	0	-1.216542	3.654880	2.014264
15	6	0	2.523279	1.006419	-0.616252
16	6	0	3.527030	1.595454	0.160137
17	6	0	2.875584	0.436354	-1.846468
18	6	0	4.841195	1.613790	-0.289402
19	1	0	3.278408	2.029909	1.115505
20	6	0	4.189307	0.457836	-2.290811
21	1	0	2.128133	-0.044109	-2.465241
22	6	0	5.180355	1.044676	-1.511596
23	1	0	5.604189	2.074476	0.325097
24	1	0	4.436938	0.009578	-3.244276
25	1	0	6.206483	1.060454	-1.855454
26	16	0	-0.563684	-0.939965	1.613933
27	6	0	-2.575315	-1.471224	-0.177152
28	6	0	-3.528039	-1.131939	0.803312
29	6	0	-3.015785	-1.512344	-1.514683
30	6	0	-4.830661	-0.802161	0.461913
31	1	0	-3.243141	-1.128653	1.848455
32	6	0	-4.323609	-1.192521	-1.848145
33	1	0	-2.314031	-1.787923	-2.288592
34	6	0	-5.240998	-0.821345	-0.868169
35	1	0	-5.533883	-0.538090	1.242805
36	1	0	-4.627649	-1.224060	-2.887830
37	1	0	-6.259630	-0.569473	-1.134171
38	6	0	-0.182950	-2.258011	-0.656146
39	8	0	-0.284234	-2.981894	-1.646550
40	6	0	2.301052	-2.726102	-0.298173
41	6	0	3.397244	-2.051060	0.522570
42	1	0	2.048356	-3.706852	0.111482
43	1	0	2.611677	-2.847034	-1.334214
44	1	0	4.003300	-1.375168	-0.073238
45	1	0	4.041181	-2.774846	1.016322
46	7	0	1.123915	-1.861216	-0.207188
47	16	0	2.523972	-1.074499	1.811525
48	6	0	1.111213	-0.930464	0.790358
49	8	0	-0.495515	-1.902663	2.759695

Structure of **TS6c**

```
Zero-point correction=                           0.359323 (Hartree/Particle)
 Thermal correction to Energy=                    0.386206
 Thermal correction to Enthalpy=                  0.387150
 Thermal correction to Gibbs Free Energy=         0.300988
 Sum of electronic and zero-point Energies=          -2777.411757
 Sum of electronic and thermal Energies=             -2777.384874
 Sum of electronic and thermal Enthalpies=           -2777.383929
 Sum of electronic and thermal Free Energies=        -2777.470092
One imaginary frequency: 340.3020i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.422678	0.420800	-0.464434
2	6	0	-0.504368	1.928041	-1.058498
3	6	0	-1.647158	-1.046053	0.569686
4	6	0	1.300089	1.632678	0.377872
5	8	0	2.014238	1.986938	1.290837
6	7	0	0.121706	2.322760	0.054393
7	16	0	0.141309	0.544355	-1.761018
8	16	0	-1.904729	2.832746	-1.440935
9	6	0	-0.402613	3.527546	0.701054
10	6	0	-1.848770	3.637440	0.225400
11	1	0	-2.176628	4.667999	0.123261
12	1	0	-2.532881	3.086901	0.866897
13	1	0	0.198735	4.383102	0.392099
14	1	0	-0.345634	3.411747	1.780474
15	6	0	2.763688	0.023974	-0.982625
16	6	0	2.916494	-1.166734	-1.702606
17	6	0	3.889744	0.824927	-0.766916
18	6	0	4.160599	-1.544509	-2.188191
19	1	0	2.057660	-1.801554	-1.868232
20	6	0	5.133304	0.438348	-1.249604
21	1	0	3.801922	1.746343	-0.212350
22	6	0	5.276668	-0.747134	-1.960897
23	1	0	4.256462	-2.470972	-2.740057
24	1	0	5.993053	1.070820	-1.067669
25	1	0	6.247807	-1.046702	-2.333687
26	16	0	-0.293974	-2.104370	0.140117
27	6	0	-2.955925	-1.207312	-0.021773
28	6	0	-3.200904	-2.135781	-1.055914
29	6	0	-4.049799	-0.419201	0.400699
30	6	0	-4.460174	-2.270648	-1.622853
31	1	0	-2.394119	-2.747021	-1.434726
32	6	0	-5.301484	-0.557748	-0.178833
33	1	0	-3.897617	0.294418	1.195735
34	6	0	-5.524884	-1.483750	-1.195154
35	1	0	-4.606616	-2.997530	-2.413122
36	1	0	-6.115989	0.065472	0.172097
37	1	0	-6.504866	-1.588814	-1.642756
38	6	0	-1.314700	-0.261371	1.692527
39	8	0	-2.014157	0.431789	2.438063
40	6	0	0.717337	-0.130600	3.265820
41	6	0	1.783310	-1.214024	3.388850
42	1	0	-0.050744	-0.228817	4.030170
43	1	0	1.156267	0.862806	3.328944
44	1	0	2.622422	-0.906192	4.008725
45	1	0	1.369518	-2.147340	3.767094
46	7	0	0.099406	-0.349316	1.959116
47	16	0	2.393451	-1.495794	1.675993
48	6	0	0.865818	-0.912377	0.982872
49	8	0	-0.014723	-2.158580	-1.330509

Structure of **TS6d**

```
Zero-point correction=                           0.359551 (Hartree/Particle)
 Thermal correction to Energy=                    0.386442
 Thermal correction to Enthalpy=                  0.387386
 Thermal correction to Gibbs Free Energy=         0.300950
 Sum of electronic and zero-point Energies=          -2777.419328
 Sum of electronic and thermal Energies=             -2777.392437
 Sum of electronic and thermal Enthalpies=           -2777.391493
 Sum of electronic and thermal Free Energies=        -2777.477929
One imaginary frequency: 333.9206i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.476663	-0.012688	-0.718843
2	6	0	0.172114	1.997935	-1.403710
3	6	0	-1.850717	-0.548357	0.853373
4	6	0	2.165162	1.263106	-0.447629
5	8	0	3.258647	1.460110	0.038147
6	7	0	1.289102	2.325583	-0.753126
7	16	0	0.007645	0.347134	-1.703702
8	16	0	-0.836942	3.313763	-1.817281
9	6	0	1.543574	3.761985	-0.611111
10	6	0	0.171473	4.419550	-0.727712
11	1	0	0.219052	5.404252	-1.183384
12	1	0	-0.343248	4.473480	0.228911
13	1	0	2.219859	4.076342	-1.406554
14	1	0	2.001273	3.959065	0.355074
15	6	0	2.219881	-1.243704	-1.060422
16	6	0	1.611085	-2.268096	-1.797669
17	6	0	3.530266	-1.440784	-0.603753
18	6	0	2.285518	-3.447861	-2.070321
19	1	0	0.598882	-2.157859	-2.163813
20	6	0	4.199379	-2.627023	-0.878682
21	1	0	4.020971	-0.665672	-0.039300
22	6	0	3.584084	-3.635636	-1.608707
23	1	0	1.791525	-4.222583	-2.642265
24	1	0	5.210974	-2.758288	-0.516024
25	1	0	4.109387	-4.558470	-1.818378
26	16	0	-0.551112	-1.706163	0.776054
27	6	0	-3.135149	-0.891165	0.270944
28	6	0	-3.483496	-2.229753	0.002172
29	6	0	-4.075150	0.098827	-0.080260
30	6	0	-4.688261	-2.556934	-0.603639
31	1	0	-2.810251	-3.028703	0.287437
32	6	0	-5.282859	-0.237438	-0.674217
33	1	0	-3.843587	1.133621	0.123417
34	6	0	-5.601886	-1.565271	-0.947526
35	1	0	-4.919064	-3.597972	-0.795634
36	1	0	-5.982172	0.549647	-0.931343
37	1	0	-6.546010	-1.822130	-1.410674
38	6	0	-1.480783	0.713627	1.366141
39	8	0	-2.152217	1.715118	1.618249
40	6	0	0.600637	1.646032	2.529768
41	6	0	1.488469	0.738453	3.377281
42	1	0	-0.164449	2.145873	3.118963
43	1	0	1.196216	2.403145	2.019057
44	1	0	2.377513	1.247877	3.741159
45	1	0	0.944204	0.302768	4.213361
46	7	0	-0.055202	0.771014	1.562936
47	16	0	2.001395	-0.630582	2.255660
48	6	0	0.659190	-0.310818	1.163979
49	8	0	-0.520093	-2.611595	1.968964

Structure of **TSb_{rac}**

```
Zero-point correction=                           0.355876 (Hartree/Particle)
 Thermal correction to Energy=                    0.382055
 Thermal correction to Enthalpy=                  0.382999
 Thermal correction to Gibbs Free Energy=         0.300913
 Sum of electronic and zero-point Energies=          -2777.348286
 Sum of electronic and thermal Energies=             -2777.322107
 Sum of electronic and thermal Enthalpies=           -2777.321163
 Sum of electronic and thermal Free Energies=        -2777.403249
One imaginary frequency: 582.5724i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.426738	-0.080808	0.014023
2	6	0	1.383505	2.366167	-0.789936
3	6	0	-2.447238	-0.563634	-0.134723
4	6	0	1.831928	0.999776	1.062631
5	8	0	2.087120	0.761926	2.227440
6	7	0	1.873771	2.237240	0.489492
7	16	0	0.812757	0.902565	-1.466988
8	16	0	1.353246	3.999164	-1.372695
9	6	0	2.102466	3.504293	1.182634
10	6	0	2.400239	4.513373	0.074938
11	1	0	2.127062	5.538580	0.353582
12	1	0	3.452070	4.480602	-0.241398
13	1	0	1.189210	3.766960	1.740542
14	1	0	2.941219	3.403568	1.883501
15	6	0	2.596135	-0.982690	-0.369467
16	6	0	3.577738	-1.325413	0.573139
17	6	0	2.668228	-1.537625	-1.656911
18	6	0	4.611226	-2.200462	0.228488
19	1	0	3.529792	-0.914836	1.580130
20	6	0	3.697873	-2.416171	-1.996066
21	1	0	1.911105	-1.295824	-2.403876
22	6	0	4.675136	-2.750544	-1.053850
23	1	0	5.369469	-2.453266	0.973368
24	1	0	3.733997	-2.839054	-3.002665
25	1	0	5.484014	-3.435269	-1.319772
26	16	0	-1.186633	0.359930	0.612783
27	6	0	-3.836293	-0.171415	-0.155832
28	6	0	-4.278970	1.005046	0.499130
29	6	0	-4.803466	-0.953111	-0.838063
30	6	0	-5.622130	1.375160	0.476334
31	1	0	-3.558980	1.632147	1.028120
32	6	0	-6.142612	-0.568889	-0.852601
33	1	0	-4.479558	-1.860054	-1.346009
34	6	0	-6.567556	0.594320	-0.198286
35	1	0	-5.932605	2.287253	0.993204
36	1	0	-6.867804	-1.190643	-1.385022
37	1	0	-7.619841	0.887797	-0.214576
38	6	0	-1.818338	-1.737483	-0.656104
39	8	0	-2.365588	-2.664901	-1.248378
40	6	0	0.105053	-3.176938	-0.138977
41	6	0	0.001825	-3.389849	1.370088
42	1	0	-0.524292	-3.873475	-0.704341
43	1	0	1.142996	-3.270769	-0.477388
44	1	0	0.666835	-4.191013	1.721787
45	1	0	-1.030064	-3.607971	1.682334
46	7	0	-0.385032	-1.815519	-0.403692
47	16	0	0.562289	-1.806493	2.112409
48	6	0	0.186044	-0.879103	0.533137
49	8	0	-1.109972	1.772548	1.186860

Structure of **TSd_{rac}**

```
Zero-point correction=                           0.357869 (Hartree/Particle)
 Thermal correction to Energy=                    0.384991
 Thermal correction to Enthalpy=                  0.385935
 Thermal correction to Gibbs Free Energy=         0.298853
 Sum of electronic and zero-point Energies=          -2777.353478
 Sum of electronic and thermal Energies=             -2777.326356
 Sum of electronic and thermal Enthalpies=           -2777.325412
 Sum of electronic and thermal Free Energies=        -2777.412494
One imaginary frequency: 659.6827i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.462561	0.351622	0.102543
2	6	0	0.615193	2.789886	-0.109581
3	6	0	-1.802770	-1.233290	-0.269483
4	6	0	0.309183	0.785485	1.059093
5	8	0	-0.154838	0.116587	1.963925
6	7	0	-0.056661	2.102481	0.813541
7	16	0	1.849056	1.895973	-0.899738
8	16	0	0.109525	4.416050	-0.319854
9	6	0	-1.090211	2.855675	1.531503
10	6	0	-1.435828	4.027956	0.618911
11	1	0	-1.738370	4.911698	1.173430
12	1	0	-2.196535	3.762034	-0.111260
13	1	0	-0.679297	3.182612	2.487191
14	1	0	-1.948989	2.212348	1.706305
15	6	0	2.689386	-0.217942	0.790339
16	6	0	3.977675	0.087859	0.352704
17	6	0	2.532857	-1.137076	1.832127
18	6	0	5.087983	-0.498763	0.946564
19	1	0	4.133364	0.786304	-0.457504
20	6	0	3.644934	-1.719882	2.425842
21	1	0	1.544167	-1.396054	2.173449
22	6	0	4.925774	-1.405171	1.986702
23	1	0	6.078428	-0.245577	0.590997
24	1	0	3.504851	-2.427013	3.233428
25	1	0	5.789997	-1.863332	2.450461
26	16	0	-0.941847	-0.011092	-1.153898
27	6	0	-3.198305	-1.152534	0.063526
28	6	0	-3.977324	-0.024214	-0.272127
29	6	0	-3.838033	-2.199663	0.764728
30	6	0	-5.315976	0.051996	0.079542
31	1	0	-3.530198	0.794174	-0.818446
32	6	0	-5.175121	-2.105490	1.113906
33	1	0	-3.265370	-3.074044	1.030779
34	6	0	-5.930097	-0.983652	0.777440
35	1	0	-5.884529	0.932217	-0.195703
36	1	0	-5.635514	-2.923320	1.655387
37	1	0	-6.975585	-0.920570	1.050222
38	6	0	-0.860708	-2.253021	0.035936
39	8	0	-1.085752	-3.349517	0.549394
40	6	0	1.331554	-3.016888	-0.877807
41	6	0	1.526314	-2.704984	-2.354383
42	1	0	0.822775	-3.962630	-0.712703
43	1	0	2.289926	-3.032034	-0.359547
44	1	0	2.400382	-3.200119	-2.773156
45	1	0	0.644072	-2.953478	-2.942564
46	7	0	0.493401	-1.941059	-0.337483
47	16	0	1.811045	-0.904011	-2.403375
48	6	0	0.814843	-0.667914	-0.883752
49	8	0	-1.436725	1.252449	-1.809441

Structure of **TS7**

```
Zero-point correction=                           0.360610 (Hartree/Particle)
 Thermal correction to Energy=                    0.386560
 Thermal correction to Enthalpy=                  0.387504
 Thermal correction to Gibbs Free Energy=         0.304191
 Sum of electronic and zero-point Energies=          -2777.416857
 Sum of electronic and thermal Energies=             -2777.390907
 Sum of electronic and thermal Enthalpies=           -2777.389963
 Sum of electronic and thermal Free Energies=        -2777.473275
One imaginary frequency: 405.7988i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.545809	0.195408	-0.022648
2	6	0	-0.371816	2.334451	-0.614623
3	6	0	2.077514	-0.852479	-0.082927
4	6	0	-1.800063	1.391069	0.931983
5	8	0	-2.336545	1.325407	2.010693
6	7	0	-1.262335	2.543913	0.413397
7	16	0	-0.831872	0.956056	-1.571112
8	16	0	0.252221	3.831374	-1.235710
9	6	0	-1.080286	3.811284	1.117731
10	6	0	-0.687226	4.803314	0.028610
11	1	0	-0.044109	5.593726	0.405097
12	1	0	-1.555432	5.232893	-0.465648
13	1	0	-0.292564	3.699309	1.864231
14	1	0	-2.009812	4.094715	1.604735
15	6	0	-2.810999	-0.569534	-0.378378
16	6	0	-3.802897	-0.814035	0.572673
17	6	0	-2.968551	-1.096148	-1.661536
18	6	0	-4.926938	-1.560641	0.239042
19	1	0	-3.699954	-0.424492	1.571446
20	6	0	-4.088855	-1.845789	-1.991457
21	1	0	-2.207003	-0.953585	-2.416542
22	6	0	-5.074563	-2.081080	-1.040207
23	1	0	-5.687518	-1.735621	0.989094
24	1	0	-4.185380	-2.247146	-2.991774
25	1	0	-5.949803	-2.664789	-1.295160
26	16	0	1.200324	0.176627	0.941391
27	6	0	3.532659	-0.746471	-0.115689
28	6	0	4.181631	0.424207	0.321216
29	6	0	4.346136	-1.807176	-0.558506
30	6	0	5.566820	0.516316	0.347911
31	1	0	3.598466	1.284477	0.622318
32	6	0	5.729155	-1.699426	-0.546851
33	1	0	3.877551	-2.713682	-0.908021
34	6	0	6.354390	-0.542864	-0.088308
35	1	0	6.030346	1.431456	0.696086
36	1	0	6.326110	-2.534653	-0.893565
37	1	0	7.434191	-0.466147	-0.080506
38	6	0	1.291678	-1.862637	-0.708027
39	8	0	1.681748	-2.784061	-1.419377
40	6	0	-0.751377	-3.051384	-0.066184
41	6	0	-0.642238	-3.244413	1.442239
42	1	0	-0.235155	-3.832642	-0.618372
43	1	0	-1.792954	-3.026212	-0.372206
44	1	0	-1.406186	-3.917538	1.826706
45	1	0	0.343634	-3.601602	1.735268
46	7	0	-0.101723	-1.774772	-0.384395
47	16	0	-0.922920	-1.581795	2.145005
48	6	0	-0.432364	-0.755731	0.562879
49	8	0	1.062785	1.659143	0.398305

Structure of **TS8**

```
Zero-point correction=                           0.360592 (Hartree/Particle)
 Thermal correction to Energy=                    0.386735
 Thermal correction to Enthalpy=                  0.387679
 Thermal correction to Gibbs Free Energy=         0.303739
 Sum of electronic and zero-point Energies=          -2777.436680
 Sum of electronic and thermal Energies=             -2777.410536
 Sum of electronic and thermal Enthalpies=           -2777.409592
 Sum of electronic and thermal Free Energies=        -2777.493532
One imaginary frequency: 38.0538i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.304619	0.162246	-0.010502
2	6	0	0.226926	2.394477	-0.284161
3	6	0	2.035472	-1.023990	0.171375
4	6	0	-1.581571	1.318929	0.988301
5	8	0	-2.339096	1.201293	1.945572
6	7	0	-0.867969	2.414211	0.712108
7	16	0	-0.333373	0.900044	-1.377613
8	16	0	-0.103451	4.042393	-1.229359
9	6	0	-1.106409	3.734270	1.256657
10	6	0	-1.297033	4.632696	0.033499
11	1	0	-1.096306	5.676963	0.266159
12	1	0	-2.311178	4.538124	-0.353866
13	1	0	-0.245687	4.054994	1.845819
14	1	0	-1.988792	3.708891	1.892099
15	6	0	-2.568840	-0.488961	-0.580153
16	6	0	-3.773665	-0.538922	0.121570
17	6	0	-2.506935	-1.107233	-1.832441
18	6	0	-4.885298	-1.174053	-0.423929
19	1	0	-3.842439	-0.080889	1.093633
20	6	0	-3.612204	-1.750117	-2.371074
21	1	0	-1.585847	-1.097650	-2.398000
22	6	0	-4.811689	-1.784879	-1.668192
23	1	0	-5.811392	-1.191661	0.136857
24	1	0	-3.533219	-2.220614	-3.342801
25	1	0	-5.677620	-2.280771	-2.088189
26	16	0	1.154437	-0.210732	1.315947
27	6	0	3.426076	-0.770933	-0.052450
28	6	0	3.981195	0.452180	0.388221
29	6	0	4.259894	-1.707717	-0.700783
30	6	0	5.320060	0.720492	0.190202
31	1	0	3.337540	1.203223	0.824716
32	6	0	5.600374	-1.426600	-0.884427
33	1	0	3.848187	-2.645668	-1.034179
34	6	0	6.134195	-0.218174	-0.442077
35	1	0	5.732198	1.666031	0.516053
36	1	0	6.236457	-2.152789	-1.372776
37	1	0	7.184429	-0.004784	-0.594360
38	6	0	1.221798	-2.105468	-0.496975
39	8	0	1.670488	-2.958856	-1.232183
40	6	0	-0.865144	-3.267940	0.110031
41	6	0	-0.997492	-3.392588	1.621919
42	1	0	-0.315307	-4.094289	-0.333740
43	1	0	-1.836546	-3.181394	-0.368084
44	1	0	-1.834808	-4.022973	1.915268
45	1	0	-0.079479	-3.766730	2.072622
46	7	0	-0.085759	-2.041994	-0.092164
47	16	0	-1.342461	-1.690700	2.197322
48	6	0	-0.459542	-0.953048	0.759162
49	8	0	1.403630	2.307860	0.176583

Structure of ^{3}**TS-*i*Pr**$_{Re}$

```
Zero-point correction=                           0.266024 (Hartree/Particle)
 Thermal correction to Energy=                    0.285038
 Thermal correction to Enthalpy=                  0.285982
 Thermal correction to Gibbs Free Energy=         0.216324
 Sum of electronic and zero-point Energies=          -1619.394655
 Sum of electronic and thermal Energies=             -1619.375642
 Sum of electronic and thermal Enthalpies=           -1619.374698
 Sum of electronic and thermal Free Energies=        -1619.444356
One imaginary frequency: 187.0013i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.210687	-0.130849	-0.040889
2	6	0	-1.043261	-1.234275	-0.090149
3	6	0	0.158795	0.664677	0.593263
4	8	0	0.277053	1.729271	1.180615
5	7	0	-1.073976	0.041158	0.402978
6	16	0	0.549771	-1.549563	-0.813822
7	16	0	-2.552655	-1.631092	-0.914863
8	6	0	-2.402382	0.655294	0.581660
9	6	0	-3.406276	-0.453792	0.210964
10	1	0	-3.733199	-1.000795	1.091259
11	1	0	-4.277932	-0.066119	-0.308409
12	1	0	-2.529284	0.891526	1.638922
13	6	0	2.608670	0.163874	-0.088372
14	6	0	3.139863	1.336299	0.496942
15	6	0	3.506646	-0.716078	-0.734497
16	6	0	4.496214	1.601597	0.431244
17	1	0	2.473797	2.022358	0.994591
18	6	0	4.858524	-0.437500	-0.795757
19	1	0	3.141523	-1.629782	-1.186657
20	6	0	5.364655	0.723323	-0.213030
21	1	0	4.881853	2.504497	0.887508
22	1	0	5.524124	-1.128998	-1.296138
23	1	0	6.424246	0.938588	-0.259750
24	8	0	-0.319686	-1.888251	2.228907
25	8	0	-1.096982	-2.296728	1.296287
26	6	0	-2.541452	1.960822	-0.223525
27	1	0	-1.724058	2.600440	0.111379
28	6	0	-2.405070	1.769444	-1.732111
29	1	0	-1.467296	1.278984	-1.997968
30	1	0	-3.225513	1.176381	-2.141369
31	1	0	-2.421776	2.741822	-2.228160
32	6	0	-3.850715	2.660349	0.138510
33	1	0	-3.937160	2.809918	1.217142
34	1	0	-3.896753	3.639691	-0.340807
35	1	0	-4.721070	2.090415	-0.195425

Structure of ^{3}**TS-*i*Pr**$_{Si}$

```
Zero-point correction=                           0.266220 (Hartree/Particle)
 Thermal correction to Energy=                    0.285205
 Thermal correction to Enthalpy=                  0.286149
 Thermal correction to Gibbs Free Energy=         0.216995
 Sum of electronic and zero-point Energies=          -1619.394541
 Sum of electronic and thermal Energies=             -1619.375556
 Sum of electronic and thermal Enthalpies=           -1619.374612
 Sum of electronic and thermal Free Energies=        -1619.443765
One imaginary frequency: 293.0440i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.303527	-0.150984	-0.210428
2	6	0	0.945675	-1.254846	-0.104983
3	6	0	-0.193809	0.789652	-0.326808
4	8	0	-0.251734	1.997154	-0.503336
5	7	0	1.021213	0.099355	-0.258672
6	16	0	-0.730590	-1.794638	-0.207470
7	16	0	2.260228	-2.076473	-0.941371
8	6	0	2.314014	0.632303	-0.742962
9	6	0	3.276115	-0.564301	-0.735557
10	1	0	3.820398	-0.643525	0.201515
11	1	0	3.982544	-0.517071	-1.559320
12	1	0	2.145972	0.953234	-1.773868
13	6	0	-2.699094	0.160359	-0.145357
14	6	0	-3.159826	1.496265	-0.145359
15	6	0	-3.662646	-0.870349	-0.074312
16	6	0	-4.514371	1.772114	-0.079453
17	1	0	-2.442886	2.299555	-0.198974
18	6	0	-5.012508	-0.581632	-0.011265
19	1	0	-3.350684	-1.907263	-0.063452
20	6	0	-5.449483	0.741967	-0.013767
21	1	0	-4.845409	2.802875	-0.079088
22	1	0	-5.729563	-1.390666	0.042615
23	1	0	-6.507036	0.966261	0.036685
24	8	0	0.660348	-0.840824	2.434342
25	8	0	1.359785	-1.573207	1.662870
26	6	0	2.828813	1.841694	0.058159
27	1	0	2.098047	2.633628	-0.106743
28	6	0	4.167473	2.305711	-0.517276
29	1	0	4.104838	2.467856	-1.596046
30	1	0	4.961734	1.579623	-0.328202
31	1	0	4.465856	3.247689	-0.054328
32	6	0	2.914281	1.592596	1.561152
33	1	0	1.944999	1.320122	1.978114
34	1	0	3.251466	2.501967	2.062217
35	1	0	3.623191	0.799723	1.809316

Structure of ^{3}**TS-Ph**$_{Re}$

```
Zero-point correction=                           0.262387 (Hartree/Particle)
 Thermal correction to Energy=                    0.281941
 Thermal correction to Enthalpy=                  0.282885
 Thermal correction to Gibbs Free Energy=         0.210393
 Sum of electronic and zero-point Energies=          -1732.559302
 Sum of electronic and thermal Energies=             -1732.539749
 Sum of electronic and thermal Enthalpies=           -1732.538805
 Sum of electronic and thermal Free Energies=        -1732.611297
One imaginary frequency: 264.4438i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.524674	-0.151446	-0.023601
2	6	0	-0.395378	-1.748035	-0.295152
3	6	0	0.369528	0.191563	0.802690
4	8	0	0.252342	1.104299	1.603415
5	7	0	-0.678171	-0.687772	0.516748
6	16	0	1.161425	-1.480806	-1.096552
7	16	0	-1.842284	-2.302598	-1.141034
8	6	0	-2.090132	-0.462805	0.845035
9	6	0	-2.816881	-1.711527	0.301767

10	1	0	-2.844351	-2.503761	1.046030
11	1	0	-3.826136	-1.484048	-0.028998
12	1	0	-2.205374	-0.441389	1.928046
13	6	0	2.802693	0.489415	-0.032462
14	6	0	3.072627	1.609129	0.787156
15	6	0	3.837334	0.020407	-0.873035
16	6	0	4.314646	2.218061	0.756344
17	1	0	2.297277	1.985049	1.435064
18	6	0	5.072290	0.639510	-0.896107
19	1	0	3.674595	-0.842499	-1.506729
20	6	0	5.321002	1.743158	-0.081636
21	1	0	4.500784	3.074182	1.392296
22	1	0	5.848060	0.259648	-1.548337
23	1	0	6.289556	2.225609	-0.099751
24	8	0	0.646705	-2.748945	1.800997
25	8	0	-0.066564	-3.121025	0.809507
26	6	0	-2.615547	0.831574	0.263264
27	6	0	-3.611227	1.518841	0.954020
28	6	0	-2.172918	1.325676	-0.961561
29	6	0	-4.163761	2.679554	0.426723
30	1	0	-3.950558	1.145760	1.913084
31	6	0	-2.722612	2.488604	-1.488613
32	1	0	-1.393007	0.813081	-1.508060
33	6	0	-3.720415	3.167514	-0.797950
34	1	0	-4.933347	3.206818	0.976154
35	1	0	-2.367235	2.865511	-2.439261
36	1	0	-4.144719	4.075103	-1.208038

Structure of ^{3}**TS-Ph**$_{Si}$

```
Zero-point correction=                           0.262362 (Hartree/Particle)
 Thermal correction to Energy=                    0.281928
 Thermal correction to Enthalpy=                  0.282872
 Thermal correction to Gibbs Free Energy=         0.210841
 Sum of electronic and zero-point Energies=          -1732.558928
 Sum of electronic and thermal Energies=             -1732.539362
 Sum of electronic and thermal Enthalpies=           -1732.538418
 Sum of electronic and thermal Free Energies=        -1732.610448
One imaginary frequency: 284.2142i
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.722935	0.153736	-0.196877
2	6	0	-0.177925	1.784870	-0.009737
3	6	0	0.422704	-0.446110	-0.475182
4	8	0	0.175294	-1.589638	-0.820045
5	7	0	-0.579419	0.523799	-0.343347
6	16	0	1.583700	1.877406	0.014917
7	16	0	-1.194541	3.010318	-0.767522
8	6	0	-1.917528	0.402751	-0.947105
9	6	0	-2.563359	1.787093	-0.762788
10	1	0	-3.085287	1.853104	0.188926
11	1	0	-3.249937	2.019147	-1.572615
12	1	0	-1.772116	0.203868	-2.010371
13	6	0	2.987536	-0.513102	-0.137775
14	6	0	3.091011	-1.912879	-0.302274
15	6	0	4.175710	0.215492	0.092610
16	6	0	4.324158	-2.537563	-0.240172
17	1	0	2.197207	-2.489462	-0.478445
18	6	0	5.401201	-0.420259	0.150326
19	1	0	4.138610	1.288885	0.231611
20	6	0	5.485334	-1.801670	-0.016189
21	1	0	4.380981	-3.611123	-0.367672
22	1	0	6.296695	0.161064	0.328217
23	1	0	6.445904	-2.297962	0.030386

24	8	0	-0.233220	0.969857	2.446126
25	8	0	-0.614912	1.980702	1.772016
26	6	0	-2.772822	-0.689108	-0.353140
27	6	0	-3.628807	-1.400814	-1.189037
28	6	0	-2.766254	-0.963104	1.012885
29	6	0	-4.475517	-2.372382	-0.667384
30	1	0	-3.626125	-1.198505	-2.253403
31	6	0	-3.606091	-1.939353	1.533239
32	1	0	-2.094907	-0.425823	1.668834
33	6	0	-4.465391	-2.644488	0.695887
34	1	0	-5.135273	-2.921599	-1.327118
35	1	0	-3.586716	-2.152077	2.594647
36	1	0	-5.118317	-3.405725	1.103620

Structure of **5**

```
Zero-point correction=                           0.261571 (Hartree/Particle)
 Thermal correction to Energy=                    0.278234
 Thermal correction to Enthalpy=                  0.279179
 Thermal correction to Gibbs Free Energy=         0.216371
 Sum of electronic and zero-point Energies=          -1469.028757
 Sum of electronic and thermal Energies=             -1469.012093
 Sum of electronic and thermal Enthalpies=           -1469.011149
 Sum of electronic and thermal Free Energies=        -1469.073956
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.381356	0.588631	-0.880046
2	6	0	-2.438113	-0.608662	-0.653463
3	1	0	-4.350091	0.449073	-0.409681
4	1	0	-3.521896	0.790175	-1.938775
5	1	0	-2.406676	-1.212988	-1.559001
6	6	0	-1.069122	1.272023	-0.157206
7	6	0	0.151314	-0.705825	-0.505744
8	7	0	-1.108617	-0.010559	-0.475202
9	16	0	-2.591569	2.082705	-0.132364
10	8	0	0.191685	-1.903842	-0.815415
11	16	0	0.499305	1.807292	0.157635
12	6	0	1.162810	0.210601	-0.146714
13	6	0	2.583620	-0.037503	-0.029205
14	6	0	3.481690	0.974361	0.359357
15	6	0	3.119178	-1.312322	-0.300401
16	6	0	4.841093	0.727473	0.471030
17	1	0	3.118058	1.970960	0.581226
18	6	0	4.481511	-1.549351	-0.185384
19	1	0	2.450288	-2.104869	-0.599562
20	6	0	5.355505	-0.537268	0.199749
21	1	0	5.502688	1.530127	0.773063
22	1	0	4.863645	-2.540102	-0.400505
23	1	0	6.417110	-0.729146	0.287313
24	6	0	-2.788687	-1.528247	0.529993
25	1	0	-1.979863	-2.261183	0.567685
26	6	0	-4.089316	-2.276871	0.245555
27	1	0	-4.274431	-3.015366	1.027283
28	1	0	-4.947911	-1.601164	0.222252
29	1	0	-4.044633	-2.802768	-0.710734
30	6	0	-2.837618	-0.803842	1.873451
31	1	0	-3.017240	-1.525296	2.672562
32	1	0	-1.898398	-0.295236	2.098230
33	1	0	-3.642638	-0.066717	1.908213

Structure of **6**

```
Zero-point correction=                           0.258144 (Hartree/Particle)
 Thermal correction to Energy=                    0.275239
 Thermal correction to Enthalpy=                  0.276183
 Thermal correction to Gibbs Free Energy=         0.210811
 Sum of electronic and zero-point Energies=          -1582.191566
 Sum of electronic and thermal Energies=             -1582.174471
 Sum of electronic and thermal Enthalpies=           -1582.173527
 Sum of electronic and thermal Free Energies=        -1582.238899
No imaginary frequencies
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.625070	1.826582	-1.057232
2	6	0	-1.978163	0.427497	-1.106037
3	1	0	-3.687798	1.783841	-0.838693
4	1	0	-2.455896	2.370476	-1.983882
5	1	0	-1.950869	0.084562	-2.138619
6	6	0	-0.398412	1.735076	0.080264
7	6	0	0.514660	-0.230571	-0.841031
8	7	0	-0.603337	0.656664	-0.661958
9	16	0	-1.777892	2.752587	0.298446
10	8	0	0.389105	-1.253968	-1.522889
11	16	0	1.185860	1.823883	0.646084
12	6	0	1.612269	0.312842	-0.136915
13	6	0	2.951387	-0.226172	-0.030354
14	6	0	3.957048	0.430599	0.703145
15	6	0	3.293505	-1.437123	-0.663719
16	6	0	5.236839	-0.093079	0.798730
17	1	0	3.742222	1.364919	1.208882
18	6	0	4.577808	-1.952709	-0.562555
19	1	0	2.538274	-1.959778	-1.230772
20	6	0	5.560718	-1.290103	0.166163
21	1	0	5.986403	0.439028	1.371569
22	1	0	4.811472	-2.885858	-1.061006
23	1	0	6.560537	-1.697790	0.241105
24	6	0	-2.690987	-0.602830	-0.255707
25	6	0	-3.790327	-1.262958	-0.802982
26	6	0	-2.315576	-0.877557	1.056007
27	6	0	-4.510338	-2.178743	-0.047461
28	1	0	-4.077730	-1.061702	-1.828277
29	6	0	-3.035296	-1.796524	1.812626
30	1	0	-1.455745	-0.390552	1.495639
31	6	0	-4.134563	-2.446930	1.265289
32	1	0	-5.358767	-2.688799	-0.485712
33	1	0	-2.731320	-2.005605	2.830361
34	1	0	-4.690757	-3.164926	1.854365