

Supporting Information Part -1

Oxidation of Norbornane Derivates and Relevant Structures by Dioxiranes

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The ^{13}C NMR chemical shifts calculated and experimental for the
alkanes, alkanols

The calculated activation parameters and geometries of the TSes

The total and ZPVE-corrected energies of *exo-exo-exo*- and *exo-endo-endo*
heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecan-2-ol

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¹³C NMR of alkanes and alkanols

All compounds for NMR calculation was optimized using B3LYP/6-31G(d,p).

The ¹³C NMR chemical shifts calculations were carried out with use of MPW1PW91/6-311+G(2d,p), CSGT.

TMS (which was used as standard) is 182.6026

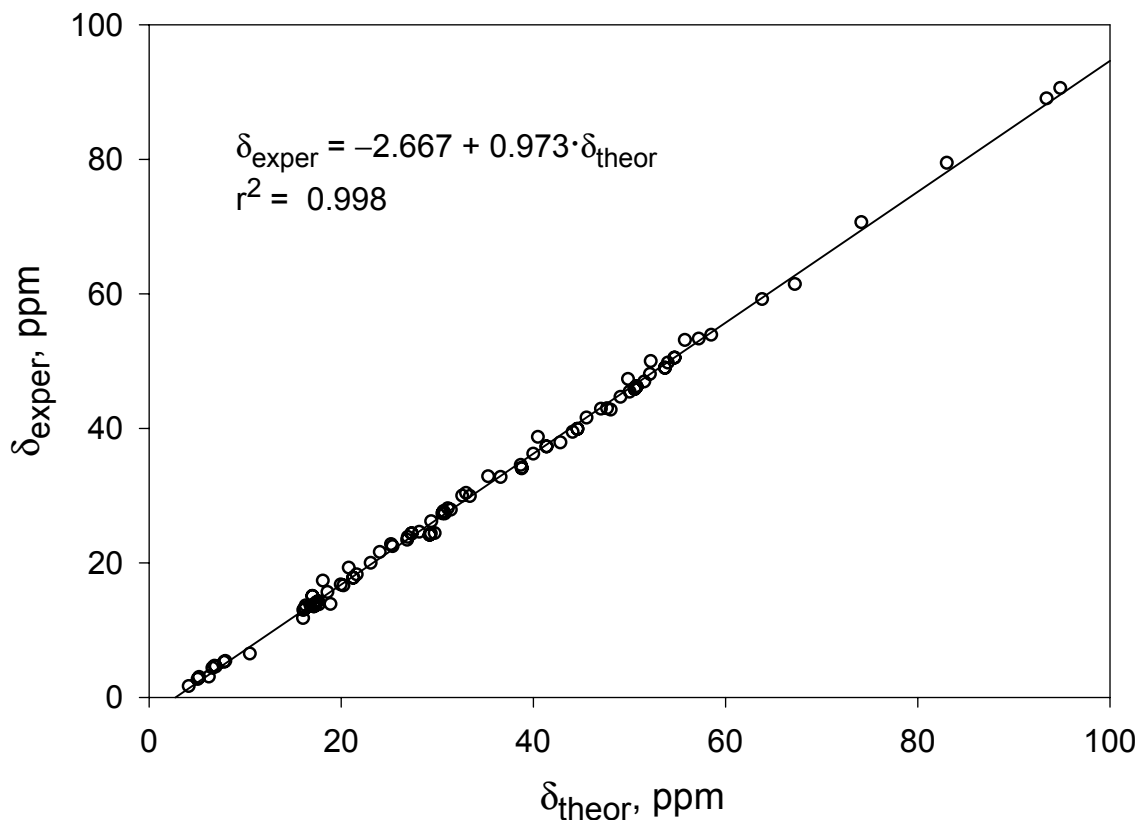


Figure S1. Dependence of experimental (δ_{exper}) vs. calculated (δ_{theor}) ¹³C NMR chemical shifts of different carbon atoms of cage hydrocarbons **1–4** and their corresponding alcohols **1a–4a**.

Spiro{1',7-cyclopropan-2-(*E*)-methyl-bicyclo[2.2.1]heptane}

No. of carbon	δ_{Exper} , ppm	$\delta_{\text{Theor}}^{\text{CSGT}}$, ppm
1	46.96	51.55
2	34.13	38.80
3	38.74	40.47
4	42.98	47.67
5	30.38	33.00
6	22.46	25.35
7	36.21	39.98
2'	5.28	7.81
3'	5.41	7.95
Me	17.37	18.10

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Spiro{cyclopropan-1',7-2-methyl-bicyclo[2.2.1]heptan-(Z)-2-ol}

No. of carbon	$\delta_{\text{Exper,}}$ ppm	$\delta_{\text{Theor}}^{\text{CSGT}},$ ppm	$\delta_{\text{Theor}}^{\text{GIAO}},$ ppm
1	53.14	52.35	52.95
2	79.48	79.65	79.27
3	49.99	48.79	49.20
4	42.77	44.62	44.81
5	27.68	27.18	27.03
6	23.85	23.47	23.26
7	34.57	35.23	34.48
2'	6.50	6.99	7.05
3'	3.06	2.72	2.77
Me	24.61	24.65	24.82

$$\delta_{\text{Experim}} = 1.002 \cdot \delta_{\text{Theor}}^{\text{CSGT}} - 3.514; r^2 = 0.9986$$

Tricyclo[3.2.2.0^{2,4}]nonane

No. of carbon	$\delta_{\text{Exper,}}$ ppm	$\delta_{\text{Theor}}^{\text{CSGT}},$ ppm
1	24.15	29.20
2	13.70	17.26
3	2.72	5.08
6	24.36	29.33
8	26.20	27.31

Tricyclo[3.2.2.0^{2,4}]nonanol-1

No. of carbon	$\delta_{\text{Exper,}}$ ppm	$\delta_{\text{Theor}}^{\text{CSGT}},$ ppm
1	70.64	69.64
2	19.26	17.64
3	3.02	2.47
4	15.88	15.49
5	24.41	26.36
6	29.93	29.93
7	34.04	35.20
8	32.75	33.06
9	23.42	23.58

$$\delta_{\text{Experim}} = 0.975 \cdot \delta_{\text{Theor}}^{\text{CSGT}} - 2.616; r^2 = 0.9966$$

Exo-endo-endo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane

No. of carbon	$\delta_{\text{Exper,}}$ ppm	$\delta_{\text{Theor}}^{\text{CSGT}},$ ppm
1	39.90	40.37
2	48.98	49.46
3	45.83	46.32
4	13.54	12.92

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No. of carbon	$\delta_{\text{Exper,}}$ ppm	$\delta_{\text{Theor}}^{\text{CSGT}},$ ppm
5	13.88	14.67
8	49.77	49.75
9	27.35	26.30
12	15.07	12.78
13	1.67	-0.10
15	32.86	31.06

Exo-endo-endo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]*pentadecanol-2*

No. of carbon	$\delta_{\text{Exper,}}$ ppm	$\delta_{\text{Theor}}^{\text{CSGT}},$ ppm
1	47.34	45.91
2	89.04	88.34
3	53.32	53.09
4	14.07	14.26
5	13.67	13.72
6	16.64	17.06
7	27.34	27.33
8	48.06	48.13
9	45.45	46.07
10	61.44	62.83
11	39.46	40.30
12	13.84	14.58
13	4.39	3.76
14	13.66	13.24
15	29.98	29.10

$$\delta_{\text{Experim}} = 0.974 \cdot \delta_{\text{Theor}}^{\text{CSGT}} - 2.650; r^2 = 0.9990$$

Exo-exo-exo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]*pentadecane*

No. of carbon	$\delta_{\text{Experim,}}$ ppm	$\delta_{\text{Theor}}^{\text{CSGT}},$ ppm
1	37.02	37.13
2	50.49	50.46
3	46.19	46.51
4	13.18	11.99
5	18.27	17.38
8	44.67	44.84
9	28.09	26.86
12	17.78	17.03
13	4.60	2.72
15	21.62	19.78

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Exo-exo-exo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecanol-2

No. of carbon	δ_{Experm} , ppm	$\delta_{\text{Theor}}^{\text{CSGT}}$, ppm
1	41.6	41.61
2	90.6	89.71
3	53.9	54.27
4	14.3	14.38
5	13.0	12.86
6	20.0	19.70
7	27.9	27.85
8	42.9	43.07
9	46.2	46.61
10	59.2	59.44
11	37.9	38.97
12	16.8	16.67
13	4.7	3.86
14	11.8	12.84
15	22.8	21.77

$$\delta_{\text{Experm}} = 0.975 \cdot \delta_{\text{Theor}}^{\text{CSGT}} - 2.793; r^2 = 0.9993$$

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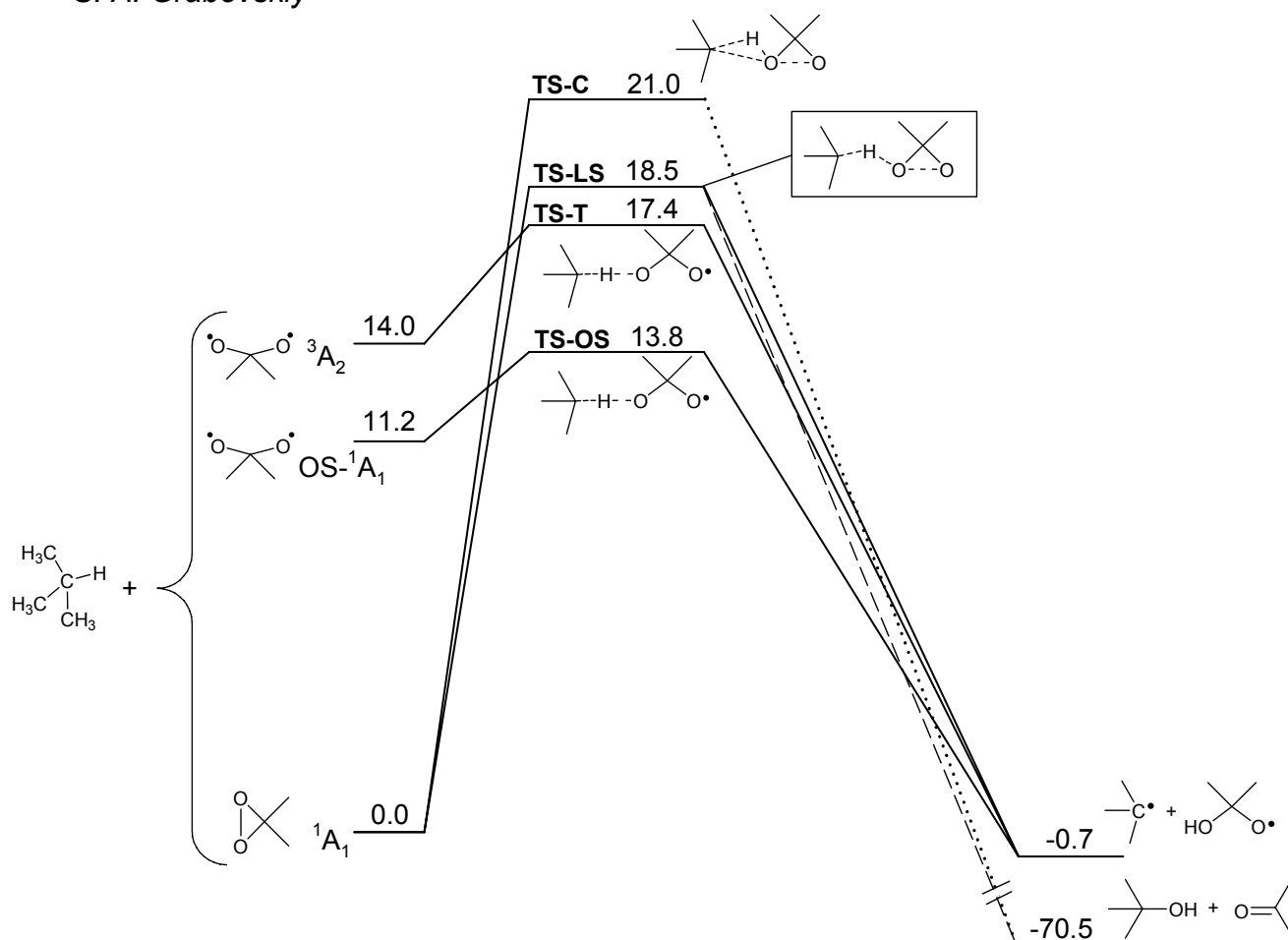


Figure S2. Reaction pathways for the 2-methylpropane – DMD system calculated at the B3PW91/6-311+G(d,p) level of theory (ΔE , kcal·mol⁻¹).

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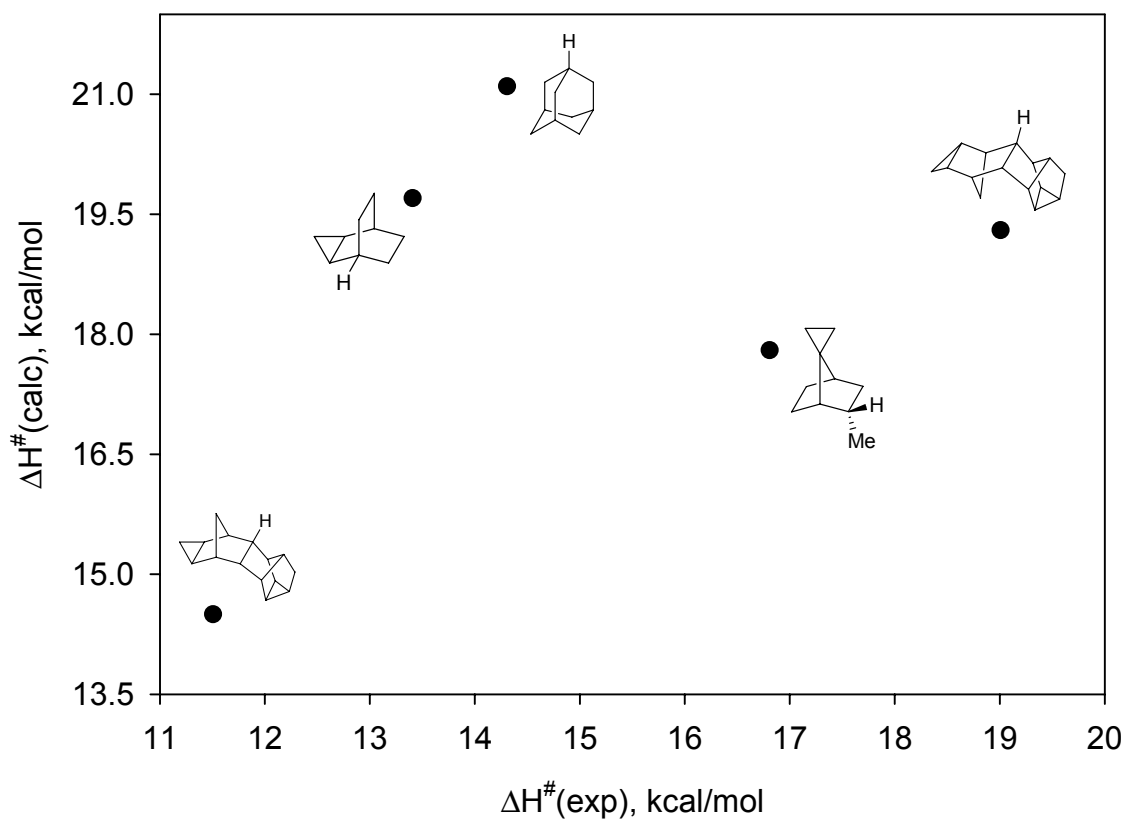
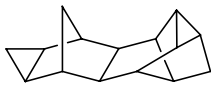
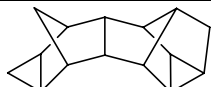
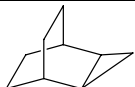
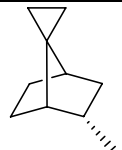


Figure S3. Experimental *vs.* calculated activation enthalpies at B3LYP/6-31G* level for the reaction of caged hydrocarbons with DMD. Experimental data for adamantane is taken from Ref. 17 (see article).

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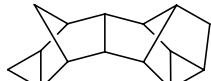
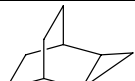
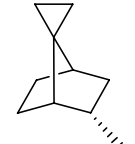
B3LYP/6-31G*; T=298.150 K; P=1.0Atm.; scaled by 0.9806.

TS/Compounds	E, a.u.	ZPVE, a.u.	E + ZPVE a.u.	S ₂₉₈ , cal/(mol·K)	E _a , kcal/mol	ΔS [‡] ₂₉₈ , cal/(mol·K)	ΔG _{solv} , kcal/mol	E _{solv} , a.u.	ΔG [‡] _{solv} , kcal/mol
DMD	-268.268936 ^a -268.349489 ^b	0.086971 ^a -	-268.181965375 ^a -268.262518108	72.249 ^a			-0.67 ^a	-268.269978 ^a	
	-582.346693 ^a -582.486482 ^b	0.290898 ^a -	-582.055795 ^a -582.195584 ^b	94.515 ^a			-0.89 ^a	-582.348124 ^a	
TS-4	-850.567871 ^a -850.799654 ^b	0.372875 ^a -	-850.194996 ^a -850.426779 ^b	132.720 ^a	26.8 ^a 19.7 ^b	-34.044 ^a	-0.82 ^a	-850.568601 ^a	0.74
	-582.338007 ^a -582.477382 ^b	0.291237 ^a -	-582.046770 ^a -582.1861447 ^b	94.446 ^a			-0.94 ^a	-582.339146 ^a	
TS-3	-850.566341 ^a -850.798113 ^b	0.373341 ^a -	-850.193000 ^a -850.424772 ^b	131.714 ^a	22.4 ^a 15.0 ^b	-34.981 ^a	-1.96 ^a	-850.568973 ^a	-0.35
	-351.356324 ^a -351.446312 ^b	0.209165 ^a -	-351.147159 ^a -351.237147 ^b	81.432 ^a			-0.50 ^a	-351.357253 ^a	
TS-2	-619.574343 ^a -619.756682 ^b	0.291615 ^a -	-619.282727 ^a -619.465067 ^b	119.566 ^a	29.1 ^a 21.7 ^b	-34.115 ^a	-2.11 ^a	-619.577469 ^a	-0.94
	-390.663782 ^a -390.764903 ^b	0.234934 ^a -	-390.428848 ^a -390.529969 ^b	90.975 ^a			1.02 ^a	-390.661902 ^a	
TS-1	-658.887125 ^a -659.079894 ^b	0.316792 ^a -	-658.570333 ^a -658.763102 ^b	127.621 ^a	25.4 ^a 18.4 ^b	-35.603 ^a	-0.04 ^a	-658.887155 ^a	-0.39
Adamantane	-390.725203 ^a -390.823497 ^b	0.239958 ^a -	-390.485245 ^a -390.583538 ^b	79.351 ^a			-1.12 ^a	-390.727556 ^a	
TS-5	-658.944576 ^a -659.135761 ^b	0.322121 ^a -	-658.622454 ^a -658.813640 ^b	122.073 ^a	28.1 ^a 20.3 ^b	-29.527 ^a	-2.56 ^a	-658.949033 ^a	-0.77

^a - B3LYP/6-31G(d); ^b - B3LYP/6-311+G(d,p)//B3LYP/6-31G(d).

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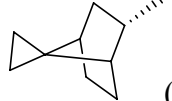
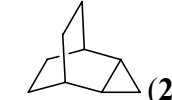
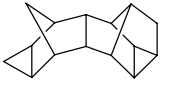
B3PW91/6-31+G*//B3LYP/6-31G*; T=298.150 K; P=1.0 Atm.; scaled by 0.9806. (1Hartree = 627.5095 kcal·mol⁻¹)

TS/Compounds	E, a.u.	ZPVE, a.u.	E + ZPVE a.u.	ΔE , $\frac{kcal}{mol}$	ΔH , a.u.	ΔH , $\frac{kcal}{mol}$	ΔG , a.u.	$\Delta G^\ddagger$, $\frac{kcal}{mol}$
DMD	-268.244155	0.086971	-268.157168		-268.150527		-268.184827	
	-582.295049	0.290898	-582.004151		-581.993625		-582.038532	
TS-4	-850.499232	0.372875	-850.126357	21.9	-850.108225	22.6	-850.171284	32.7
	-582.285571	0.291237	-581.994334		-581.983855		-582.028730	
TS-3	-850.497640	0.373341	-850.124299	17.1	-850.106316	17.6	-850.168898	28.0
	-351.324174	0.209165	-351.115009		-351.10705		-351.14574	
TS-2	-619.526051	0.291615	-619.234436	23.7	-619.219104	24.1	-619.275914	34.3
	-390.628389	0.234934	-390.393455		-390.383457		-390.426682	
TS-1	-658.834795	0.316792	-658.518003	20.5	-658.500679	20.9	-658.561316	31.5
Adamantane	-390.687723	0.239958	-390.447765		-390.439663		-390.477366	
TS-5	-658.891671	0.322121	-658.56955	22.2	-658.554009	22.7	-658.612009	31.5

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B3PW91/6-31+G*; T=298.150 K; P=1.0 Atm.; no scaled. (1Hartree = 627.5095 kcal·mol⁻¹)

TS/Compounds	E, a.u.	ZPVE, a.u.	E + ZPVE a.u.	S ₂₉₈ , cal/(mol·K)	$\frac{\Delta E,}{kcal}$ mol	$\Delta S^\ddagger_{298}$, cal/(mol·K)	ΔH , a.u.	$\frac{\Delta H,}{kcal}$ mol	ΔG , a.u.	$\frac{\Delta G^\ddagger,}{kcal}$ mol
DMD/ 6-31+G*	-268.177747	0.088767	-268.088980	71.891			-268.082419		-268.116577	
6-311+G**	-268.244530	0.088072	-268.156458	73.117			-268.149917		-268.184657	
TFD/ 6-31+G*	-565.796801	0.065599	-565.731202	86.024			-565.722747		-565.763620	
•OC(Me₂)O• / 6-31+G*	-268.154799 (S ² =0.9122)	0.085690	-268.069109	75.395			-268.061993		-268.097815	
6-311+G**	-268.223334 (S ² =0.9060)	0.084696	-268.138638	75.800			-268.131432		-268.167447	
³A₂ •OC(Me₂)O•	-268.219120	0.084965	-268.134155	77.280			-268.127082		-268.163801	
6-311+G**	(S ² =2.0078)									
DMD vs •OC(Me₂)O•					12.5	3.504		12.8		11.8
6-31+G*										
6-311+G**					11.2	2.683		11.6		10.8
DMD vs •OC(Me₂)O• (³A₂)					14.0	4.163		14.3		13.1
6-311+G**										
HOC(Me₂)O• / 6-311+G**	-268.901309	0.097779	-268.803530	79.608			-268.795959		-268.833783	
(CH₃)₃C• / 6-311+G**	-157.785169	0.116102	-157.669067	75.241			-157.661736		-157.697485	
H₃CC(O)CH₃ / 6-311+G**	-193.140037	0.083327	-193.056710	72.659			-193.050368		-193.084891	
(CH₃)₃COH / 6-311+G**	-233.662170	0.135026	-233.527144	77.546			-233.519378		-233.556222	
DMD + (CH₃)₃CH →										
HOC(Me₂)O• + (CH₃)₃C•					-0.7	9.563		0.4		-2.4
(U)B3PW91/6-311+G**										
DMD + (CH₃)₃CH →										
Me₂CO• + (CH₃)₃COH					-70.5	4.919		-69.9		-71.4
B3PW91/6-311+G**										
 (4)	-582.173914	0.296908	-581.877006	93.643			-581.866734		-581.911227	
TS (4 + DMD)	-850.304920	0.380639	-849.924281	130.640	26.2	-34.894	-849.906562	26.7	-849.968633	37.1

TS/Compounds	E, a.u.	ZPVE, a.u.	E + ZPVE a.u.	S ₂₉₈ , cal/(mol·K)	$\frac{\Delta E,}{mol}$ <i>kcal</i>	$\Delta S^\ddagger_{298}$, cal/(mol·K)	ΔH , a.u.	$\frac{\Delta H,}{mol}$ <i>kcal</i>	ΔG , a.u.	$\frac{\Delta G^\ddagger,}{mol}$ <i>kcal</i>
RB3PW91/6-31+G* TS (4 + DMD) UB3PW91/6-31+G*	-850.313074 (S ² =0.4600)	0.379785	-849.933288	129.664	20.5	-35.87	-849.915944	20.8	-849.977551	31.5
TS (4 + [•]OC(Me₂)O[•]) UB3PW91/6-31+G*	-850.320580 (S ² =0.9137)	0.378605	-849.941975	130.644	2.60	-38.394	-849.924408	2.7	-849.986481	14.2
 (1) TS (1 + DMD) RB3PW91/6-31+G*	-390.542296	0.239534	-390.302761	90.404			-390.292932		-390.335886	
TS (1 + DMD) UB3PW91/6-31+G*	-658.675315	0.322956	-658.352359	127.816	24.7	-34.479	-658.335285	25.1	-658.396015	35.4
TS (1 + DMD) UB3PW91/6-31+G*	-658.682125 (S ² =0.4286)	0.322441	-658.359684	126.873	20.1	-35.422	-658.342869	20.4	-658.403150	30.9
TS (1 + [•]OC(Me₂)O[•]) UB3PW91/6-31+G*	-658.688999 (S ² =0.9384)	0.321463	-658.367536	127.145	2.7	-38.654	-658.350565	2.7	-658.410976	14.3
 (2) TS (2 + DMD) RB3PW91/6-31+G*	-351.247380	0.213290	-351.034090	80.989			-351.026268		-351.064749	
TS (2 + DMD) UB3PW91/6-31+G*	-619.375943	0.297390	-619.078554	119.591	27.9	-33.289	-619.063399	28.4	-619.120221	38.3
TS (2 + DMD) UB3PW91/6-31+G*	-619.386569 (S ² =0.5020)	0.295943	-619.090626	119.728	20.4	-33.152	-619.075686	20.7	-619.132573	30.6
TS (2 + [•]OC(Me₂)O[•]) UB3PW91/6-31+G*	-619.393904 (S ² =0.9323)	0.295044	-619.098860	119.314	2.7	-37.070	-619.083783	2.8	-619.140473	13.9
 (3) TS (3 + DMD) RB3PW91/6-31+G*	-582.164543	0.297242	-581.867300	93.592			-581.857075		-581.901544	
TS (3 + DMD) UB3PW91/6-31+G*	-850.303319	0.381021	-849.922297	129.561	21.3	-35.922	-849.904938	21.7	-849.966497	32.4
TS (3 + DMD) UB3PW91/6-31+G*	-850.308429 (S ² =0.3874)	0.380725	-849.927704	129.838	17.93	-35.645	-849.910424	18.24	-849.972115	28.9

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TS/Compounds	E, a.u.	ZPVE, a.u.	E + ZPVE a.u.	S ₂₉₈ , cal/(mol·K)	$\frac{\Delta E,}{mol}$ <i>kcal</i>	$\Delta S^\ddagger_{298}$, cal/(mol·K)	ΔH , a.u.	$\frac{\Delta H,}{mol}$ <i>kcal</i>	ΔG , a.u.	$\frac{\Delta G^\ddagger,}{mol}$ <i>kcal</i>
TS (3 + [•]OC(Me₂)O[•]) UB3PW91/6-31+G*	-850.314946 (S ² =0.9306)	0.379515	-849.935432	130.660	13.1	-34.823	-849.917982	13.5	-849.980063	23.9
Adamantane / 6-31+G*	-390.602405	0.244574	-390.357831	78.818			-390.349895		-390.387344	
TS AdH – DMD RB3PW91/6-31+G*	-658.733148	0.328483	-658.404666	120.982	26.4	-29.727	-658.389327	27.0	-658.446809	35.8
TS AdH – DMD UB3PW91/6-31+G*	-658.742652 (S ² =0.4650)	0.327515	-658.415137	119.783	19.88	-30.926	-658.400114	20.2	-658.457027	29.4
TS AdH-[•]OC(Me₂)O[•] UB3PW91/6-31+G*	-658.749905 (S ² =0.9330)	0.326455	-658.423449	119.667	2.1	-34.546	-658.408252	2.3	-658.465110	12.6
(CH₃)₃CH / 6-31+G*	-158.406348	0.132245	-158.274104	72.039			-158.267479		-158.301707	
6-311+G**	-158.446128	0.131035	-158.315093	72.169			-158.308430		-158.342720	
TS iPrH-DMD RB3PW91/6-31+G*	-426.534793	0.215772	-426.319021	111.803	27.7	-32.127	-426.305065	28.1	-426.358187	37.7
RB3PW91/6-311+G**	-426.648733	0.213365	-426.435368	113.964	22.7	-31.322	-426.421249	23.3	-426.475397	32.6
TS iPrH-DMD UB3PW91/6-31+G*	-426.544735 (S ² =0.4584)	0.215136	-426.329600	109.987	21.0	-33.943	-426.316053	21.2	-426.368311	31.4
UB3PW91/6-311+G**	-426.655624 (S ² =0.3743)	0.213553	-426.442071	110.515	18.5	-34.771	-426.428459	18.8	-426.480968	29.1
TS iPrH-[•]OC(Me₂)O[•] UB3PW91/6-31+G*	-426.552348 (S ² =0.9362)	0.214243	-426.338105	110.894	3.2	-36.54	-426.324379	3.2	-426.377068	14.1
UB3PW91/6-311+G**	-426.662506 (S ² =0.9283)	0.212879	-426.449628	112.092	2.6	-35.877	-426.435839	2.5	-426.489098	13.2
TS iPrH-[•]OC(Me₂)O[•] ³A₂ UB3PW91/6-311+G**	-426.657051 (S ² =2.0125)	0.213223	-426.443828	114.984	3.4	-34.465	-426.430173	3.4	-426.484806	13.6
H₃CC(O)CH₃ / 6-31+G*	-193.090439	0.084148	-193.006291	72.430			-192.999987		-193.034401	
TS-2 (Acetone+ DMD) RB3PW91/6-31+G*	-461.202813 (S ² =0.0000)	0.169843	-461.032970	110.746	39.1	-33.575	-461.020152	39.1	-461.072771	49.1
TS-1 (Acetone+ DMD) UB3PW91/6-31+G*	-461.224451 (S ² =1.0144)	0.166289	-461.058163	110.367	23.3	-33.954	-461.045213	23.3	-461.097651	33.5
TS-2 (Acetone+ DMD)	461.217940	0.166534	-461.051405	111.575	27.5	-32.746	-461.038435	27.6	-461.091448	37.4

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TS/Compounds	E, a.u.	ZPVE, a.u.	E + ZPVE a.u.	S ₂₉₈ , cal/(mol·K)	$\frac{\Delta E,}{mol}$ <i>kcal</i>	$\Delta S^\ddagger_{298}$, cal/(mol·K)	ΔH , a.u.	$\frac{\Delta H,}{mol}$ <i>kcal</i>	ΔG , a.u.	$\frac{\Delta G^\ddagger,}{mol}$ <i>kcal</i>
UB3PW91/6-31+G* TS-2 (Acetone+ DMDBR) UB3PW91/6-31+G*	(S ² =0.6800) -461.231308 (S ² =0.9382)	0.166256	-461.065052	111.418	19.0	-32.903	-461.052046	19.1	-461.104984	28.9
c-C₆H₁₂ / 6-31+G* TS (c-C₆H₁₂ + TFD) RB3PW91/6-31+G*	-235.804083 -801.563187	0.171078 0.230868	-235.633004 -801.332318	74.508 124.587			-235.626365 -801.316485		-235.661766 -801.375680	
TS (c-C₆H₁₂ + TFD) UB3PW91/6-31+G* TS (c-C₆H₁₂ + TFD) UB3PW91/6-31+G*	-801.568904 (S ² =0.3888) -801.574206 (S ² =0.9182)	0.231242	-801.337662	123.489	16.66	-37.043	-801.322111	16.94	-801.380785	27.99
		0.231280	-801.342926	123.550	13.4	-36.982	-801.327435	13.6	-801.386137	24.6

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The total and ZPVE-corrected energies for TSs of reaction methylcyclohexane h_{14} and d_{14} with DMD- h_6 at (U)B3PW91/6-311+G(d,p) level of theory (T=273.150 K; P=1.0 Atm.; no scaled; 1Hartree = 627.5095 kcal·mol⁻¹)

TS	E, a.u.	ZPVE, a.u.	E + ZPVE a.u.	G, a.u.	$\Delta G^\ddagger$, a.u.	$-\delta\Delta G^\ddagger$, a.u.	$-\delta\Delta G^\ddagger$, $\frac{cal}{mol}$	k_H/k_D , at 0°C
DMD h_6	-268.244518	0.088008	-268.156510	-268.181885				
C ₇ H ₁₄	-275.170361	0.197410	-274.972951	-275.000374				
C ₇ D ₁₄	-275.170361	0.151223	-275.019138	-275.047930				
TS-C h	-543.374989	0.279859	-543.095130	-543.131885	0.050374			
TS-C d	-543.374989	0.234896	-543.140092	-543.178232	0.051583	0.001209	758.66	4.05
TS-LS h	-543.380253 $\langle S^2 \rangle = 0.3582$	0.279898	-543.100355	-543.137533	0.044726			
TS-LS d	-543.380253 $\langle S^2 \rangle = 0.3582$	0.235119	-543.145134	-543.183582	0.046233	0.001507	945.66	5.72
TS-OS h	-543.386680 $\langle S^2 \rangle = 0.9292$	0.279582	-543.107098	-543.143897	0.038362			
TS-OS d	-543.386680 $\langle S^2 \rangle = 0.9292$	0.234584	-543.152096	-543.190171	0.039644	0.001282	804.47	4.41
TS-OS2 h	-543.379096 $\langle S^2 \rangle = 1.0074$	0.279319	-543.099778	-543.136808	0.045451			
TS-OS2 d	-543.379096 $\langle S^2 \rangle = 1.0074$	0.234353	-543.144744	-543.183050	0.046765	0.001314	824.55	4.58
Experiment ^a							6.05 ± 0.27	

^a G. Asensio, R. Mello, M. E. Gonzalez-Nuñez, C. Boix, J. Royo, *Tetrahedron Letters*, Vol. 38, No.13, pp.2373-2376.

**The total and ZPVE-corrected energies of *exo-exo-exo*- and *exo-endo-endo*-
Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecan-2-ol**

Exo-endo-endo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecan-2-ol

Method/Basis set	E, a.u.	ZPVE, a.u.	E+ZPVE, a.u.
B3LYP/6-31G(d)	-657.550296	0.294544	-657.255752
B3LYP/6-311+G(3df,2p)	-657.762838		-657.468294
B3PW91/6-311+G(d,p)	-657.501501	0.299064	-657.202438

Exo-exo-exo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecan-2-ol

Method/Basis set	E, a.u.	ZPVE, a.u.	E+ZPVE, a.u.
B3LYP/6-31G(d)	-657.556701	0.294398	-657.262302
B3LYP/6-311+G(3df,2p)	-657.769521		-657.475123
B3PW91/6-311+G(d,p)	-657.508499	0.299012	-657.209487

The total energies of *exo-exo-exo*- and *exo-endo-endo*-
heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecan-2-ols.

B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d) (Method A)

B3PW91/6-311+G(d,p) (Method B)

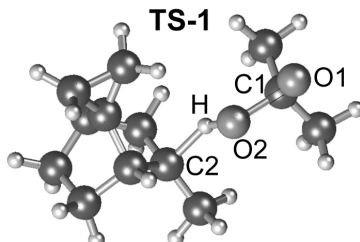
Compound	E+ZPVE, a.u. (Method A)	E+ZPVE, a.u. (Method B)
<i>exo-endo-endo</i> -	-657.468294	-657.202438
<i>exo-exo-exo</i> -	-657.475123	-657.209487
$\Delta E + \Delta ZPVE$	4.3 kcal/mol	4.4 kcal/mol

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All compounds was optimized using B3LYP/6-31G(d). Zero-point corrections (ZPVE) were scaled by a 0.9806 for the B3LYP.

Spiro{1',7-cyclopropan-2-(*E*)-methyl-bicyclo[2.2.1]heptane} + DMD
RB3LYP/6-31G*



Zero-point correction= 0.316792 (Hartree/Particle)
Thermal correction to Energy= 0.333171
Thermal correction to Enthalpy= 0.334116
Thermal correction to Gibbs Free Energy= 0.273479
Sum of electronic and zero-point Energies= -658.570333
Sum of electronic and thermal Energies= -658.553953
Sum of electronic and thermal Enthalpies= -658.553009
Sum of electronic and thermal Free Energies= -658.613646

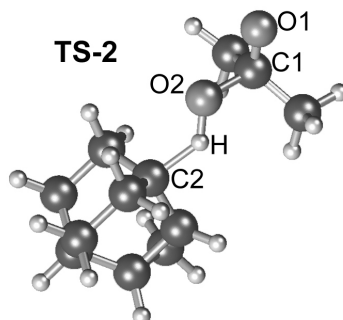
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.632205	0.951987	-0.069653
2	6	0	1.319666	-0.273445	-0.939609
3	6	0	2.722276	-0.982301	-0.933796
4	6	0	3.271832	-0.685345	0.496719
5	6	0	2.139614	0.157144	1.135076
6	6	0	0.928860	-0.781636	1.394598
7	6	0	0.438105	-1.083100	-0.020430
8	6	0	-0.097577	-2.428346	-0.390325
9	6	0	2.219657	2.233318	-0.585924
10	6	0	0.816246	2.209272	-0.010505
11	1	0	0.163837	-0.269913	1.996298
12	1	0	-0.807118	-0.202764	-0.021615
13	1	0	0.904190	-0.105735	-1.934182
14	1	0	2.660902	-2.050053	-1.164698
15	1	0	3.342701	-0.515149	-1.705335
16	1	0	4.199522	-0.106909	0.446956
17	1	0	1.181878	-1.705846	1.932857
18	1	0	2.438526	0.739025	2.010957
19	1	0	3.483525	-1.596704	1.067020
20	1	0	0.665018	2.671189	0.962972
21	1	0	-0.032597	2.297874	-0.681624
22	1	0	2.327648	2.355898	-1.661238
23	1	0	3.004927	2.712423	-0.005166
24	1	0	-0.495224	-2.436141	-1.407724
25	1	0	0.711656	-3.174033	-0.325832
26	1	0	-0.884397	-2.753181	0.298234
27	8	0	-1.560782	0.143435	-0.664449
28	6	0	-2.933421	0.256991	-0.041501
29	8	0	-3.377434	1.131272	-0.918565
30	6	0	-3.614422	-1.118902	-0.100112
31	6	0	-2.788633	0.793299	1.394518
32	1	0	-4.656653	-1.025972	0.226866
33	1	0	-3.606317	-1.472223	-1.134527
34	1	0	-3.123967	-1.861853	0.543084
35	1	0	-3.783360	0.973108	1.817786
36	1	0	-2.265684	0.091107	2.059577
37	1	0	-2.249715	1.744574	1.369121

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Tricyclo[3.2.2.0^{2,4}]nonane + DMD

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RB3LYP/6-31G*



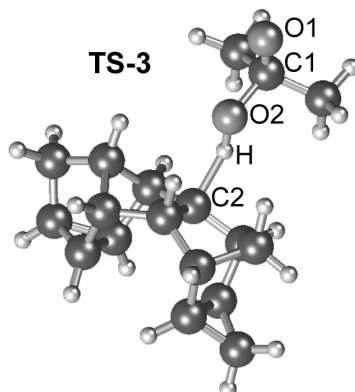
Zero-point correction= 0.291615 (Hartree/Particle)
Thermal correction to Energy= 0.306003
Thermal correction to Enthalpy= 0.306947
Thermal correction to Gibbs Free Energy= 0.250137
Sum of electronic and zero-point Energies= -619.282727
Sum of electronic and thermal Energies= -619.268340
Sum of electronic and thermal Enthalpies= -619.267396
Sum of electronic and thermal Free Energies= -619.324205

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.731255	-1.320801	-0.681560
2	6	0	-3.009586	-0.062296	0.186165
3	6	0	-2.301240	-0.239637	1.542022
4	6	0	-0.751626	-0.401238	1.306663
5	6	0	-0.537271	-0.310471	-0.181163
6	6	0	-1.172076	-1.473849	-0.914889
7	6	0	-0.918537	0.984735	-0.810148
8	6	0	-2.447326	1.137381	-0.579980
9	6	0	-1.471087	2.129978	-0.003915
10	1	0	-0.553482	1.176784	-1.816565
11	1	0	0.889577	-0.405112	-0.591045
12	1	0	-0.941503	-1.441253	-1.984320
13	1	0	-0.803050	-2.424709	-0.522377
14	1	0	-3.131180	-2.213731	-0.188131
15	1	0	-3.030047	1.457843	-1.441728
16	1	0	-4.089349	0.053286	0.338850
17	1	0	-3.240363	-1.232517	-1.647883
18	1	0	-0.396408	-1.368831	1.666802
19	1	0	-0.187293	0.370392	1.836185
20	1	0	-2.504883	0.613480	2.197251
21	1	0	-2.697700	-1.128728	2.043799
22	1	0	-1.438316	3.108465	-0.474583
23	1	0	-1.300635	2.160252	1.067480
24	8	0	1.707206	-0.917160	-0.170241
25	6	0	2.975159	-0.068708	0.009591
26	8	0	3.783652	-1.093060	-0.074134
27	6	0	3.050060	0.934398	-1.155507
28	6	0	2.903607	0.608336	1.385805
29	1	0	3.849992	1.124313	1.587018
30	1	0	2.094478	1.347395	1.450568
31	1	0	2.760449	-0.159568	2.150549
32	1	0	3.997957	1.481568	-1.099799
33	1	0	3.026576	0.384708	-2.100830
34	1	0	2.235387	1.670746	-1.134752

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Exo-endo-endo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]*pentadecane* + **DMD**
RB3LYP/6-31G*



Zero-point correction= 0.373341 (Hartree/Particle)
Thermal correction to Energy= 0.390380
Thermal correction to Enthalpy= 0.391324
Thermal correction to Gibbs Free Energy= 0.328742
Sum of electronic and zero-point Energies= -850.193000
Sum of electronic and thermal Energies= -850.175962
Sum of electronic and thermal Enthalpies= -850.175017
Sum of electronic and thermal Free Energies= -850.237599

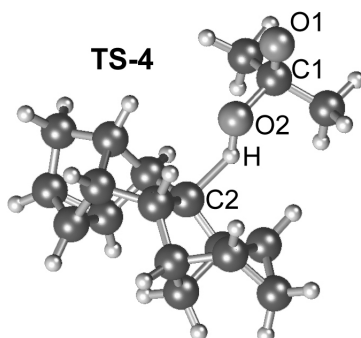
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.510187	-3.044014	-0.623452
2	6	0	-1.763323	-1.806849	-1.081796
3	6	0	-0.264078	-1.646152	-0.725460
4	6	0	-0.164504	-2.405571	0.626363
5	6	0	-1.356966	-1.661032	1.290966
6	6	0	-2.481200	-1.820840	0.258633
7	6	0	-0.766158	-0.214065	1.191629
8	6	0	-0.162350	-0.220369	-0.201374
9	6	0	-1.453794	1.177081	1.244507
10	6	0	-0.378226	2.049284	0.507377
11	6	0	-0.360983	1.153158	-0.782060
12	6	0	-2.572140	1.376255	0.211196
13	6	0	-2.311165	2.676673	-0.527993
14	6	0	-1.096804	3.335868	0.099241
15	6	0	-1.863149	1.351803	-1.126574
16	1	0	-2.149216	-1.261697	-1.935170
17	1	0	-3.405194	-1.272797	0.407200
18	1	0	0.437138	-1.926267	-1.514627
19	1	0	-3.446317	-3.221970	-1.146787
20	1	0	-1.991609	-3.957709	-0.354000
21	1	0	-1.600478	-1.974930	2.309351
22	1	0	0.786480	-2.205834	1.125315
23	1	0	-0.289965	-3.485038	0.536491
24	1	0	0.051554	-0.168094	1.924472
25	1	0	1.395475	-0.172074	-0.060589
26	1	0	-1.700099	1.511703	2.256313
27	1	0	0.324798	1.448872	-1.579807
28	1	0	-2.309773	0.946155	-2.025832
29	1	0	0.586512	2.131527	1.007659
30	1	0	-3.575001	0.986555	0.340042
31	1	0	-3.120200	3.235260	-0.987476
32	1	0	-1.346016	3.965223	0.961690
33	1	0	-0.518674	3.936754	-0.612710
34	8	0	2.162569	-0.038882	0.625357

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35	6	0	3.543633	0.001386	-0.009635
36	8	0	4.228999	0.133906	1.100181
37	6	0	3.762789	-1.331621	-0.752221
38	6	0	3.594723	1.218901	-0.953592
39	1	0	4.780617	-1.362367	-1.158312
40	1	0	3.651616	-2.154339	-0.040488
41	1	0	3.064036	-1.474431	-1.588795
42	1	0	4.603458	1.318351	-1.371350
43	1	0	2.890752	1.136502	-1.793868
44	1	0	3.370839	2.121083	-0.377553

Exo-exo-exo-Heptacyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane +DMD
RB3LYP/6-31G*



Zero-point correction=	0.372875 (Hartree/Particle)
Thermal correction to Energy=	0.390063
Thermal correction to Enthalpy=	0.391007
Thermal correction to Gibbs Free Energy=	0.327948
Sum of electronic and zero-point Energies=	-850.194996
Sum of electronic and thermal Energies=	-850.177807
Sum of electronic and thermal Enthalpies=	-850.176863
Sum of electronic and thermal Free Energies=	-850.239923

Standard orientation:

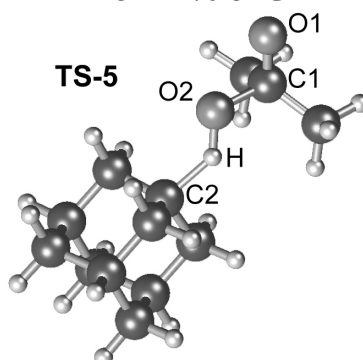
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			X	Y	Z
1	6	0	-0.389180	3.897590	-0.075425
2	6	0	-0.763987	2.462458	-0.353167
3	6	0	0.196407	1.541907	-1.136255
4	6	0	1.593866	2.123518	-0.736389
5	6	0	1.333224	2.078601	0.787657
6	6	0	-0.002284	2.828588	0.915870
7	6	0	0.928026	0.583015	1.001160
8	6	0	0.278475	0.244686	-0.341564
9	6	0	1.917776	-0.603789	1.177414
10	6	0	1.066825	-1.799143	0.634335
11	6	0	0.777429	-1.118740	-0.744149
12	6	0	3.011551	-0.664411	0.101993
13	6	0	3.054712	-2.073887	-0.457512
14	6	0	2.069323	-2.916764	0.332868
15	6	0	2.263268	-0.992995	-1.177060
16	1	0	-1.807827	2.172950	-0.305200
17	1	0	-0.503824	2.803421	1.879564
18	1	0	0.000814	1.433113	-2.205784
19	1	0	0.350612	4.425878	-0.669065
20	1	0	-1.218561	4.530918	0.228150

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21	1	0	2.144400	2.438194	1.427108
22	1	0	2.423505	1.495771	-1.052471
23	1	0	1.755684	3.124474	-1.142197
24	1	0	0.193570	0.506693	1.811052
25	1	0	-1.242580	-0.029879	-0.163767
26	1	0	2.279523	-0.721180	2.203216
27	1	0	0.152345	-1.671714	-1.448995
28	1	0	2.552734	-0.606753	-2.148310
29	1	0	0.174675	-2.043863	1.208844
30	1	0	3.884894	-0.020807	0.110414
31	1	0	3.958759	-2.475840	-0.903369
32	1	0	2.505035	-3.344709	1.243299
33	1	0	1.631874	-3.730349	-0.257755
34	8	0	-1.841677	-0.433982	0.586661
35	6	0	-3.150416	-1.072510	0.078425
36	8	0	-3.701596	-1.210927	1.253492
37	6	0	-3.837417	-0.055320	-0.853440
38	6	0	-2.791800	-2.386755	-0.636714
39	1	0	-3.247270	0.172702	-1.751359
40	1	0	-4.802765	-0.458058	-1.181552
41	1	0	-4.024869	0.865550	-0.293754
42	1	0	-2.190563	-2.229029	-1.542573
43	1	0	-2.245904	-3.031438	0.057441
44	1	0	-3.712870	-2.903081	-0.932435

Adamantane + DMD

RB3LYP/6-31G*



Zero-point correction=	0.322121 (Hartree/Particle)
Thermal correction to Energy=	0.336718
Thermal correction to Enthalpy=	0.337662
Thermal correction to Gibbs Free Energy=	0.279662
Sum of electronic and zero-point Energies=	-658.622454
Sum of electronic and thermal Energies=	-658.607858
Sum of electronic and thermal Enthalpies=	-658.606914
Sum of electronic and thermal Free Energies=	-658.664914

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.912668	-1.212158	-1.073855
2	6	0	0.259521	-0.171995	-0.199665
3	6	0	0.553632	1.237614	-0.628923
4	6	0	2.090302	1.430909	-0.406145

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5	6	0	2.854575	0.402754	-1.265662
6	6	0	2.453670	-1.027447	-0.850993
7	6	0	2.773279	-1.250924	0.641179
8	6	0	2.012188	-0.221150	1.500800
9	6	0	2.412821	1.209005	1.085858
10	6	0	0.470392	-0.407421	1.274731
11	1	0	2.363419	2.450615	-0.704374
12	1	0	3.485787	1.359495	1.264805
13	1	0	1.881405	1.945663	1.702722
14	1	0	0.294312	1.389943	-1.680664
15	1	0	-0.011625	1.960570	-0.031899
16	1	0	2.638088	0.563255	-2.329897
17	1	0	3.936917	0.537043	-1.137239
18	1	0	2.224893	-0.383009	2.565000
19	1	0	-1.165653	-0.562867	-0.363883
20	1	0	2.982774	-1.764979	-1.467318
21	1	0	2.499962	-2.271735	0.939761
22	1	0	3.853423	-1.149146	0.810366
23	1	0	0.170646	-1.418102	1.575867
24	1	0	-0.086695	0.314739	1.882073
25	1	0	0.614020	-2.228173	-0.790616
26	1	0	0.657498	-1.059744	-2.127568
27	8	0	-1.978966	-0.129783	-0.874427
28	6	0	-3.262138	0.014215	-0.050987
29	8	0	-4.046850	0.020592	-1.097963
30	6	0	-3.392097	-1.216987	0.863980
31	6	0	-3.183636	1.338303	0.723569
32	1	0	-4.358974	-1.182798	1.378667
33	1	0	-3.361949	-2.121320	0.249698
34	1	0	-2.606353	-1.265165	1.630138
35	1	0	-4.135878	1.519733	1.236004
36	1	0	-2.387471	1.339224	1.480444
37	1	0	-3.013074	2.151979	0.013707

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Acetone at B3PW91/6-31+G(d) level

Zero-point correction=	0.084148 (Hartree/Particle)
Thermal correction to Energy=	0.089508
Thermal correction to Enthalpy=	0.090452
Thermal correction to Gibbs Free Energy=	0.056038
Sum of electronic and zero-point Energies=	-193.006291
Sum of electronic and thermal Energies=	-193.000931
Sum of electronic and thermal Enthalpies=	-192.999987
Sum of electronic and thermal Free Energies=	-193.034401

C,0,0.025120309,1.2882938404,-0.6120145913
H,0,0.9817865185,1.3785389534,-1.1432194225
C,0,0.0026501031,-0.0000843133,0.1831827032
O,0,0.0019455288,-0.0000920584,1.399809976
H,0,-0.0964945034,2.1448008023,0.0545346407
H,0,-0.7630878147,1.2930461266,-1.3748066561
C,0,-0.0189097354,-1.2884535696,-0.6120551584
H,0,-0.975016154,-1.378740335,-1.1442608278
H,0,0.7700953786,-1.2931577589,-1.3740217585
H,0,0.1020413695,-2.1449626876,0.0546120947

Acetone at B3PW91/6-311+G(d,p) level

Zero-point correction=	0.083327 (Hartree/Particle)
Thermal correction to Energy=	0.088725
Thermal correction to Enthalpy=	0.089669
Thermal correction to Gibbs Free Energy=	0.055147
Sum of electronic and zero-point Energies=	-193.056710
Sum of electronic and thermal Energies=	-193.051312
Sum of electronic and thermal Enthalpies=	-193.050368
Sum of electronic and thermal Free Energies=	-193.084891

C,0,0.0273567245,1.2853180325,-0.611964754
H,0,0.9920479993,1.3786825048,-1.1230763087
C,0,0.0026640598,-0.0000853815,0.1837347
O,0,0.0019982083,-0.0000913391,1.3936342006
H,0,-0.1112513628,2.1393362548,0.050315635
H,0,-0.7442688581,1.2810351343,-1.3879595221
C,0,-0.0211582318,-1.2854793318,-0.6120054056
H,0,-0.985298929,-1.3788400421,-1.1241623358
H,0,0.7513059001,-1.2811824855,-1.3871694921
H,0,0.1167354281,-2.1395061409,0.0504127871

Dimethyldioxirane at B3PW91/6-31+G(d) level

Zero-point correction=	0.088767 (Hartree/Particle)
Thermal correction to Energy=	0.094383
Thermal correction to Enthalpy=	0.095328
Thermal correction to Gibbs Free Energy=	0.061170
Sum of electronic and zero-point Energies=	-268.088980
Sum of electronic and thermal Energies=	-268.083364

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Sum of electronic and thermal Enthalpies= -268.082419
Sum of electronic and thermal Free Energies= -268.116577

C,0,0.0817544688,0.,0.049127692
C,0,0.0819428935,0.,1.5541497338
C,0,1.4107575682,0.,-0.6571598866
O,0,-0.9337700696,-0.7452848589,-0.5611187868
O,0,-0.9337700696,0.7452848589,-0.5611187868
H,0,-0.9461926047,0.,1.9230235864
H,0,1.2538638387,0.,-1.7381385541
H,0,0.6022006555,-0.8863280304,1.9344431758
H,0,0.6022006555,0.8863280304,1.9344431758
H,0,1.9907594931,0.8863280304,-0.3762880153
H,0,1.9907594931,-0.8863280304,-0.3762880153

Dimethyldioxirane at B3PW91/6-311+G(d,p) level

Zero-point correction= 0.088072 (Hartree/Particle)
Thermal correction to Energy= 0.093669
Thermal correction to Enthalpy= 0.094613
Thermal correction to Gibbs Free Energy= 0.059873
Sum of electronic and zero-point Energies= -268.156458
Sum of electronic and thermal Energies= -268.150861
Sum of electronic and thermal Enthalpies= -268.149917
Sum of electronic and thermal Free Energies= -268.184657

O,0,0.5403009533,-0.0084677843,-1.1996821691
C,0,-0.0809930762,0.0007772058,0.0495131409
O,0,1.3140710216,-0.0093272298,0.0661710505
C,0,-0.7506672595,-1.2797688489,0.4579874273
C,0,-0.7319137944,1.2939960832,0.4482613507
H,0,-0.1672666955,-2.128449266,0.1008596665
H,0,-0.8358583069,-1.3318586678,1.5470313585
H,0,-1.7587396335,-1.3308749981,0.0370755081
H,0,-0.8163457297,1.3555213855,1.5368720132
H,0,-0.1361911224,2.1313618364,0.0848222233
H,0,-1.7391295308,1.356633182,0.026856666

•OC(Me₂)O• OS-¹A₁ at UB3PW91/6-31+G(d) level

Zero-point correction= 0.085690 (Hartree/Particle)
Thermal correction to Energy= 0.091862
Thermal correction to Enthalpy= 0.092806
Thermal correction to Gibbs Free Energy= 0.056984
Sum of electronic and zero-point Energies= -268.069109
Sum of electronic and thermal Energies= -268.062937
Sum of electronic and thermal Enthalpies= -268.061993
Sum of electronic and thermal Free Energies= -268.097815
<S²> = 0.9122

O,0,0.0038089879,0.0041649558,-0.0017012048
C,0,0.0087053223,0.0093222398,1.3515409967
O,0,1.2105941927,0.0027740349,1.9732516588

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C,0,-0.7689849322,-1.268177026,1.8256616697
C,0,-0.7502681186,1.3014808091,1.816043176
H,0,-0.2322777969,-2.1608083565,1.4966483009
H,0,-0.8283802746,-1.2558021808,2.9159180449
H,0,-1.7663343781,-1.2540156727,1.3812777172
H,0,-0.8093914675,1.2983755164,2.9063789302
H,0,-0.2008638965,2.1837167286,1.4800032042
H,0,-1.7478938286,1.298334285,1.3720897887

$\bullet\text{OC}(\text{Me}_2)\text{O}\bullet$ $\text{OS-}^1\text{A}_1$ at UB3PW91/6-311+G(d,p) level

Zero-point correction= 0.084696 (Hartree/Particle)
Thermal correction to Energy= 0.090957
Thermal correction to Enthalpy= 0.091901
Thermal correction to Gibbs Free Energy= 0.055886
Sum of electronic and zero-point Energies= -268.138638
Sum of electronic and thermal Energies= -268.132376
Sum of electronic and thermal Enthalpies= -268.131432
Sum of electronic and thermal Free Energies= -268.167447
<S²> = 0.9060

O,0,0.0003521147,-0.8378889422,1.1539174603
C,0,-0.0000029195,-0.1419541092,0.0001680257
O,0,0.0002248305,-0.8387375334,-1.1530733813
C,0,1.2830865358,0.7621871146,-0.0002396482
C,0,-1.2837225004,0.7612618926,-0.0000957336
H,0,2.1682433555,0.1260705282,-0.0000561747
H,0,1.2719755723,1.3785316042,-0.898740572
H,0,1.2720807435,1.3791966431,0.8978058634
H,0,-1.2731687874,1.377613526,-0.8985986966
H,0,-2.1684240195,0.124510971,0.0001927268
H,0,-1.2730669255,1.378283305,0.8979461303

$\bullet\text{OC}(\text{Me}_2)\text{O}\bullet$ $^3\text{A}_2$ at UB3PW91/6-311+G(d,p) level

Zero-point correction= 0.084965 (Hartree/Particle)
Thermal correction to Energy= 0.091093
Thermal correction to Enthalpy= 0.092037
Thermal correction to Gibbs Free Energy= 0.055319
Sum of electronic and zero-point Energies= -268.134155
Sum of electronic and thermal Energies= -268.128027
Sum of electronic and thermal Enthalpies= -268.127082
Sum of electronic and thermal Free Energies= -268.163801
<S²> = 2.0078

O,0,-0.0380804679,-0.8790398187,1.1275433321
C,0,0.0147643302,-0.1123763634,0.0001576615
O,0,-0.0381496127,-0.8798830482,-1.126650622
C,0,1.2821438256,0.7753005343,-0.0002314128
C,0,-1.2801689768,0.7573644356,-0.0001103578
H,0,2.1685266263,0.1384613016,-0.0000954035
H,0,1.2943667045,1.3985498918,-0.8954646574
H,0,1.2945016489,1.3991233727,0.8946005792

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H,0,-1.2730370982,1.3816537525,-0.8952423481
H,0,-2.1543528223,0.1075511936,0.000198675
H,0,-1.2729361576,1.3823697481,0.8945205539

HOC(Me₂)O• at UB3PW91/6-311+G(d,p) level

Zero-point correction= 0.097779 (Hartree/Particle)
Thermal correction to Energy= 0.104406
Thermal correction to Enthalpy= 0.105350
Thermal correction to Gibbs Free Energy= 0.067526
Sum of electronic and zero-point Energies= -268.803530
Sum of electronic and thermal Energies= -268.796903
Sum of electronic and thermal Enthalpies= -268.795959
Sum of electronic and thermal Free Energies= -268.833783
<S²> = 0.7541

C,0,0.0553743682,-0.0052964542,0.0764798575
O,0,0.1560473654,0.0639183171,1.4038901418
O,0,1.2986935644,0.1271457859,-0.601477467
C,0,-0.8800246788,1.1639604895,-0.3605659445
C,0,-0.5518636903,-1.3645311725,-0.337706166
H,0,-1.5535906259,-1.4732208218,0.0779795629
H,0,-0.5882323068,-1.4067832963,-1.4276124152
H,0,0.0892725329,-2.1681172243,0.0265505794
H,0,-1.8733503396,1.0385400152,0.0701982327
H,0,-0.9302061912,1.1513119034,-1.4504667471
H,0,-0.4531184119,2.1129957382,-0.0333544503
H,0,1.9303819092,0.451963685,0.048157358

2-Methylpropane at B3PW91/6-311+G(d,p) level

Zero-point correction= 0.131035 (Hartree/Particle)
Thermal correction to Energy= 0.136754
Thermal correction to Enthalpy= 0.137698
Thermal correction to Gibbs Free Energy= 0.103409
Sum of electronic and zero-point Energies= -158.315093
Sum of electronic and thermal Energies= -158.309374
Sum of electronic and thermal Enthalpies= -158.308430
Sum of electronic and thermal Free Energies= -158.342720

C,0,-0.2049631918,1.4414057175,0.0944216777
C,0,0.0002104768,-0.0000466234,-0.3732412372
C,0,-1.1461141315,-0.898065349,0.093809096
C,0,1.3511579743,-0.5435458978,0.0937273898
H,0,0.000045292,0.0002292124,-1.47215152
H,0,0.5956219432,2.0957703221,-0.2652411992
H,0,-1.1561499185,1.8465982411,-0.2655179333
H,0,-0.2130849781,1.4964557083,1.1893887221
H,0,-1.0210825815,-1.9246802243,-0.2651482873
H,0,-1.191135358,-0.9312507303,1.1887276549
H,0,-2.1125407238,-0.532032326,-0.267518714
H,0,1.4035910459,-0.5631116655,1.1886404886
H,0,1.5166736143,-1.5643977429,-0.2654687116

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H,0,2.1777705366,0.0766743578,-0.2676024266

2-Methylpropan-2-ol at B3PW91/6-311+G(d,p) level

Zero-point correction= 0.135026 (Hartree/Particle)
Thermal correction to Energy= 0.141848
Thermal correction to Enthalpy= 0.142792
Thermal correction to Gibbs Free Energy= 0.105948
Sum of electronic and zero-point Energies= -233.527144
Sum of electronic and thermal Energies= -233.520322
Sum of electronic and thermal Enthalpies= -233.519378
Sum of electronic and thermal Free Energies= -233.556222

C,0,-0.0052100458,-0.0000000026,0.0144998543
C,0,-1.4868617649,-0.0000007539,-0.3417693543
O,0,0.0298672771,0.0000000151,1.4487829367
C,0,0.6824909191,1.2598025919,-0.5157458633
C,0,0.6824921966,-1.2598018999,-0.5157458633
H,0,-1.6258530657,-0.0000008243,-1.4261359241
H,0,-1.9749769035,0.8853692352,0.0734119156
H,0,-1.9749760057,-0.8853712379,0.0734119156
H,0,0.9500386993,0.0000004817,1.7274020188
H,0,1.7451995892,1.2669642075,-0.2482991252
H,0,0.2163218531,2.1514592197,-0.0885055203
H,0,0.6131567695,1.3197303608,-1.6060883845
H,0,1.745200874,-1.2669624378,-0.2482991252
H,0,0.6131581078,-1.3197297391,-1.6060883845
H,0,0.2163240348,-2.1514590003,-0.0885055203

Me₃C[•] at UB3PW91/6-311+G(d,p) level

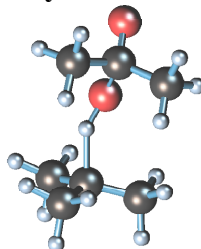
Zero-point correction= 0.116102 (Hartree/Particle)
Thermal correction to Energy= 0.122489
Thermal correction to Enthalpy= 0.123433
Thermal correction to Gibbs Free Energy= 0.087684
Sum of electronic and zero-point Energies= -157.669067
Sum of electronic and thermal Energies= -157.662680
Sum of electronic and thermal Enthalpies= -157.661736
Sum of electronic and thermal Free Energies= -157.697485
<S²> = 0.7546

C,0,-0.2084006343,1.4670722883,0.0153218477
C,0,0,0,-0.1535026748
C,0,-1.1663215537,-0.9140163876,0.0153218477
C,0,1.374722188,-0.5530559006,0.0153218477
H,0,0.6050332627,2.047133237,-0.4329942054
H,0,-1.1511937027,1.7976575864,-0.4329942054
H,0,-0.2494837931,1.7562842856,1.0810626742
H,0,-0.9812202858,-1.8957917845,-0.4329942054
H,0,-1.3962449111,-1.0942014454,1.0810626742
H,0,-2.0753860196,-0.4995924428,-0.4329942054
H,0,1.6457287041,-0.6620828402,1.0810626742
H,0,1.4703527568,-1.5475407942,-0.4329942054

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H,0,2.1324139885,0.098134198,-0.4329942054

TS-C **2-Methylpropane + Dimethyldioxirane** at RB3PW91/6-31+G(d) level

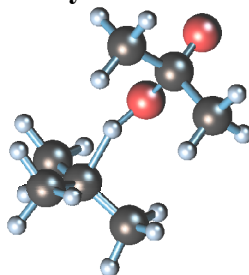


Zero-point correction= 0.215772 (Hartree/Particle)
Thermal correction to Energy= 0.228783
Thermal correction to Enthalpy= 0.229727
Thermal correction to Gibbs Free Energy= 0.176606
Sum of electronic and zero-point Energies= -426.319021
Sum of electronic and thermal Energies= -426.306010
Sum of electronic and thermal Enthalpies= -426.305065
Sum of electronic and thermal Free Energies= -426.358187
<S²> = 0.0000

C,0,-0.4607756942,0.3063987529,-1.737626666
H,0,-0.4128836808,0.2822050359,-0.218123159
C,0,0.952926032,0.3004743465,-2.2196381551
H,0,1.4828660419,1.2101185809,-1.9286080171
H,0,1.507056231,-0.5677470999,-1.8515613322
H,0,0.9464684953,0.2443795369,-3.3221715448
C,0,-1.2250952648,-0.9783828892,-1.8604483619
H,0,-1.4605167702,-1.1386764843,-2.9272274364
H,0,-0.6388247673,-1.8416606551,-1.5295942248
H,0,-2.1768052357,-0.9548325852,-1.3202581121
C,0,-1.2281132452,1.5826925804,-1.8801525386
H,0,-2.1930484527,1.5469595453,-1.3657922439
H,0,-0.6557414978,2.4366197307,-1.508038676
H,0,-1.4285829175,1.7536005076,-2.9521959783
O,0,0.1566086634,0.7080466803,0.54900518
C,0,0.4434044109,-0.2239243789,1.6975747557
O,0,0.7496604935,0.7398273023,2.5395746413
C,0,1.6080496471,-1.1396948548,1.3101875662
C,0,-0.8367075613,-0.9969918448,2.0403902594
H,0,2.4614907442,-0.5242754578,1.0119953437
H,0,1.9018603216,-1.7431417326,2.1770880542
H,0,1.3470227755,-1.8275406834,0.4939106958
H,0,-0.6684579081,-1.5845495115,2.9499585846
H,0,-1.645013093,-0.2859204222,2.235549822
H,0,-1.139173488,-1.6919604381,1.2447084954

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TS-C 2-Methylpropane + Dimethyldioxirane at RB3PW91/6-311+G(d,p) level

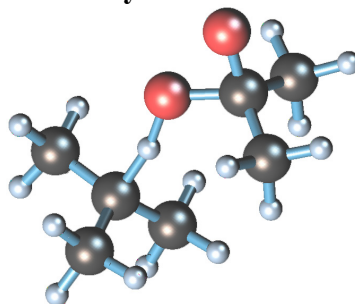


Zero-point correction= 0.213365 (Hartree/Particle)
Thermal correction to Energy= 0.226540
Thermal correction to Enthalpy= 0.227484
Thermal correction to Gibbs Free Energy= 0.173336
Sum of electronic and zero-point Energies= -426.435368
Sum of electronic and thermal Energies= -426.422193
Sum of electronic and thermal Enthalpies= -426.421249
Sum of electronic and thermal Free Energies= -426.475397
<S²> = 0.0000

C,0,-0.4486595732,0.3008937268,-1.7425348107
H,0,-0.3090743791,0.2654933108,-0.2703811567
C,0,0.9536396728,0.2971422308,-2.2524689152
H,0,1.491895106,1.1968340039,-1.9533147575
H,0,1.5090195258,-0.5804425402,-1.9160140939
H,0,0.9261804581,0.266512953,-3.3534109641
C,0,-1.2197863086,-0.9775586816,-1.8600401144
H,0,-1.4960812628,-1.1156102024,-2.9178018004
H,0,-0.6266880073,-1.8472563365,-1.5684396857
H,0,-2.1484563747,-0.9581472917,-1.285402042
C,0,-1.2156974176,1.5767173513,-1.8639727381
H,0,-2.1624716653,1.5417450612,-1.3218217394
H,0,-0.6322884185,2.4277928624,-1.5097724983
H,0,-1.4469030113,1.7463239239,-2.9277446965
O,0,0.1577037106,0.7095655057,0.5584998961
C,0,0.4332685447,-0.2232550041,1.6999510562
O,0,0.7211844401,0.7461563987,2.5393364649
C,0,1.6086994803,-1.1306072412,1.3332033678
C,0,-0.8426818536,-1.00212074,2.0320610994
H,0,2.4594272518,-0.5096506264,1.047592779
H,0,1.8920902574,-1.7278293808,2.2048605622
H,0,1.3649401849,-1.821210645,0.5171861477
H,0,-0.6801092557,-1.5849594328,2.9430465631
H,0,-1.653327585,-0.2944968131,2.2156101228
H,0,-1.1319532981,-1.6981439327,1.2359227019

S. A. Grabovskiy

TS-LS 2-Methylpropane + Dimethyldioxirane at UB3PW91/6-31+G(d) level

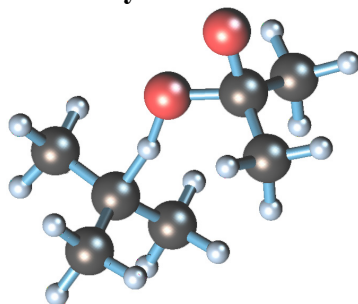


Zero-point correction=	0.215136 (Hartree/Particle)
Thermal correction to Energy=	0.227739
Thermal correction to Enthalpy=	0.228683
Thermal correction to Gibbs Free Energy=	0.176425
Sum of electronic and zero-point Energies=	-426.329600
Sum of electronic and thermal Energies=	-426.316997
Sum of electronic and thermal Enthalpies=	-426.316053
Sum of electronic and thermal Free Energies=	-426.368311
$\langle S^2 \rangle =$	0.4584

C,0,-0.0022407111,-0.463031473,-1.6926115786
H,0,0.0006408934,-0.4542617933,-0.4192376791
C,0,1.4692027732,-0.4371571737,-2.0440071174
H,0,1.9537170207,0.4839363743,-1.7031556756
H,0,1.999923648,-1.2898337937,-1.60875361
H,0,1.5876315137,-0.4897038874,-3.1375171254
C,0,-0.6991203132,-1.7713229896,-1.9955930627
H,0,-0.7404896237,-1.923412928,-3.0853672353
H,0,-0.1643434397,-2.620375051,-1.5583061893
H,0,-1.7261283524,-1.7784454775,-1.6166319325
C,0,-0.7747706642,0.7718511183,-2.1003500556
H,0,-1.8005869814,0.7547087658,-1.7175837399
H,0,-0.2868675897,1.6924802201,-1.7616633591
H,0,-0.8333303035,0.8189907184,-3.1989412098
O,0,0.0337589036,-0.7120843622,0.797696185
C,0,0.0020785289,0.4059073353,1.680589437
O,0,0.1186194537,-0.4881627444,2.7113780899
C,0,-1.3325508735,1.1403279515,1.6664611092
C,0,1.2116224234,1.3192735961,1.5242901725
H,0,-2.1452688082,0.4132743339,1.746386518
H,0,-1.3886172648,1.8248435894,2.5208177524
H,0,-1.4600238312,1.7318286419,0.7522176765
H,0,1.2565652118,2.025298043,2.3614892691
H,0,2.1233448763,0.7158516976,1.524649643
H,0,1.1594791921,1.9017072102,0.5963292721

S. A. Grabovskiy

TS-LS 2-Methylpropane + Dimethyldioxirane at UB3PW91/6-311+G(d,p) level

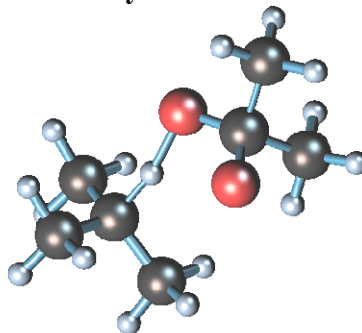


Zero-point correction=	0.213553 (Hartree/Particle)
Thermal correction to Energy=	0.226221
Thermal correction to Enthalpy=	0.227165
Thermal correction to Gibbs Free Energy=	0.174656
Sum of electronic and zero-point Energies=	-426.442071
Sum of electronic and thermal Energies=	-426.429403
Sum of electronic and thermal Enthalpies=	-426.428459
Sum of electronic and thermal Free Energies=	-426.480968
<S ² > = 0.3743	

C,0,-1.7515136256,-0.0052477385,0.0131928485
H,0,-0.547955004,-0.0202305083,-0.3207845458
C,0,-2.0986508533,1.4664710059,0.0322509486
H,0,-1.5247965853,2.0099372809,0.787142462
H,0,-1.9190961665,1.9318264246,-0.9395936049
H,0,-3.1636228135,1.591617106,0.2723417541
C,0,-2.4055667723,-0.7854160191,-1.104975963
H,0,-3.4925159044,-0.816708987,-0.9472269802
H,0,-2.2217979131,-0.3206781195,-2.0763382789
H,0,-2.0431737033,-1.8153696352,-1.1425123512
C,0,-1.8097100036,-0.6822009957,1.3637435306
H,0,-1.4434250921,-1.7107965062,1.3181475826
H,0,-1.2375674773,-0.1378856872,2.1199443598
H,0,-2.8520990393,-0.7193992011,1.7092320792
O,0,0.5793490869,-0.0176660695,-0.8913064704
C,0,1.7349192584,0.0016275202,-0.0601971635
O,0,2.439109426,0.0319136606,-1.2287615674
C,0,1.9235100786,-1.2792438678,0.7356440914
C,0,1.8536547369,1.2714337841,0.7666941846
H,0,1.786494014,-2.135976768,0.0742065472
H,0,2.936538532,-1.3113963791,1.147186791
H,0,1.21878352,-1.3435712053,1.5698673342
H,0,2.8577972107,1.3422407236,1.1946049552
H,0,1.6836771555,2.1363757075,0.1239764972
H,0,1.1352342489,1.2814928911,1.5922348386

S. A. Grabovskiy

TS-OS 2-Methylpropane + Dimethyldioxirane at UB3PW91/6-31+G(d) level

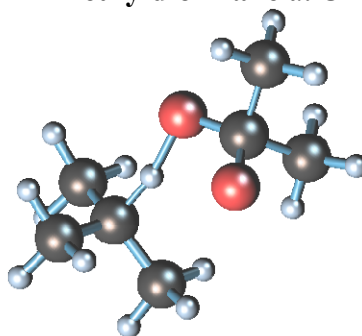


Zero-point correction= 0.214243 (Hartree/Particle)
Thermal correction to Energy= 0.227025
Thermal correction to Enthalpy= 0.227969
Thermal correction to Gibbs Free Energy= 0.175280
Sum of electronic and zero-point Energies= -426.338105
Sum of electronic and thermal Energies= -426.325323
Sum of electronic and thermal Enthalpies= -426.324379
Sum of electronic and thermal Free Energies= -426.377068
<S²> = 0.9362

C,0,0.5703136406,0.1738606532,-1.670902018
H,0,0.4976863356,0.2053717954,-0.4512433497
C,0,2.0662187156,0.1951698003,-1.9315562654
H,0,2.536873448,1.0754882789,-1.4806736485
H,0,2.5587433346,-0.6987065318,-1.5326169035
H,0,2.259753793,0.2291189814,-3.0148226939
C,0,-0.1141046975,-1.094561667,-2.1476045365
H,0,-0.0763340042,-1.1450245394,-3.2467862641
H,0,0.3803876677,-1.9946483256,-1.7644469451
H,0,-1.1689774595,-1.1197146444,-1.8532662899
C,0,-0.1418930764,1.444255482,-2.0986885013
H,0,-1.1940442427,1.4321865287,-1.7966610307
H,0,0.3290089696,2.3306852225,-1.6604529224
H,0,-0.1012052414,1.5473456668,-3.1941316843
O,0,0.5589891773,0.4779552274,0.8974181923
C,0,-0.5254811366,-0.0966672503,1.539258322
O,0,-1.7403232821,0.2103362202,1.0424439041
C,0,-0.4480287272,0.4917191046,2.9890876313
C,0,-0.4247549644,-1.6484886944,1.6019872584
H,0,-0.5591229066,1.5770312215,2.9429927087
H,0,-1.2532142214,0.0590028147,3.5877248651
H,0,0.5243849011,0.2409984051,3.419376314
H,0,-1.2230305946,-2.0619121479,2.2231317248
H,0,-0.5060082729,-2.0651054002,0.5949777941
H,0,0.5521528076,-1.9101734772,2.0185102114

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TS-OS 2-Methylpropane + Dimethyldioxirane at UB3PW91/6-311+G(d,p) level

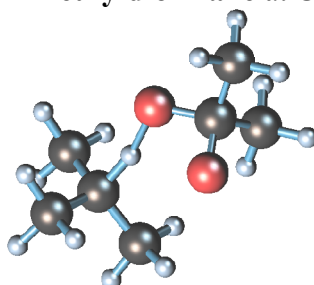


Zero-point correction= 0.212879 (Hartree/Particle)
Thermal correction to Energy= 0.225723
Thermal correction to Enthalpy= 0.226667
Thermal correction to Gibbs Free Energy= 0.173409
Sum of electronic and zero-point Energies= -426.449628
Sum of electronic and thermal Energies= -426.436783
Sum of electronic and thermal Enthalpies= -426.435839
Sum of electronic and thermal Free Energies= -426.489098
<S²> = 0.9283

C,0,0.5761174257,0.170671493,-1.6802002556
H,0,0.4887382966,0.2106778484,-0.4903941027
C,0,2.0726349769,0.185012308,-1.936855702
H,0,2.5437312752,1.06546326,-1.4921880665
H,0,2.5600850847,-0.7049538274,-1.5291281131
H,0,2.2708641966,0.2090181457,-3.0170055418
C,0,-0.1042860371,-1.0971382119,-2.1641582086
H,0,-0.0506467509,-1.1527550093,-3.2598530085
H,0,0.380335232,-1.9954655868,-1.7707099493
H,0,-1.1615173445,-1.1189568162,-1.886369114
C,0,-0.1247134769,1.4364104157,-2.1391553882
H,0,-1.1799485159,1.431858887,-1.8557462137
H,0,0.3393889288,2.3258644742,-1.7054503451
H,0,-0.0657851477,1.5251768975,-3.2324949899
O,0,0.5218124233,0.5108437433,0.9106059623
C,0,-0.5380100414,-0.0901271707,1.5531440483
O,0,-1.7638804378,0.2109830788,1.0941351898
C,0,-0.4359318963,0.4739571346,3.0144301478
C,0,-0.4148335524,-1.6402896256,1.5878189079
H,0,-0.5618647216,1.5558356331,2.9883125794
H,0,-1.2241905936,0.0189342478,3.6147036187
H,0,0.5462292566,0.2263545496,3.4171201537
H,0,-1.1929374266,-2.071869122,2.2178416865
H,0,-0.5146116807,-2.0363633875,0.5767874551
H,0,0.5728096349,-1.8944128293,1.9765034357

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TS-T 2-Methylpropane + Dimethyldioxirane at UB3PW91/6-311+G(d,p) level

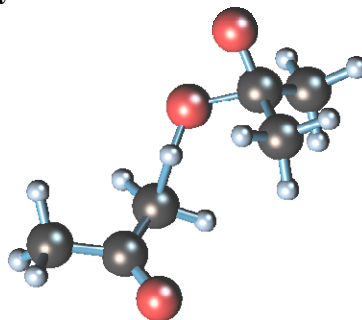


Zero-point correction= 0.213223 (Hartree/Particle)
Thermal correction to Energy= 0.225934
Thermal correction to Enthalpy= 0.226878
Thermal correction to Gibbs Free Energy= 0.172245
Sum of electronic and zero-point Energies= -426.443828
Sum of electronic and thermal Energies= -426.431118
Sum of electronic and thermal Enthalpies= -426.430173
Sum of electronic and thermal Free Energies= -426.484806
<S²> = 2.0125

C,0,-1.775322346,-0.0189265737,0.003959475
H,0,-0.604102632,-0.2161883167,0.2124062744
C,0,-2.4173302354,-0.1351871387,1.3736968356
H,0,-2.2180119634,-1.1093628226,1.8276003763
H,0,-2.059105372,0.6415027658,2.0549091414
H,0,-3.5066925192,-0.024151692,1.2863313431
C,0,-1.9094887551,1.3572000417,-0.6188667527
H,0,-2.9601480905,1.5402543649,-0.8829537197
H,0,-1.6067996845,2.1493101313,0.0717170202
H,0,-1.3167903202,1.4436142718,-1.5327074583
C,0,-2.1503805205,-1.1455822562,-0.9401292811
H,0,-1.603441448,-1.0732817715,-1.8830251649
H,0,-1.94084439,-2.1228623773,-0.4980789773
H,0,-3.2246947272,-1.1019384894,-1.1658571281
O,0,0.669816433,-0.7802054335,0.509597407
C,0,1.7067545885,-0.009030557,-0.0058466734
O,0,1.4619189487,-0.10638249,-1.3626933209
C,0,2.9961186239,-0.7547353108,0.3876044381
C,0,1.7064835787,1.4347088166,0.4859379221
H,0,2.9368006548,-1.7867863285,0.0416772287
H,0,3.8423572032,-0.261575944,-0.0984982617
H,0,3.1391945632,-0.7330636839,1.4698937615
H,0,2.5334493807,1.9834660158,0.026959153
H,0,0.7728640691,1.9226230664,0.2040149134
H,0,1.8210726173,1.4704620669,1.5722430275

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TS-C Acetone + Dimethyldioxirane at RB3PW91/6-31+G(d) level

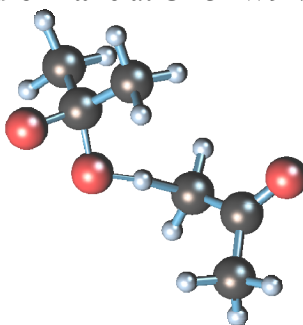


Zero-point correction= 0.169843 (Hartree/Particle)
Thermal correction to Energy= 0.181717
Thermal correction to Enthalpy= 0.182661
Thermal correction to Gibbs Free Energy= 0.130042
Sum of electronic and zero-point Energies= -461.032970
Sum of electronic and thermal Energies= -461.021096
Sum of electronic and thermal Enthalpies= -461.020152
Sum of electronic and thermal Free Energies= -461.072771
<S²> = 0.0000

C,0,-3.1776629861,-0.8386358333,-0.5105659167
H,0,-2.5742309861,-1.6282478333,-0.9739799167
C,0,-2.3033349861,0.1911171667,0.1664740833
O,0,-2.4754969861,1.3951991667,0.0273890833
H,0,-3.8051219861,-0.3566968333,-1.2628649167
H,0,-3.8232609861,-1.3224158333,0.2338910833
C,0,-1.2055559861,-0.3084828333,1.0339480833
H,0,-1.2826149861,-1.3162948333,1.4338890833
H,0,-0.2582509861,-0.4316238333,-0.1298529167
H,0,-0.7532479861,0.4326991667,1.6870140833
O,0,0.6768960139,-0.9087668333,0.0272930833
O,0,2.4129890139,-1.0086628333,-0.8646689167
C,0,1.4955510139,1.2293531667,-0.9604619167
H,0,2.4096000139,1.7780441667,-1.2119459167
H,0,1.0069400139,0.9386621667,-1.8952109167
H,0,0.8424100139,1.9037401667,-0.3955269167
C,0,1.8778140139,-0.0142218333,-0.1667089167
C,0,2.5198670139,0.2685011667,1.1816690833
H,0,1.9156330139,0.9498981667,1.7910000833
H,0,2.6694890139,-0.6717668333,1.7183550833
H,0,3.4974830139,0.7360601667,1.0189990833

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TS-LS Acetone + Dimethyldioxirane at UB3PW91/6-31+G(d) level

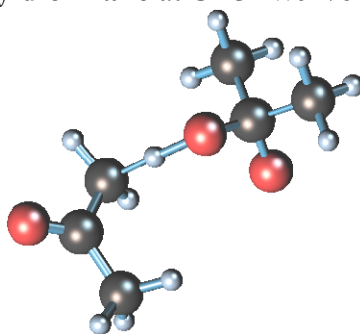


Zero-point correction= 0.166534 (Hartree/Particle)
Thermal correction to Energy= 0.178561
Thermal correction to Enthalpy= 0.179505
Thermal correction to Gibbs Free Energy= 0.126492
Sum of electronic and zero-point Energies= -461.051405
Sum of electronic and thermal Energies= -461.039379
Sum of electronic and thermal Enthalpies= -461.038435
Sum of electronic and thermal Free Energies= -461.091448
<S²> = 0.6800

C,0,-1.2510637577,-2.6677445223,-0.9947660858
H,0,-1.6809539339,-2.2775835138,-0.0640696406
C,0,-0.1688185768,-1.7434157536,-1.4917005624
O,0,0.9665805944,-2.1224464537,-1.7356134718
H,0,-0.8433077864,-3.666465877,-0.827379025
H,0,-2.0664606988,-2.7252678812,-1.7267515808
C,0,-0.522837559,-0.3080631502,-1.686237208
H,0,-1.5322525563,-0.0919249264,-2.0432739646
H,0,-0.6139096627,0.1593470734,-0.4599875939
H,0,0.2610388088,0.2935022906,-2.1470350638
O,0,-0.861646495,0.6675739951,0.585119467
O,0,-0.4670117716,1.5303120055,2.325702609
C,0,1.4587693682,0.4256559911,1.355485136
H,0,2.2110904841,0.9292630776,1.9727840294
H,0,1.1435926572,-0.4889283065,1.8649969527
H,0,1.9265893363,0.1641430456,0.3996460517
C,0,0.2566928776,1.3393012202,1.1597506728
C,0,0.5786337192,2.6489219757,0.4536260433
H,0,1.0459768169,2.4705898647,-0.5217589339
H,0,-0.3410218671,3.2237870953,0.316584508
H,0,1.2779833497,3.2380871167,1.0576274524

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TS-OS Acetone + Dimethyldioxirane at UB3PW91/6-31+G(d) level



Zero-point correction= 0.166256 (Hartree/Particle)
Thermal correction to Energy= 0.178317
Thermal correction to Enthalpy= 0.179262
Thermal correction to Gibbs Free Energy= 0.126323
Sum of electronic and zero-point Energies= -461.065052
Sum of electronic and thermal Energies= -461.052990
Sum of electronic and thermal Enthalpies= -461.052046
Sum of electronic and thermal Free Energies= -461.104984
<S²> = 0.9382

C,0,-0.1645153713,-0.5192316856,-1.5616769574
H,0,-0.0792156233,-0.5164149764,-0.2960914808
C,0,1.2273517958,-0.8337140521,-2.0079387627
O,0,1.4774324683,-1.9184619524,-2.5085628319
H,0,-0.8871899039,-1.2986624713,-1.8076163699
H,0,-0.503760367,0.4941609564,-1.7927305924
O,0,-0.0278745193,-0.4406851895,0.970780094
C,0,-0.8712174316,0.5707041344,1.4174332493
O,0,-0.6321606153,1.7950355113,0.9110596315
C,0,-0.5854055987,0.6321112712,2.9559610575
C,0,-2.3684542959,0.2354856392,1.1714761469
H,0,-0.7843718185,-0.3511515796,3.3881452476
H,0,0.4606629393,0.8993889771,3.1184625471
H,0,-1.2377373649,1.3860589348,3.4022457842
H,0,-3.0118629626,0.9826644282,1.6417220538
H,0,-2.5707765721,0.2186940638,0.0966908772
H,0,-2.5713992146,-0.7550337814,1.587952164
C,0,2.2743532189,0.2346548441,-1.8138587835
H,0,2.0426060229,1.1067068609,-2.4383148445
H,0,2.271488358,0.5779341117,-0.7726438167
H,0,3.2597039344,-0.1515133865,-2.0824124188

Adamantane at B3PW91/6-31+G(d) level

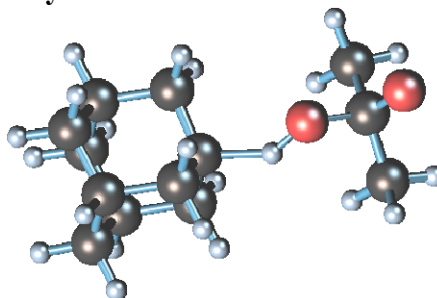
Zero-point correction= 0.244574 (Hartree/Particle)
Thermal correction to Energy= 0.251566
Thermal correction to Enthalpy= 0.252510
Thermal correction to Gibbs Free Energy= 0.215061
Sum of electronic and zero-point Energies= -390.357831
Sum of electronic and thermal Energies= -390.350839
Sum of electronic and thermal Enthalpies= -390.349895

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Sum of electronic and thermal Free Energies= -390.387344

C,0,0.,1.2580846082,0.8890634193
C,0,0.,0.,1.773650972
C,0,-1.2551928113,1.2551928113,0.
C,0,1.2551928113,1.2551928113,0.
H,0,0.,2.1552109146,1.5242296903
C,0,0.,-1.2580846082,0.8890634193
C,0,-1.2580846082,0.,-0.8890634193
C,0,1.2580846082,0.,-0.8890634193
H,0,0.8830846362,0.,2.429486779
H,0,-0.8830846362,0.,2.429486779
H,0,-1.2769411523,2.1600846985,-0.6247354627
H,0,-2.1600846985,1.2769411523,0.6247354627
H,0,1.2769411523,2.1600846985,-0.6247354627
H,0,2.1600846985,1.2769411523,0.6247354627
C,0,1.2551928113,-1.2551928113,0.
C,0,-1.2551928113,-1.2551928113,0.
C,0,0.,0.,-1.773650972
H,0,0.,-2.1552109146,1.5242296903
H,0,-2.1552109146,0.,-1.5242296903
H,0,2.1552109146,0.,-1.5242296903
H,0,1.2769411523,-2.1600846985,-0.6247354627
H,0,2.1600846985,-1.2769411523,0.6247354627
H,0,-1.2769411523,-2.1600846985,-0.6247354627
H,0,-2.1600846985,-1.2769411523,0.6247354627
H,0,0.,-0.8830846362,-2.429486779
H,0,0.,0.8830846362,-2.429486779

TS-C Adamantane + Dimethyldioxirane at RB3PW91/6-31+G(d) level



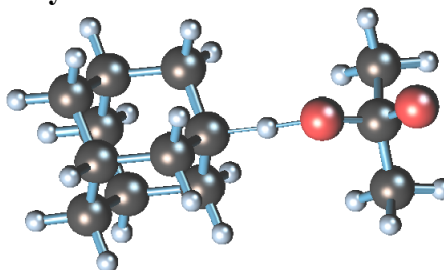
Zero-point correction= 0.328483 (Hartree/Particle)
Thermal correction to Energy= 0.342878
Thermal correction to Enthalpy= 0.343822
Thermal correction to Gibbs Free Energy= 0.286340
Sum of electronic and zero-point Energies= -658.404666
Sum of electronic and thermal Energies= -658.390271
Sum of electronic and thermal Enthalpies= -658.389327
Sum of electronic and thermal Free Energies= -658.446809
<S²> = 0.0000

C,0,0.9004999724,-1.1389467045,-1.0887795559
C,0,0.2871203726,-0.1592989298,-0.1384604896
C,0,0.5316264733,1.2695924967,-0.4975893962

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C,0,2.0708413361,1.4677225581,-0.3153861928
C,0,2.8109554441,0.5023413262,-1.254154285
C,0,2.4423656769,-0.9482344907,-0.9077490487
C,0,2.8136305385,-1.2501636683,0.5519364135
C,0,2.0766574692,-0.2823445068,1.4895676528
C,0,2.4436793098,1.1684979291,1.1445113465
C,0,0.5329902766,-0.4749720587,1.3073621082
H,0,2.3182524041,2.5073984584,-0.5661352287
H,0,3.5208054077,1.3237902591,1.2959660632
H,0,1.9255017672,1.8629325378,1.8200364412
H,0,0.23686387,1.4738940506,-1.5314844625
H,0,-0.0185705611,1.9519503809,0.1596296397
H,0,2.5555227146,0.7195194193,-2.3000728092
H,0,3.896202819,0.6440683723,-1.1562696351
H,0,2.3237024537,-0.5014934786,2.5368465473
H,0,-1.167502337,-0.5131429414,-0.2244725013
H,0,2.9556256535,-1.644486419,-1.5837966169
H,0,2.5609644157,-2.2896994948,0.8022976163
H,0,3.8985532548,-1.145969638,0.6906840594
H,0,0.2548722743,-1.5054111459,1.5582945312
H,0,-0.0088130309,0.207306188,1.9727954595
H,0,0.618549384,-2.1710210572,-0.8504442813
H,0,0.6049709149,-0.9290198013,-2.121808788
O,0,-1.980151488,-0.2811514764,-0.8449369483
C,0,-3.271187259,-0.0275639666,-0.1007528819
O,0,-4.0495109372,-0.215433954,-1.1414512265
C,0,-3.4082704372,-1.0799484145,1.0092088901
C,0,-3.246487427,1.4062998407,0.4402099517
H,0,-4.3898663547,-0.9744998691,1.4851546754
H,0,-3.3469618871,-2.0784308442,0.565938159
H,0,-2.6433399852,-0.9757330261,1.7915475624
H,0,-4.219523052,1.6441602214,0.886286496
H,0,-2.4763532321,1.5527664224,1.2104535401
H,0,-3.0686879704,2.0959163826,-0.3898881452

TS-LS Adamantane + Dimethyldioxirane at UB3PW91/6-31+G(d) level



Zero-point correction=	0.327515 (Hartree/Particle)
Thermal correction to Energy=	0.341594
Thermal correction to Enthalpy=	0.342538
Thermal correction to Gibbs Free Energy=	0.285626
Sum of electronic and zero-point Energies=	-658.415137
Sum of electronic and thermal Energies=	-658.401058
Sum of electronic and thermal Enthalpies=	-658.400114
Sum of electronic and thermal Free Energies=	-658.457027

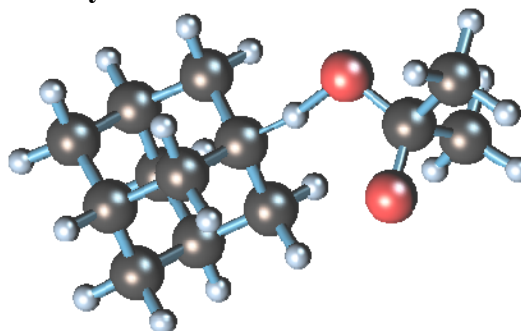
S. A. Grabovskiy

S**2 = 0.4650

C,0,0.882055704,-0.6763110869,-1.4278283626
C,0,0.2357041242,-0.0315459549,-0.2175182278
C,0,0.6287385754,1.4256120612,-0.0763051894
C,0,2.1618734538,1.4579692289,0.1606194783
C,0,2.8717879188,0.8137687465,-1.0403042209
C,0,2.4150060019,-0.6452755899,-1.1942005862
C,0,2.7446206821,-1.4290102213,0.0860663079
C,0,2.0352168976,-0.7866412904,1.2883016261
C,0,2.4906891448,0.6728500034,1.4400800965
C,0,0.5007290541,-0.8175423104,1.0511035529
H,0,2.4813178142,2.5033834129,0.2692295674
H,0,3.5722725992,0.7082256579,1.6330068857
H,0,1.9983715189,1.1362944209,2.3067983388
H,0,0.370634829,1.9873726081,-0.9824752311
H,0,0.1084221706,1.8958202409,0.7679374664
H,0,2.6528555754,1.3783794521,-1.9574042382
H,0,3.9608798524,0.8526657074,-0.8959115131
H,0,2.2623746498,-1.3491857574,2.204121345
H,0,-1.0097042332,-0.0580488834,-0.4614816764
H,0,2.9150852215,-1.1069697244,-2.0563165998
H,0,2.4353549712,-2.4782118541,-0.0210850157
H,0,3.8310761151,-1.4341314517,0.2536179676
H,0,0.1548936648,-1.854271076,0.9518616598
H,0,-0.0169295921,-0.3709098378,1.9104205282
H,0,0.5355170448,-1.7100886668,-1.5496247109
H,0,0.6229643063,-0.1301584009,-2.3430850742
O,0,-2.1544151041,-0.0873809149,-0.9483068313
C,0,-3.2276931172,0.0034937106,-0.0170668722
O,0,-4.0924342791,-0.0274319188,-1.0777950879
C,0,-3.3352038827,-1.2209411259,0.8849542287
C,0,-3.2414360203,1.3264814633,0.74086583
H,0,-4.2925188876,-1.2080148339,1.4190024828
H,0,-3.2879518702,-2.1249400944,0.2716271732
H,0,-2.5321838568,-1.2445723125,1.6312383303
H,0,-4.1938803168,1.4432586631,1.2708539689
H,0,-2.4349885272,1.3743452629,1.4829330242
H,0,-3.1315992025,2.1508143321,0.030944707

TS-OS

Adamantane + Dimethyldioxirane at UB3PW91/6-31+G(d) level



Zero-point correction=

0.326455 (Hartree/Particle)

S. A. Grabovskiy

Thermal correction to Energy= 0.340708
Thermal correction to Enthalpy= 0.341652
Thermal correction to Gibbs Free Energy= 0.284795
Sum of electronic and zero-point Energies= -658.423449
Sum of electronic and thermal Energies= -658.409197
Sum of electronic and thermal Enthalpies= -658.408252
Sum of electronic and thermal Free Energies= -658.465110
S**2 = 0.9330

C,0,0.6424073157,-1.1952721453,0.792550906
C,0,0.2423685184,-0.1425969422,-0.2312681925
C,0,0.944788688,-0.3742227359,-1.5621963824
C,0,2.4685547029,-0.2419684282,-1.3226447502
C,0,2.9107016442,-1.2913689677,-0.2905044541
C,0,2.1651393652,-1.0656220685,1.034745096
C,0,2.472053889,0.3435983748,1.5658456382
C,0,2.0299098953,1.3952432926,0.5360373638
C,0,2.7750142096,1.1664061438,-0.7886256871
C,0,0.5061047755,1.2617182732,0.2926356142
H,0,2.997052553,-0.404979681,-2.2723295901
H,0,3.8576859653,1.2824184848,-0.6349735195
H,0,2.4763615062,1.9243825384,-1.5272102964
H,0,0.7069146828,-1.3715922083,-1.9543763485
H,0,0.6145307023,0.3600598658,-2.3092728373
H,0,2.7095818764,-2.3033114328,-0.670013556
H,0,3.9961949143,-1.2225843799,-0.1279139203
H,0,2.2442683578,2.4039767522,0.9158931771
H,0,-0.9501242735,-0.3129234297,-0.4375163312
H,0,2.4772654824,-1.8184174626,1.7719245342
H,0,1.9543975622,0.508814806,2.5213178205
H,0,3.5488529683,0.4449052334,1.7648939917
H,0,-0.0412432728,1.4370282783,1.2278719776
H,0,0.1815525889,2.0189945147,-0.434221789
H,0,0.089635767,-1.0485746315,1.7287971598
H,0,0.3994218449,-2.1999384071,0.4228168366
O,0,-2.2248425545,-0.7308352931,-0.7166535244
C,0,-3.1206844979,-0.0098812113,0.0535598707
O,0,-2.89088171,-0.0022681778,1.3824235172
C,0,-3.2428048768,1.4704696247,-0.4112593016
C,0,-4.4867443916,-0.7423001131,-0.1756356426
H,0,-4.0416596664,1.9817550383,0.1316326633
H,0,-2.2995446598,1.9923972239,-0.2306926868
H,0,-3.4521282928,1.4756403584,-1.4848509046
H,0,-5.2697195702,-0.2109199047,0.3708354369
H,0,-4.7055803748,-0.7484451314,-1.246049501
H,0,-4.4087779702,-1.7690772389,0.1878372703

S. A. Grabovskiy

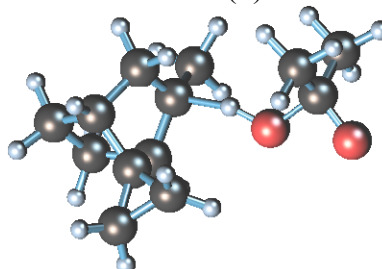
Spiro{cyclopropan-1',7-2-(E)-methyl-bicyclo[2.2.1]heptane at RB3PW91/6-31+G(d) level



Zero-point correction=	0.239534 (Hartree/Particle)
Thermal correction to Energy=	0.248419
Thermal correction to Enthalpy=	0.249363
Thermal correction to Gibbs Free Energy=	0.206410
Sum of electronic and zero-point Energies=	-390.302761
Sum of electronic and thermal Energies=	-390.293877
Sum of electronic and thermal Enthalpies=	-390.292932
Sum of electronic and thermal Free Energies=	-390.335886

C,0,-0.4264307427,-0.8781908185,-1.4374379107
C,0,-0.4239288828,-0.8780437367,0.1047690646
C,0,1.0250892313,-0.8845377785,0.6549458467
C,0,1.5467426623,0.5317541491,0.2447100851
C,0,0.3181731464,1.1954954137,-0.4121231601
C,0,0.0941857554,0.5478167634,-1.7948702406
C,0,-0.81988351,0.5682072448,0.3885013353
C,0,1.9182682606,-2.0414728808,0.2178542842
C,0,-2.2218851252,1.0870721037,0.4496042196
C,0,-1.3485946835,1.0817443688,1.6906704407
H,0,1.883950678,1.0975158656,1.1214866317
H,0,0.9459180157,-0.9207111494,1.750430528
H,0,-1.0628383304,-1.6486743311,0.551646944
H,0,0.1870228767,-1.6776332827,-1.8662356981
H,0,-1.4469309667,-1.0249958795,-1.8100977602
H,0,-0.6546005571,1.1059235383,-2.3693238866
H,0,2.3953543711,0.4729748062,-0.4499058592
H,0,0.3502695031,2.2903739598,-0.4293583874
H,0,1.0143025412,0.5275324039,-2.3916477761
H,0,-0.9847772044,2.0393201222,2.0591426235
H,0,-1.5869432115,0.3653769741,2.4751144923
H,0,-3.043084079,0.3738572394,0.4047476807
H,0,-2.4422056677,2.0480936315,-0.012045821
H,0,1.4718221451,-3.0122242701,0.4692585865
H,0,2.1094820075,-2.0296598494,-0.8619917267
H,0,2.8928412082,-1.9861387527,0.7190356397

TS-C Spiro{cyclopropan-1',7-2-methyl-bicyclo[2.2.1]heptane + Dimethyldioxirane
at RB3PW91/6-31+G(d) level



Zero-point correction=	0.322956 (Hartree/Particle)
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S. A. Grabovskiy

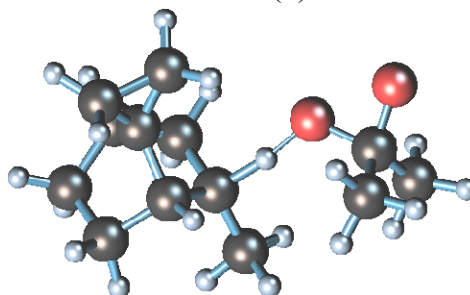
Thermal correction to Energy= 0.339086
Thermal correction to Enthalpy= 0.340030
Thermal correction to Gibbs Free Energy= 0.279301
Sum of electronic and zero-point Energies= -658.352359
Sum of electronic and thermal Energies= -658.336230
Sum of electronic and thermal Enthalpies= -658.335285
Sum of electronic and thermal Free Energies= -658.396015
S**2 = 0.0000

C,0,1.6449850932,0.956873874,-0.0725581096
C,0,1.3200249301,-0.2565916301,-0.9451276108
C,0,2.7123695284,-0.9765682741,-0.9301761385
C,0,3.2481309556,-0.7014189106,0.5025300602
C,0,2.1291423897,0.1560666255,1.1311500483
C,0,0.9044863334,-0.7573003626,1.3765884339
C,0,0.4439608547,-1.0717507225,-0.0354102898
C,0,-0.070570419,-2.4201431065,-0.4062672889
C,0,2.268797384,2.2202535669,-0.580295992
C,0,0.8636847425,2.2311291329,-0.0177926414
H,0,0.1351809521,-0.2118130084,1.9436807834
H,0,-0.830536426,-0.2508725737,-0.0871843789
H,0,0.9120318756,-0.0841096336,-1.942917152
H,0,2.6479855209,-2.0404884843,-1.179432758
H,0,3.3407675677,-0.4996400754,-1.690405969
H,0,4.1884218458,-0.1411278198,0.468233531
H,0,1.1213186309,-1.6740502846,1.9430718627
H,0,2.428535528,0.7335935307,2.0105103066
H,0,3.4353996015,-1.6206553056,1.070222003
H,0,0.7152859191,2.6940872959,0.9559558653
H,0,0.0271126918,2.3470785592,-0.7011136975
H,0,2.3850824301,2.3438010363,-1.6551815874
H,0,3.0620933971,2.6754558276,0.0095954147
H,0,-0.4438662213,-2.4442061916,-1.4331193607
H,0,0.7472628191,-3.154120658,-0.31494335
H,0,-0.8656829052,-2.7505736567,0.2699962683
O,0,-1.5961338402,0.1670117979,-0.6766837223
C,0,-2.9370662238,0.239709414,-0.0305001316
O,0,-3.4338237862,1.1039598826,-0.8979630691
C,0,-3.5972796245,-1.1425587051,-0.0680025021
C,0,-2.7883236966,0.7832996198,1.3969844384
H,0,-4.6354482431,-1.0592103078,0.2742948757
H,0,-3.6008558806,-1.5072690795,-1.0990985669
H,0,-3.0874781811,-1.8712173232,0.5769388305
H,0,-3.782861019,0.951657971,1.8257323562
H,0,-2.2529136331,0.088584459,2.060340105
H,0,-2.2612287458,1.7413191492,1.3652652925

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TS-LS

Spiro{cyclopropan-1',7-2-methyl-bicyclo[2.2.1]heptane + Dimethyldioxirane
at UB3PW91/6-31+G(d) level



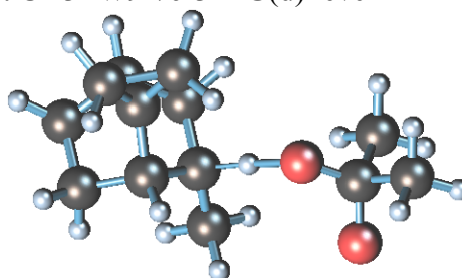
Zero-point correction= 0.322441 (Hartree/Particle)
Thermal correction to Energy= 0.338312
Thermal correction to Enthalpy= 0.339256
Thermal correction to Gibbs Free Energy= 0.278975
Sum of electronic and zero-point Energies= -658.359684
Sum of electronic and thermal Energies= -658.343813
Sum of electronic and thermal Enthalpies= -658.342869
Sum of electronic and thermal Free Energies= -658.403150
S**2 = 0.4286

C,0,-1.7126942132,0.9463934097,0.0159569833
C,0,-1.1501688356,-0.1728410833,0.8896625845
C,0,-2.4526132492,-0.9668670159,1.1885694535
C,0,-3.2527852543,-0.852629816,-0.1419077005
C,0,-2.3398682259,0.0250384804,-1.0253475025
C,0,-1.1148988489,-0.8150528225,-1.4475542308
C,0,-0.3387948217,-0.9769552416,-0.1293602862
C,0,0.1643083295,-2.3549207099,0.2271464946
C,0,-2.3385071296,2.2053116697,0.5345010474
C,0,-1.0575085507,2.2582128797,-0.2717567014
H,0,-0.5928386591,0.1235552048,1.7832996904
H,0,-2.2665635388,-2.0003067208,1.4982510112
H,0,-2.9832341168,-0.4732627045,2.0106795843
H,0,-4.2186493035,-0.3626632369,0.0240959527
H,0,-3.4556359778,-1.8279704516,-0.6007394947
H,0,-2.8496449539,0.5161171806,-1.8602092959
H,0,-0.5120282159,-0.2802469156,-2.1922165201
H,0,-1.3854864896,-1.7870461181,-1.8821648139
H,0,0.697696182,-2.365638171,1.1844513397
H,0,-0.6755997592,-3.0596406428,0.3063014341
H,0,0.8331771764,-2.7412989695,-0.5496056034
H,0,-2.276940951,2.4148038477,1.6009908292
H,0,-3.2552194051,2.5566909904,0.0646334913
H,0,-1.1096546604,2.642291374,-1.2884369319
H,0,-0.1298500195,2.4975399009,0.2402875525
H,0,0.7143511521,-0.2929885418,-0.2882349004
O,0,1.6817414316,0.4390547567,-0.6203673812
C,0,2.9332000128,0.2205476688,0.0227335709
O,0,3.3918482794,1.310928181,-0.6660378401
C,0,2.8713266424,0.4274302101,1.5314339571
C,0,3.6092698076,-1.0799341827,-0.3925232064

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H,0,3.8859757546,0.4633532789,1.9447571085
H,0,2.3728260355,1.3762113209,1.7478795243
H,0,2.3342304783,-0.388825272,2.0297121411
H,0,4.6617250462,-1.0621235927,-0.0859794894
H,0,3.1374635284,-1.9518701148,0.0746584965
H,0,3.5635890299,-1.1789458256,-1.4804961158

TS-OS **Spiro{cyclopropan-1',7-2-methyl-bicyclo[2.2.1]heptane + Dimethyldioxirane**
at UB3PW91/6-31+G(d) level



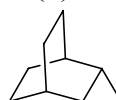
Zero-point correction= 0.321463 (Hartree/Particle)
Thermal correction to Energy= 0.337490
Thermal correction to Enthalpy= 0.338434
Thermal correction to Gibbs Free Energy= 0.278023
Sum of electronic and zero-point Energies= -658.367536
Sum of electronic and thermal Energies= -658.351509
Sum of electronic and thermal Enthalpies= -658.350565
Sum of electronic and thermal Free Energies= -658.410976
S**2 = 0.9384

C,0,1.8308335876,0.9515508826,0.036769116
C,0,1.3285016535,-0.091393337,-0.9579953067
C,0,2.6128061348,-0.9429535342,-1.1300583113
C,0,3.2268206632,-0.9499097208,0.3013615648
C,0,2.2605288039,-0.0505229521,1.1034511452
C,0,0.9421050118,-0.8229807293,1.3235384249
C,0,0.3277303488,-0.8775535241,-0.094431702
C,0,-0.1461742585,-2.2277095063,-0.5920450715
C,0,2.5806217965,2.1945625316,-0.3315591277
C,0,1.2054530292,2.2834936403,0.2996632435
H,0,0.9061582364,0.2815516162,-1.8958243965
H,0,2.4165373496,-1.9454273123,-1.5232396582
H,0,3.2803058441,-0.4419454412,-1.8408382917
H,0,4.2378612559,-0.52680387,0.2968588716
H,0,3.2970186202,-1.9580677869,0.7278736413
H,0,2.6884267461,0.3716070415,2.0188818921
H,0,0.291496877,-0.2800606142,2.0208336623
H,0,1.1010664494,-1.8276804463,1.7389545541
H,0,-0.56309167,-2.1615075383,-1.602088538
H,0,0.6820814452,-2.9502512171,-0.604968127
H,0,-0.9212575537,-2.642781392,0.0615667737
H,0,2.6730772613,2.4508453002,-1.3855537761
H,0,3.4402335975,2.4811647933,0.2720362806
H,0,1.1422829632,2.6271768957,1.330714545
H,0,0.3696530818,2.5894338221,-0.3236422406

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H,0,-0.6586115825,-0.1577362567,-0.1051987851
O,0,-1.7067744128,0.7312368519,-0.2566094688
C,0,-2.9258862246,0.1111413125,-0.0533367813
O,0,-3.243949552,-0.8824844063,-0.9106065722
C,0,-3.9694212035,1.2561835667,-0.2997851992
C,0,-3.0808137312,-0.4304490156,1.3945253168
H,0,-3.8787202109,1.6110794546,-1.3284864815
H,0,-4.974252435,0.8628323547,-0.1280380861
H,0,-3.7559007123,2.0750523799,0.3912899466
H,0,-4.0898501561,-0.8186629256,1.5539566007
H,0,-2.3606867627,-1.2350561999,1.5672361606
H,0,-2.8766705948,0.3844600916,2.0948199107

Tricyclo[3.2.2.0^{2,4}]nonane at RB3PW91/6-31+G(d) level

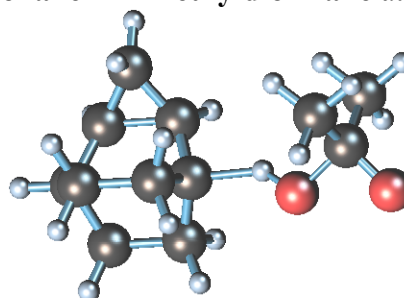


Zero-point correction=	0.213290 (Hartree/Particle)
Thermal correction to Energy=	0.220167
Thermal correction to Enthalpy=	0.221112
Thermal correction to Gibbs Free Energy=	0.182631
Sum of electronic and zero-point Energies=	-351.034090
Sum of electronic and thermal Energies=	-351.027213
Sum of electronic and thermal Enthalpies=	-351.026268
Sum of electronic and thermal Free Energies=	-351.064749

C,0,0.2961562313,1.4393064824,0.7763388575
C,0,0.2119636587,-0.003024901,1.2980820072
C,0,-1.0186024508,-0.7257468035,0.7563815745
C,0,-1.0186024508,-0.7257468035,-0.7563815745
C,0,0.2119636587,-0.003024901,-1.2980820072
C,0,0.2961562313,1.4393064824,-0.7763388575
C,0,1.4428873683,-0.7777357841,-0.7778627552
C,0,1.4428873683,-0.7777357841,0.7778627552
C,0,-2.1133691582,-0.0173662824,0.
H,0,-1.2898423689,-1.6426828557,-1.2791372031
H,0,0.2061169158,0.0014268723,-2.3959500033
H,0,1.4193471985,-1.804598513,-1.1645915739
H,0,2.3611393491,-0.3194806019,-1.1686861327
H,0,2.3611393491,-0.3194806019,1.1686861327
H,0,-1.2898423689,-1.6426828557,1.2791372031
H,0,0.2061169158,0.0014268723,2.3959500033
H,0,1.4193471985,-1.804598513,1.1645915739
H,0,1.2130948799,1.9011862315,-1.1646554329
H,0,-0.5363259868,2.0332163658,-1.1728846548
H,0,-0.5363259868,2.0332163658,1.1728846548
H,0,1.2130948799,1.9011862315,1.1646554329
H,0,-3.0904207051,-0.4953682263,0.
H,0,-2.1652820111,1.0678429971,0.

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TS-C Tricyclo[3.2.2.0^{2,4}]nonane + Dimethyldioxirane at RB3PW91/6-31+G(d) level



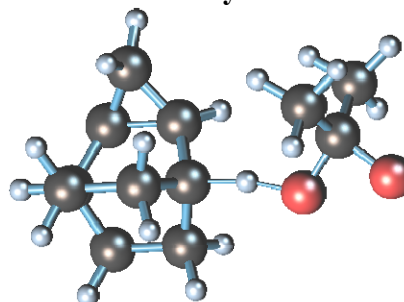
Zero-point correction= 0.297380 (Hartree/Particle)
Thermal correction to Energy= 0.311567
Thermal correction to Enthalpy= 0.312511
Thermal correction to Gibbs Free Energy= 0.255888
Sum of electronic and zero-point Energies= -619.077620
Sum of electronic and thermal Energies= -619.063433
Sum of electronic and thermal Enthalpies= -619.062489
Sum of electronic and thermal Free Energies= -619.119112
S**2 = 0.0000

C,0,0.8212795853,-0.1908967337,1.3772504736
C,0,0.5270215118,0.0635150714,-0.06993889
C,0,1.2555225618,1.1888570983,-0.6928682743
C,0,2.7560595869,0.7989611599,-0.6234264291
C,0,2.9373614401,-0.5646943138,0.0341389525
C,0,2.3401406913,-0.586052295,1.4473079665
C,0,2.1690894428,-1.5885564018,-0.8334401965
C,0,0.6412712516,-1.1886259272,-0.9060901815
C,0,2.2331313965,2.016829618,0.0851717071
H,0,3.3308574173,0.9614849445,-1.5344181291
H,0,4.0006306121,-0.8337707274,0.0709163489
H,0,2.5841831978,-1.6147550834,-1.8478675414
H,0,2.2764612399,-2.5960347083,-0.4143670954
H,0,0.0113069723,-1.9907254119,-0.5090575196
H,0,0.887146617,1.5588885808,-1.6472869414
H,0,-0.8951937898,0.4726457321,-0.3096206077
H,0,0.347335613,-1.0069196066,-1.945246625
H,0,2.4478362834,-1.5904004999,1.8724527366
H,0,2.883689324,0.0991516046,2.1070065617
H,0,0.6032032952,0.6928747759,1.9812530436
H,0,0.1881017304,-1.0019998341,1.7471092972
H,0,2.4941771839,2.9800485106,-0.3447599547
H,0,2.174945377,2.0271440175,1.1695161439
O,0,-1.6910917028,0.7935242726,0.2940248886
O,0,-3.7465214064,1.0787377826,0.4905658794
C,0,-3.0480504055,-1.1864123599,0.8776753603
H,0,-2.3030573206,-1.9269814843,0.5560084928
H,0,-2.8760114079,-0.9269010201,1.9261092272
H,0,-4.040074778,-1.6457449469,0.7927141781
C,0,-3.0064087967,0.0930666332,0.036616238
C,0,-3.135596924,-0.1761328791,-1.4691161688
H,0,-3.0249023719,0.7662847127,-2.0142377535

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H,0,-2.4001041982,-0.9052625488,-1.836207928
H,0,-4.1345541744,-0.5762754688,-1.6764254262

TS-LS **Tricyclo[3.2.2.0^{2,4}]nonane + Dimethyldioxirane** at UB3PW91/6-31+G(d) level



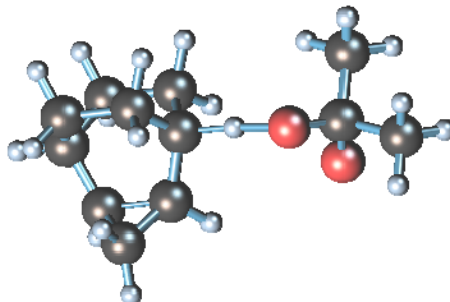
Zero-point correction= 0.295943 (Hartree/Particle)
Thermal correction to Energy= 0.309939
Thermal correction to Enthalpy= 0.310884
Thermal correction to Gibbs Free Energy= 0.253997
Sum of electronic and zero-point Energies= -619.090626
Sum of electronic and thermal Energies= -619.076630
Sum of electronic and thermal Enthalpies= -619.075686
Sum of electronic and thermal Free Energies= -619.132573
S**2 = 0.5020

C,0,-2.7113594109,-1.2925609551,-0.7591148293
C,0,-3.0293940709,-0.0171216233,0.0546030371
C,0,-2.4689823547,-0.1972906015,1.4718446289
C,0,-0.9195182477,-0.4066480681,1.4039559353
C,0,-0.5178546407,-0.3542723937,-0.0570429979
C,0,-1.1586709342,-1.5007416682,-0.8298762705
C,0,-0.8373810305,0.9404388229,-0.7391565139
C,0,-2.3569429019,1.1446923395,-0.6687282196
C,0,-1.4196836172,2.1134353916,-0.0003818365
H,0,-3.1953879978,-2.1615810719,-0.2962752244
H,0,-3.1238771161,-1.2022569813,-1.7714453211
H,0,-4.1152437825,0.1361771949,0.1013937775
H,0,-2.7153113979,0.6696374079,2.0956003493
H,0,-2.9467089317,-1.0667418602,1.9387979453
H,0,-0.6375699389,-1.3786385164,1.8221270004
H,0,-0.3929486413,0.3566061184,1.9864997575
H,0,-0.8131320035,-1.4976322098,-1.8690807417
H,0,-0.8677435546,-2.4628560697,-0.3948648273
H,0,-0.3515176644,1.1184553342,-1.6965226007
H,0,-2.8520865794,1.4813019753,-1.5787223313
H,0,-1.3088273162,3.0873701383,-0.4705862671
H,0,-1.3638073035,2.1470382099,1.0839758802
O,0,1.89051809,-0.9985026567,-0.2138326907
C,0,2.92138083,-0.0391364023,-0.0039341104
O,0,3.8477251759,-1.0256951904,-0.221496357
C,0,2.9413319983,1.0498642629,-1.0711732985
C,0,2.9414354692,0.503525061,1.4210976693
H,0,0.7402776281,-0.5684864069,-0.1153372373
H,0,3.8712088149,1.6260684038,-0.9990506828

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H,0,2.8931514656,0.5857396127,-2.0602709119
H,0,2.1021136944,1.7454448071,-0.9514356671
H,0,3.8698156658,1.059718397,1.5958076847
H,0,2.1010407571,1.1840862143,1.6033378286
H,0,2.8944415409,-0.3309729145,2.1261248069

TS-OS **Tricyclo[3.2.2.0_{2,4}]nonane + Dimethyldioxirane** at UB3PW91/6-31+G(d) level



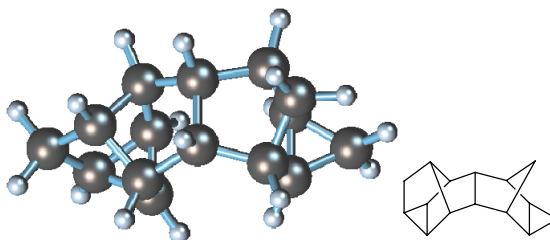
Zero-point correction= 0.295044 (Hartree/Particle)
Thermal correction to Energy= 0.309177
Thermal correction to Enthalpy= 0.310122
Thermal correction to Gibbs Free Energy= 0.253432
Sum of electronic and zero-point Energies= -619.098860
Sum of electronic and thermal Energies= -619.084727
Sum of electronic and thermal Enthalpies= -619.083783
Sum of electronic and thermal Free Energies= -619.140473
S**2 = 0.9323

C,0,0.1643077622,0.2082794346,-1.9886674827
C,0,0.1656443111,0.2714351767,-0.4679337946
C,0,1.5436334601,0.2184576803,0.134674467
C,0,2.3562255633,1.4030964491,-0.3920907294
C,0,1.5235169605,2.2482125812,-1.3504723603
C,0,0.9979075087,1.4143692386,-2.5273657616
C,0,0.31123558,2.7690544377,-0.5470119868
C,0,-0.5188916983,1.5580579155,-0.0018279017
C,0,2.7757038103,-0.0115598786,-0.6929595219
H,0,2.9575624992,1.9605518383,0.3254830497
H,0,2.1119123991,3.0942520046,-1.7295307189
H,0,0.6575027747,3.3934525356,0.2859525028
H,0,-0.3121859087,3.4095542785,-1.1841615106
H,0,-1.549524077,1.6000302394,-0.3749885068
H,0,1.5879955287,-0.0091057023,1.197405775
H,0,-0.4474224183,-0.7209485624,-0.0824600284
H,0,-0.5648965136,1.5877444056,1.0925988522
H,0,0.3755519414,2.0521047016,-3.1673303422
H,0,1.8301558546,1.0652943073,-3.149824489
H,0,0.5760335397,-0.7461893837,-2.3337030289
H,0,-0.868480527,0.2560701343,-2.352508923
H,0,3.6502779857,-0.3834821937,-0.1648156806
H,0,2.6839089619,-0.3984869174,-1.7037667205
O,0,-1.0032411615,-1.9170418737,0.2270335675
O,0,-0.8161030514,-1.341396472,2.4656277817
C,0,-2.9125902796,-1.0172689965,1.4627776147

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H,0,-3.4169888517,-1.0775809125,2.4303756402
H,0,-2.6949255588,0.0303328663,1.2399441356
H,0,-3.5550713184,-1.4224146185,0.675735419
C,0,-1.5891742748,-1.8376149416,1.478774999
C,0,-1.9065790697,-3.328480806,1.8409841665
H,0,-2.4141714995,-3.3584937996,2.8082252687
H,0,-2.5458627041,-3.7499759218,1.0615006524
H,0,-0.972256207,-3.8914322805,1.8912876102

Exo-endo-endo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at RB3PW91/6-31+G(d) level



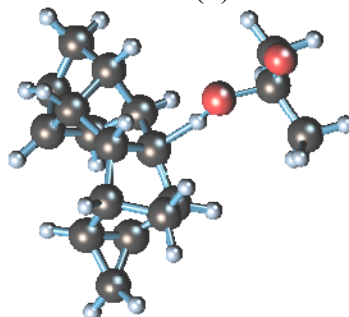
Zero-point correction=	0.297242 (Hartree/Particle)
Thermal correction to Energy=	0.306523
Thermal correction to Enthalpy=	0.307467
Thermal correction to Gibbs Free Energy=	0.262999
Sum of electronic and zero-point Energies=	-581.867300
Sum of electronic and thermal Energies=	-581.858020
Sum of electronic and thermal Enthalpies=	-581.857075
Sum of electronic and thermal Free Energies=	-581.901544

C,0,-1.2769699251,-1.5003159952,-2.6652520335
C,0,-1.2740899058,-1.4969258465,-1.1398077872
C,0,0.2275386078,-1.4967387449,-0.7106206539
C,0,0.6626477945,-0.3880803584,-1.6703579389
C,0,-0.488975586,0.5921127737,-1.6703620708
C,0,-0.3027455921,-0.3557060538,-2.8385706351
C,0,-1.5138625294,-0.014561964,-0.7106269019
C,0,-1.0970068494,-0.0717808739,0.7747305968
C,0,0.1044365522,-1.0943778364,0.7747349075
C,0,-0.5659941422,1.0939724166,1.6575405776
C,0,0.5638406667,1.8326699716,0.945360891
C,0,1.7190161051,0.8494535396,0.9453650356
C,0,1.1703519757,-0.3839018335,1.6575468074
C,0,0.2035004743,0.2391029103,2.6927798634
C,0,1.8353582933,2.1563592298,1.690566302
H,0,0.3292419957,2.4304041918,0.0716213496
H,0,2.3465611606,0.713382443,0.0716285876
H,0,-1.351716756,1.7380092326,2.0685632509
H,0,2.4680365713,2.8996873446,1.2103300435
H,0,1.8739000084,2.2016462455,2.7751590281
H,0,1.931667169,-1.0566113248,2.0685750314
H,0,-0.4376195122,-0.5141433527,3.1653126127
H,0,0.6873598062,0.8075898737,3.4909153695
H,0,-0.1863199923,-2.0064242558,1.3162879274
H,0,-1.9508736656,-0.5045414171,1.3162815964

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H,0,0.7471256633,-2.4490239742,-0.8724583247
H,0,-2.5369385266,0.3461755839,-0.8724701076
H,0,-0.3461695313,1.65930107,-1.7946496541
H,0,-1.904089717,-2.2371069533,-0.6376697675
H,0,1.6933031904,-0.0765764649,-1.7946423366
H,0,0.0141061031,0.0165571271,-3.8083530748
H,0,-0.9110555236,-2.4458197283,-3.0862942103
H,0,-2.2687940813,-1.2901936513,-3.0862990817

TS-C **Exo-endo-endo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at**
RB3PW91/6-31+G(d) level



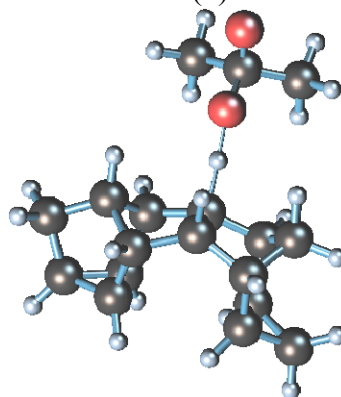
Zero-point correction=	0.381021 (Hartree/Particle)
Thermal correction to Energy=	0.397436
Thermal correction to Enthalpy=	0.398380
Thermal correction to Gibbs Free Energy=	0.336822
Sum of electronic and zero-point Energies=	-849.922297
Sum of electronic and thermal Energies=	-849.905883
Sum of electronic and thermal Enthalpies=	-849.904938
Sum of electronic and thermal Free Energies=	-849.966497
S**2	= 0.0000

C,0,-2.4028590207,-3.0669174448,-0.6432320387
C,0,-1.6671466994,-1.8199773936,-1.079268334
C,0,-0.1912999562,-1.6340182684,-0.6728600786
C,0,-0.1292213644,-2.3831271053,0.6795630878
C,0,-1.3493853591,-1.6587476519,1.2971192316
C,0,-2.4294912789,-1.8410862689,0.2301510911
C,0,-0.7830669729,-0.2079131095,1.215322414
C,0,-0.1174844247,-0.2062444246,-0.150240467
C,0,-1.5084101587,1.1584905981,1.2319446848
C,0,-0.4399772569,2.0528554708,0.5280168483
C,0,-0.3535902805,1.1553933255,-0.749161511
C,0,-2.5931020963,1.3171870427,0.1644593771
C,0,-2.3450732295,2.6175891712,-0.5724918227
C,0,-1.1768696333,3.3129641742,0.0896209306
C,0,-1.8405340611,1.3047795973,-1.143886153
H,0,-2.0347221167,-1.2885132797,-1.9498306586
H,0,-3.370992157,-1.3138056699,0.3415556257
H,0,0.5421341716,-1.9100672381,-1.4340519941
H,0,-3.3171142859,-3.2647973741,-1.1983495787
H,0,-1.8761749842,-3.9695387462,-0.350227964
H,0,-1.6242240057,-1.9748783429,2.3077831733

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H,0,0.7996431896,-2.1728966545,1.217282235
H,0,-0.2344162082,-3.4658036924,0.5911828998
H,0,-0.0040033419,-0.1412125655,1.9913503555
H,0,1.3164912508,-0.1065271889,0.0922491751
H,0,-1.7988245568,1.4948585086,2.2323995764
H,0,0.3494133705,1.4723258554,-1.5240691156
H,0,-2.2463466509,0.8860644874,-2.057104684
H,0,0.5025448972,2.1726024503,1.0652744609
H,0,-3.5907832667,0.9045050184,0.2615838357
H,0,-3.15529223,3.1479913183,-1.0639085555
H,0,-1.4740338162,3.938770386,0.9399767733
H,0,-0.5906331422,3.9255810226,-0.606210161
O,0,2.2074839215,-0.0056920137,0.6876419088
C,0,3.4939515555,0.0328946238,-0.0423209325
O,0,4.2197853373,0.1610177218,1.0593815611
C,0,3.7067024485,-1.2860570397,-0.7943640007
C,0,3.5283291846,1.2511490704,-0.9728017303
H,0,4.7202523166,-1.3070260546,-1.211598792
H,0,3.6056833845,-2.1189489094,-0.0924927976
H,0,2.999128296,-1.4169196307,-1.6245490841
H,0,4.529584999,1.3486205189,-1.4084707673
H,0,2.8089685186,1.1691651469,-1.7991370113
H,0,3.3167339217,2.1525587658,-0.3902482885

TS-LS **Exo-endo-endo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at**
UB3PW91/6-31+G(d) level



Zero-point correction=	0.380725 (Hartree/Particle)
Thermal correction to Energy=	0.397061
Thermal correction to Enthalpy=	0.398005
Thermal correction to Gibbs Free Energy=	0.336315
Sum of electronic and zero-point Energies=	-849.927704
Sum of electronic and thermal Energies=	-849.911368
Sum of electronic and thermal Enthalpies=	-849.910424
Sum of electronic and thermal Free Energies=	-849.972115
S**2 =	0.3874

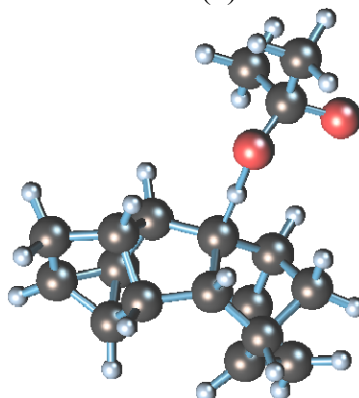
C,0,-1.2976081642,1.2051118949,-3.5097859358
C,0,-1.2896752168,1.2120999591,-1.9991996033
C,0,0.0499654541,1.2330233119,-1.252549403
C,0,0.9833371602,0.4806185964,-2.2304980381

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C,0,0.0518060131,-0.7443426742,-2.390927726
C,0,-1.2844164291,-0.1004232515,-2.7565175785
C,0,0.0372701444,-1.1893110891,-0.8979649737
C,0,-0.0208766541,0.161850704,-0.1480910484
C,0,-1.0086120454,-2.0430912275,-0.1454683901
C,0,-0.7737511759,-1.5620281051,1.3208574188
C,0,-1.0150554686,-0.0551075282,0.9886195229
C,0,-2.4524451934,-1.5484742167,-0.2506489301
C,0,-3.0341678998,-1.4739125617,1.1468826822
C,0,-1.9988935723,-2.0115202293,2.1096080206
C,0,-2.4584673699,-0.2325617162,0.4907893824
H,0,-2.1758266937,1.5745007229,-1.4901538456
H,0,-2.1699602673,-0.7241339367,-2.8114190117
H,0,0.3832988782,2.2220158734,-0.9256600897
H,0,-2.2527898012,1.4702787773,-3.9576976316
H,0,-0.445192654,1.543403749,-4.0910285401
H,0,0.4036791199,-1.516657987,-3.0826728512
H,0,1.9384347428,0.2189196394,-1.7651176465
H,0,1.195817792,1.0198646646,-3.1560083316
H,0,1.0103566304,-1.6693636383,-0.7124875924
H,0,1.0772952753,0.2705881599,0.4478416562
H,0,-0.890778247,-3.1220006201,-0.2955326982
H,0,-0.9178650885,0.6353065601,1.8322002466
H,0,-3.0919863498,0.5996275386,0.207058256
H,0,0.2092758374,-1.7908806296,1.7381397388
H,0,-3.0856603928,-1.7328001408,-1.1108572593
H,0,-4.1041554399,-1.5605966327,1.3110800354
H,0,-2.0452256381,-3.1013887585,2.2274889343
H,0,-2.0544955773,-1.5499952923,3.1036048276
O,0,2.2391149111,0.1197286624,0.9575840707
C,0,2.7618660921,1.1830185362,1.7482360691
O,0,3.8632885847,0.3930825064,1.9257127327
C,0,3.0368301251,2.4488661289,0.9465102211
C,0,1.9666787276,1.4272504845,3.0246778938
H,0,3.6612534202,3.1315732898,1.5345770891
H,0,3.5714189218,2.1887839203,0.02899382
H,0,2.1094473285,2.9757338483,0.6926274322
H,0,2.5398799813,2.0714296563,3.7016286198
H,0,1.0117618132,1.9240731833,2.8155721647
H,0,1.7800812784,0.4728266037,3.5242707453

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TS-OS Exo-endo-endo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at
UB3PW91/6-31+G(d) level



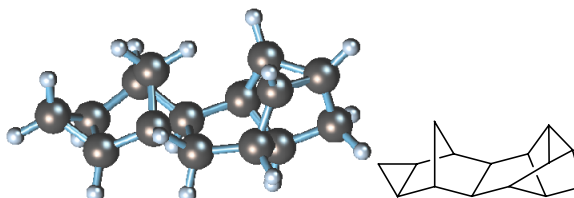
Zero-point correction=	0.379515 (Hartree/Particle)
Thermal correction to Energy=	0.396020
Thermal correction to Enthalpy=	0.396964
Thermal correction to Gibbs Free Energy=	0.334883
Sum of electronic and zero-point Energies=	-849.935432
Sum of electronic and thermal Energies=	-849.918926
Sum of electronic and thermal Enthalpies=	-849.917982
Sum of electronic and thermal Free Energies=	-849.980063
S**2 =	0.9306

C,0,-1.6628970225,-3.2099750175,-0.1066483869
 C,0,-0.7641326844,-2.061573323,-0.5547245105
 C,0,-1.7060036647,-1.0226799117,-1.2397857696
 C,0,-2.7778223606,-1.0319275979,-0.1482337784
 C,0,-2.0032818942,-1.1329061478,1.1441554382
 C,0,-2.7038135407,-2.3567510117,0.5841486309
 C,0,-0.5291202542,-1.1840362351,0.7145840007
 C,0,-0.0202363872,0.1161251522,0.0817473013
 C,0,-0.7953329326,0.224505031,-1.2603074978
 C,0,-0.0023566093,1.5603595874,0.6356514578
 C,0,-1.4220843591,1.9133453066,1.0909730489
 C,0,-2.2170434269,2.023557817,-0.1945749314
 C,0,-1.2018689136,1.7271405513,-1.2972934732
 C,0,0.1065643655,2.3088228364,-0.7124242867
 C,0,-2.0296541935,3.2348853115,0.6845901814
 H,0,-1.8257711465,1.4215729078,1.969240588
 H,0,-3.2170746268,1.6120879325,-0.2768204108
 H,0,0.7882853374,1.7699554851,1.3616007404
 H,0,-2.9064194587,3.5265721537,1.2589163474
 H,0,-1.4190565209,4.0795884671,0.3803431098
 H,0,-1.4769171219,2.0907840282,-2.2933328438
 H,0,0.9929496549,2.0018492056,-1.2750461551
 H,0,0.125971684,3.3972503195,-0.6244336692
 H,0,-0.0965883257,0.0770294242,-2.0985427666
 H,0,1.1236379183,-0.1269030962,-0.214961686
 H,0,-2.0727651114,-1.3224479841,-2.2283399448
 H,0,0.1353447588,-1.6236364602,1.4658926241
 H,0,-2.3371535757,-0.6687398641,2.0648686069

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H,0,0.1397337978,-2.3159606474,-1.1129220648
H,0,-3.7123100231,-0.4880835583,-0.2260744628
H,0,-3.5769046637,-2.7669041243,1.0831517914
H,0,-2.0670536428,-3.7826369298,-0.9512268734
H,0,-1.154055653,-3.9038926389,0.5748074179
O,0,2.3785662124,-0.4953144711,-0.7617925366
O,0,3.5729597032,1.1765451791,0.3176842805
C,0,3.311975071,-0.8538302319,1.4655586391
H,0,4.2035532185,-0.6527817017,2.0644951758
H,0,2.4334479095,-0.4880138861,2.0043080326
H,0,3.2059781069,-1.9291281542,1.2961300104
C,0,3.4097067236,-0.144439833,0.0853383221
C,0,4.6974175297,-0.6319308729,-0.6656992478
H,0,5.571565971,-0.416427727,-0.0465990894
H,0,4.6108893066,-1.7061970363,-0.8450803634
H,0,4.7784122021,-0.1069302451,-1.6198388939

Exo-exo-exo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at RB3PW91/6-31+G(d) level



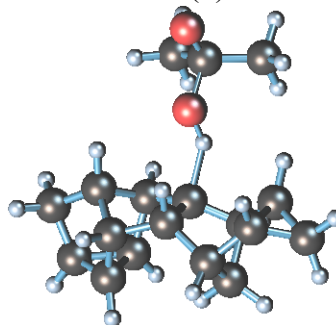
Zero-point correction=	0.296908 (Hartree/Particle)
Thermal correction to Energy=	0.306235
Thermal correction to Enthalpy=	0.307179
Thermal correction to Gibbs Free Energy=	0.262687
Sum of electronic and zero-point Energies=	-581.877006
Sum of electronic and thermal Energies=	-581.867678
Sum of electronic and thermal Enthalpies=	-581.866734
Sum of electronic and thermal Free Energies=	-581.911227

C,0,-0.017483707,3.4355067248,0.
C,0,-0.8025885027,2.1248644584,0.
C,0,-0.1896703951,1.2595395548,-1.1392036822
C,0,1.2709385816,1.5026081419,-0.7582756438
C,0,1.2709385816,1.5026081419,0.7582756438
C,0,1.3629077643,2.8106704336,0.
C,0,-0.1896703951,1.2595395548,1.1392036822
C,0,-0.7191662568,-0.1480381613,0.7883917139
C,0,-0.7191662568,-0.1480381613,-0.7883917139
C,0,0.0483080948,-1.4522513664,1.1360943329
C,0,-0.9473380701,-2.5579376756,0.7612981081
C,0,-0.9473380701,-2.5579376756,-0.7612981081
C,0,0.0483080948,-1.4522513664,-1.1360943329
C,0,1.0807849783,-1.5498780492,0.
C,0,-0.5008573484,-3.7787979468,0.
H,0,-1.8808566992,-2.6102267337,1.3191344226
H,0,-1.8808566992,-2.6102267337,-1.3191344226
H,0,0.4446349921,-1.5047185927,2.1564371939

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H,0,0.5366436719,-4.1025548974,0.
H,0,-1.2053929843,-4.607872423,0.
H,0,0.4446349921,-1.5047185927,-2.1564371939
H,0,1.798259594,-0.7329885847,0.
H,0,1.6465557021,-2.4859708303,0.
H,0,-1.7414100236,-0.220012544,-1.1843928495
H,0,-1.7414100236,-0.220012544,1.1843928495
H,0,-0.4420792195,1.5880703956,-2.1546651078
H,0,-0.4420792195,1.5880703956,2.1546651078
H,0,2.1046703218,1.1208273592,1.3399079082
H,0,-1.8940636375,2.1974479159,0.
H,0,2.1046703218,1.1208273592,-1.3399079082
H,0,2.2802259998,3.3918138919,0.
H,0,-0.2127948243,4.0455027571,-0.8914424426
H,0,-0.2127948243,4.0455027571,0.8914424426

**TS-C Exo-exo-exo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at
RB3PW91/6-31+G(d) level**



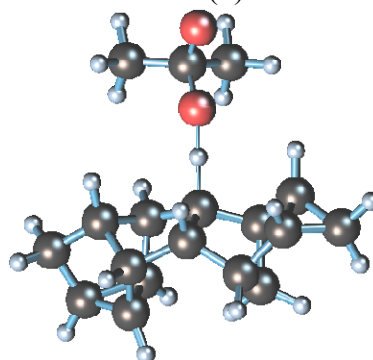
Zero-point correction=	0.380639 (Hartree/Particle)
Thermal correction to Energy=	0.397414
Thermal correction to Enthalpy=	0.398358
Thermal correction to Gibbs Free Energy=	0.336287
Sum of electronic and zero-point Energies=	-849.924281
Sum of electronic and thermal Energies=	-849.907506
Sum of electronic and thermal Enthalpies=	-849.906562
Sum of electronic and thermal Free Energies=	-849.968633
S**2 =	0.0000

C,0,-0.99142545,-1.088260553,-3.6023211486
C,0,-0.9476038608,-1.159829423,-2.0989141559
C,0,0.3989365213,-1.2684542442,-1.3641819123
C,0,1.3484946547,-0.4944158006,-2.3299139745
C,0,0.4656421219,0.765823588,-2.4208871786
C,0,-0.898324864,0.1849235684,-2.806768376
C,0,0.2861120704,1.1353119022,-0.9193956372
C,0,0.3621764502,-0.2317496615,-0.2587068126
C,0,1.2896595127,1.9496126856,-0.0629407772
C,0,0.9846198828,1.4063977478,1.3643831547
C,0,1.2042637305,-0.0853884693,0.973638829
C,0,2.7279181182,1.4346278086,-0.1454955904
C,0,3.2556553332,1.2727383575,1.2637234476
C,0,2.194776068,1.7817798732,2.2155590627

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C,0,2.6772810281,0.0796798617,0.525681704
H,0,-1.8397324187,-1.4696597005,-1.5647298983
H,0,-1.7596479872,0.8480406014,-2.7753029183
H,0,0.7134924748,-2.2727128217,-1.0684666653
H,0,-0.1706789233,-1.4389838505,-4.2217409785
H,0,-1.9676779174,-1.293544474,-4.034848057
H,0,0.8374647979,1.5723040221,-3.0602683787
H,0,2.3302180027,-0.3030072767,-1.9005394096
H,0,1.4928397266,-1.0235102624,-3.2755156821
H,0,-0.7021535332,1.5868061719,-0.7576044597
H,0,-1.0246182461,-0.5590767759,0.376896766
H,0,1.1836047057,3.033006856,-0.1779716109
H,0,1.0560233751,-0.8338715215,1.7559293277
H,0,3.2857114616,-0.7625687095,0.2117098759
H,0,-0.009315015,1.628626888,1.7537596446
H,0,3.3843745656,1.6391687708,-0.9857215475
H,0,4.3198314139,1.3157246876,1.4757774634
H,0,2.2611661429,2.8618678714,2.3931742736
H,0,2.2066450707,1.2675494811,3.1842029759
O,0,-1.8186207785,-0.0819019192,0.8548314184
C,0,-2.6122046896,-0.9586867872,1.7956271135
O,0,-3.5665603665,-0.0879413967,2.0355810769
C,0,-3.0643147547,-2.2128304231,1.0322897409
C,0,-1.7370480428,-1.2989939603,3.0097851146
H,0,-2.2235253228,-2.8390318301,0.7030545526
H,0,-3.7005884045,-2.8224103949,1.684391041
H,0,-3.6581625682,-1.9077425266,0.1653771934
H,0,-0.8798194964,-1.9366558814,2.7518148199
H,0,-1.3803027639,-0.3704449777,3.4650228713
H,0,-2.3413829611,-1.8348442464,3.7513232152

TS-LS Exo-exo-exo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at
UB3PW91/6-31+G(d) level



Zero-point correction=	0.380725 (Hartree/Particle)
Thermal correction to Energy=	0.397061
Thermal correction to Enthalpy=	0.398005
Thermal correction to Gibbs Free Energy=	0.336315
Sum of electronic and zero-point Energies=	-849.927704
Sum of electronic and thermal Energies=	-849.911368
Sum of electronic and thermal Enthalpies=	-849.910424
Sum of electronic and thermal Free Energies=	-849.972115

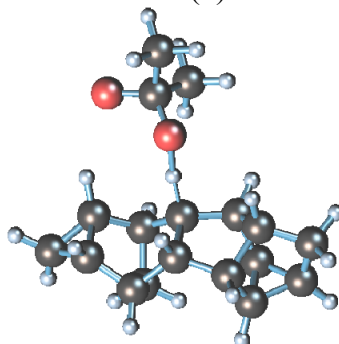
S. A. Grabovskiy

$$S^{*2} = 0.3874$$

C,0,-1.2976081642,1.2051118949,-3.5097859358
C,0,-1.2896752168,1.2120999591,-1.9991996033
C,0,0.0499654541,1.2330233119,-1.252549403
C,0,0.9833371602,0.4806185964,-2.2304980381
C,0,0.0518060131,-0.7443426742,-2.390927726
C,0,-1.2844164291,-0.1004232515,-2.7565175785
C,0,0.0372701444,-1.1893110891,-0.8979649737
C,0,-0.0208766541,0.161850704,-0.1480910484
C,0,-1.0086120454,-2.0430912275,-0.1454683901
C,0,-0.7737511759,-1.5620281051,1.3208574188
C,0,-1.0150554686,-0.0551075282,0.9886195229
C,0,-2.4524451934,-1.5484742167,-0.2506489301
C,0,-3.0341678998,-1.4739125617,1.1468826822
C,0,-1.9988935723,-2.0115202293,2.1096080206
C,0,-2.4584673699,-0.2325617162,0.4907893824
H,0,-2.1758266937,1.5745007229,-1.4901538456
H,0,-2.1699602673,-0.7241339367,-2.8114190117
H,0,0.3832988782,2.2220158734,-0.9256600897
H,0,-2.2527898012,1.4702787773,-3.9576976316
H,0,-0.445192654,1.543403749,-4.0910285401
H,0,0.4036791199,-1.516657987,-3.0826728512
H,0,1.9384347428,0.2189196394,-1.7651176465
H,0,1.195817792,1.0198646646,-3.1560083316
H,0,1.0103566304,-1.6693636383,-0.7124875924
H,0,1.0772952753,0.2705881599,0.4478416562
H,0,-0.890778247,-3.1220006201,-0.2955326982
H,0,-0.9178650885,0.6353065601,1.8322002466
H,0,-3.0919863498,0.5996275386,0.207058256
H,0,0.2092758374,-1.7908806296,1.7381397388
H,0,-3.0856603928,-1.7328001408,-1.1108572593
H,0,-4.1041554399,-1.5605966327,1.3110800354
H,0,-2.0452256381,-3.1013887585,2.2274889343
H,0,-2.0544955773,-1.5499952923,3.1036048276
O,0,2.2391149111,0.1197286624,0.9575840707
C,0,2.7618660921,1.1830185362,1.7482360691
O,0,3.8632885847,0.3930825064,1.9257127327
C,0,3.0368301251,2.4488661289,0.9465102211
C,0,1.9666787276,1.4272504845,3.0246778938
H,0,3.6612534202,3.1315732898,1.5345770891
H,0,3.5714189218,2.1887839203,0.02899382
H,0,2.1094473285,2.9757338483,0.6926274322
H,0,2.5398799813,2.0714296563,3.7016286198
H,0,1.0117618132,1.9240731833,2.8155721647
H,0,1.7800812784,0.4728266037,3.5242707453

S. A. Grabovskiy

TS-OS Exo-exo-exo-heptocyclo[9.3.1.0^{2,10}.0^{3,8}.0^{4,6}.0^{5,9}.0^{12,14}]pentadecane at
UB3PW91/6-31+G(d) level



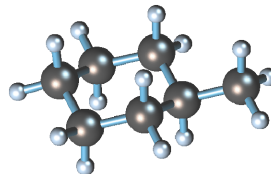
Zero-point correction=	0.379515 (Hartree/Particle)
Thermal correction to Energy=	0.396020
Thermal correction to Enthalpy=	0.396964
Thermal correction to Gibbs Free Energy=	0.334883
Sum of electronic and zero-point Energies=	-849.935432
Sum of electronic and thermal Energies=	-849.918926
Sum of electronic and thermal Enthalpies=	-849.917982
Sum of electronic and thermal Free Energies=	-849.980063
S**2 =	0.9306

C,0,-1.6628970225,-3.2099750175,-0.1066483869
 C,0,-0.7641326844,-2.061573323,-0.5547245105
 C,0,-1.7060036647,-1.0226799117,-1.2397857696
 C,0,-2.7778223606,-1.0319275979,-0.1482337784
 C,0,-2.0032818942,-1.1329061478,1.1441554382
 C,0,-2.7038135407,-2.3567510117,0.5841486309
 C,0,-0.5291202542,-1.1840362351,0.7145840007
 C,0,-0.0202363872,0.1161251522,0.0817473013
 C,0,-0.7953329326,0.224505031,-1.2603074978
 C,0,-0.0023566093,1.5603595874,0.6356514578
 C,0,-1.4220843591,1.9133453066,1.0909730489
 C,0,-2.2170434269,2.023557817,-0.1945749314
 C,0,-1.2018689136,1.7271405513,-1.2972934732
 C,0,0.1065643655,2.3088228364,-0.7124242867
 C,0,-2.0296541935,3.2348853115,0.6845901814
 H,0,-1.8257711465,1.4215729078,1.969240588
 H,0,-3.2170746268,1.6120879325,-0.2768204108
 H,0,0.7882853374,1.7699554851,1.3616007404
 H,0,-2.9064194587,3.5265721537,1.2589163474
 H,0,-1.4190565209,4.0795884671,0.3803431098
 H,0,-1.4769171219,2.0907840282,-2.2933328438
 H,0,0.9929496549,2.0018492056,-1.2750461551
 H,0,0.125971684,3.3972503195,-0.6244336692
 H,0,-0.0965883257,0.0770294242,-2.0985427666
 H,0,1.1236379183,-0.1269030962,-0.214961686
 H,0,-2.0727651114,-1.3224479841,-2.2283399448
 H,0,0.1353447588,-1.6236364602,1.4658926241
 H,0,-2.3371535757,-0.6687398641,2.0648686069
 H,0,0.1397337978,-2.3159606474,-1.1129220648
 H,0,-3.7123100231,-0.4880835583,-0.2260744628

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H,0,-3.5769046637,-2.7669041243,1.0831517914
H,0,-2.0670536428,-3.7826369298,-0.9512268734
H,0,-1.154055653,-3.9038926389,0.5748074179
O,0,2.3785662124,-0.4953144711,-0.7617925366
O,0,3.5729597032,1.1765451791,0.3176842805
C,0,3.311975071,-0.8538302319,1.4655586391
H,0,4.2035532185,-0.6527817017,2.0644951758
H,0,2.4334479095,-0.4880138861,2.0043080326
H,0,3.2059781069,-1.9291281542,1.2961300104
C,0,3.4097067236,-0.144439833,0.0853383221
C,0,4.6974175297,-0.6319308729,-0.6656992478
H,0,5.571565971,-0.416427727,-0.0465990894
H,0,4.6108893066,-1.7061970363,-0.8450803634
H,0,4.7784122021,-0.1069302451,-1.6198388939

Methylcyclohexane at B3PW91/6-311+G(d,p) level



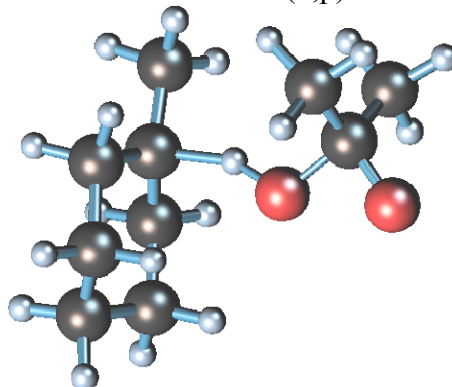
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197410 (Hartree/Particle)
Thermal correction to Energy= 0.204605
Thermal correction to Enthalpy= 0.205549
Thermal correction to Gibbs Free Energy= 0.166788
Sum of electronic and zero-point Energies= -274.972951
Sum of electronic and thermal Energies= -274.965756
Sum of electronic and thermal Enthalpies= -274.964812
Sum of electronic and thermal Free Energies= -275.003573

C,0,-0.1619247318,1.0535333314,0.0498157547
C,0,-1.3009661073,0.0289736931,-0.0108638817
C,0,-0.5258383543,2.252541739,0.9203655476
C,0,1.1306936032,0.377614899,0.5231008353
C,0,-0.9436998287,-1.1854764736,-0.8681478547
C,0,1.4974663147,-0.8353026062,-0.3323077846
C,0,0.3512625569,-1.8458782142,-0.3928363336
H,0,0.0111311383,1.4165135431,-0.9752362753
H,0,-2.2114698493,0.5067634923,-0.3918306054
H,0,-1.5310317601,-0.303390601,1.0120313368
H,0,0.2790816678,2.994428088,0.9339011765
H,0,-0.7098039419,1.9430527628,1.9555275938
H,0,-1.4316521137,2.7483028174,0.5566207379
H,0,1.9521248763,1.1040794947,0.5220504573
H,0,1.0004881512,0.0598942455,1.5680489535
H,0,-1.7659756576,-1.9096005145,-0.8578529173
H,0,-0.8242661761,-0.867727949,-1.9130262954
H,0,2.4044570279,-1.3110694643,0.0570533108
H,0,1.7366416906,-0.4996065397,-1.3506869648
H,0,0.6154708445,-2.683191548,-1.0482812171

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H,0,0.1928469283,-2.2720762523,0.6074768244

TS7-C **Methylcyclohexane** at B3PW91/6-311+G(d,p) level



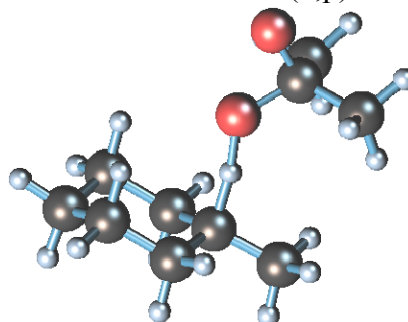
Temperature 293.149 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.279859 (Hartree/Particle)
Thermal correction to Energy= 0.293888
Thermal correction to Enthalpy= 0.294817
Thermal correction to Gibbs Free Energy= 0.239383
Sum of electronic and zero-point Energies= -543.095130
Sum of electronic and thermal Energies= -543.081100
Sum of electronic and thermal Enthalpies= -543.080172
Sum of electronic and thermal Free Energies= -543.135605
S**2 = 0.0000

C,0,-0.9665253266,1.0467901156,0.1153689004
H,0,0.263514675,0.3227206007,-0.1505586982
C,0,-1.4750740154,0.3751261117,1.3550511611
C,0,-1.9331262951,-1.0692989182,1.1468474367
C,0,-2.8575034034,-1.1963394842,-0.0626978611
C,0,-2.179378809,-0.6667052789,-1.3245335443
C,0,-1.7248036261,0.7837887026,-1.1516482818
C,0,-0.3614929589,2.4070078174,0.2752559965
O,0,0.8525419617,-0.5329281983,-0.3873122165
C,0,2.3108474725,-0.4211035657,-0.0908296852
O,0,2.5814915215,-1.5986098066,-0.6157377079
C,0,2.5205622019,-0.3272102841,1.4216301611
C,0,2.9019188016,0.767725068,-0.8512158976
H,0,3.99084101,0.7537194552,-0.7494272257
H,0,2.6524277831,0.6718611678,-1.9094290158
H,0,2.5412582375,1.7302967875,-0.4716950625
H,0,2.1316632174,0.6080109207,1.8413396908
H,0,2.0315742534,-1.1763777159,1.9020980068
H,0,3.5908631224,-0.3737320803,1.6429893683
H,0,-0.7330161349,0.4499122982,2.156441651
H,0,-2.3341905099,0.9873040389,1.6877044757
H,0,-1.0478870433,-1.6942931832,0.9953249639
H,0,-2.4321225378,-1.421747705,2.0548412302
H,0,-3.140925812,-2.243721384,-0.2048799285
H,0,-3.7897871142,-0.6434090404,0.1208016448
H,0,-2.8550684116,-0.7299363714,-2.1830348752

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H,0,-1.3020591852,-1.2786043993,-1.5544981563
H,0,-2.6120717213,1.4428467235,-1.1041723347
H,0,-1.1462567376,1.1278992628,-2.0146373316
H,0,-1.1711090915,3.1261620307,0.473515871
H,0,0.1512171898,2.7384673631,-0.6304712552
H,0,0.3263226952,2.4562435649,1.1227760619

TS7-LS **Methylcyclohexane** at UB3PW91/6-311+G(d,p) level



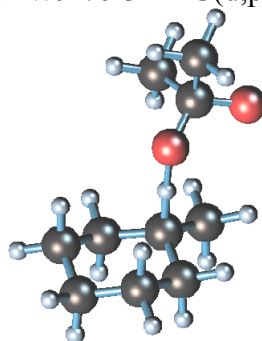
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.279899 (Hartree/Particle)
Thermal correction to Energy= 0.294130
Thermal correction to Enthalpy= 0.295074
Thermal correction to Gibbs Free Energy= 0.238030
Sum of electronic and zero-point Energies= -543.100355
Sum of electronic and thermal Energies= -543.086123
Sum of electronic and thermal Enthalpies= -543.085179
Sum of electronic and thermal Free Energies= -543.142223
S**2 = 0.3582

C,0,-0.8803781652,0.9829991011,0.0987897017
H,0,0.104828005,0.2508773594,-0.1426026783
C,0,-1.485472584,0.3791232164,1.3530102542
C,0,-2.0047273202,-1.0448339554,1.1494753348
C,0,-2.9441910771,-1.1313154011,-0.0530104132
C,0,-2.2615257555,-0.6176943403,-1.3200569109
C,0,-1.7426924799,0.8095418891,-1.1386454204
C,0,-0.3159415933,2.3726336922,0.2772451881
O,0,0.9721724938,-0.6170823705,-0.4679835161
C,0,2.3229022945,-0.3850589266,-0.0742419901
O,0,2.582568922,-1.5854939176,-0.6657462413
C,0,2.5113127306,-0.3827697833,1.4339916646
C,0,2.9612811526,0.7981361051,-0.7826667613
H,0,4.0459599845,0.7670927203,-0.6440955286
H,0,2.7423546721,0.738295112,-1.8497943339
H,0,2.5978109636,1.7502832543,-0.3858707544
H,0,2.115886003,0.5316652927,1.886826811
H,0,2.0063459922,-1.2501703184,1.8614548004
H,0,3.5768803326,-0.4426991673,1.6738298324
H,0,-0.7618555269,0.4171327238,2.1745922058
H,0,-2.320682567,1.0339871922,1.6534092164
H,0,-1.1523062447,-1.714721228,0.9911342995
H,0,-2.5120628812,-1.382981986,2.0590337623

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H,0,-3.274856954,-2.1650898044,-0.1971502167
H,0,-3.8488610684,-0.5390675551,0.1443767567
H,0,-2.9529888648,-0.6496027167,-2.1684435703
H,0,-1.4196758306,-1.2719031912,-1.5717465242
H,0,-2.5967026897,1.4996063563,-1.0332531623
H,0,-1.1915400268,1.1389283243,-2.0256799041
H,0,-1.1339816258,3.0758132838,0.4841679262
H,0,0.1953338132,2.7213849744,-0.623749564
H,0,0.3787799719,2.4272100955,1.1200548002

TS7-OS **Methylcyclohexane** at UB3PW91/6-311+G(d,p) level



Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.279582 (Hartree/Particle)
Thermal correction to Energy= 0.293837
Thermal correction to Enthalpy= 0.294781
Thermal correction to Gibbs Free Energy= 0.238127
Sum of electronic and zero-point Energies= -543.107098
Sum of electronic and thermal Energies= -543.092843
Sum of electronic and thermal Enthalpies= -543.091899
Sum of electronic and thermal Free Energies= -543.148553
S**2 = 0.9292
C,0,-0.2187443727,-0.3517892309,-1.2345742576
H,0,-0.1773260831,-0.1232673026,-0.0570468479
C,0,1.220273055,-0.2700149162,-1.7275072548
C,0,1.8403837308,1.1151872328,-1.5404614255
C,0,0.9655769413,2.206175755,-2.1576605987
C,0,-0.4535227912,2.1590960932,-1.5918069403
C,0,-1.0856809135,0.7789898083,-1.7756086701
C,0,-0.8477665891,-1.7205853241,-1.407929622
O,0,-0.2104027812,0.3216905486,1.2984163308
C,0,-0.3472065349,-0.7491006147,2.1551180936
O,0,-1.4610145377,-1.488184768,2.017272522
C,0,-0.4383616924,-0.067740882,3.5681150201
C,0,0.8786855007,-1.7013817238,2.1185167933
H,0,0.7904082326,-2.4676883334,2.8891469927
H,0,0.9336446007,-2.1846678985,1.1420641057
H,0,1.7819513568,-1.1094182845,2.2752314058
H,0,0.4606142514,0.5291126479,3.7223231375
H,0,-1.318148375,0.5740665097,3.5988301329
H,0,-0.5172240504,-0.8489254155,4.3245000707
H,0,1.830540119,-1.0361055633,-1.2356354134
H,0,1.218011928,-0.5261277111,-2.7998775321

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H,0,1.9589658047,1.3115641568,-0.4680229242
H,0,2.8440240943,1.134783791,-1.9791181105
H,0,1.4106686503,3.1915433045,-1.9817931532
H,0,0.9297729862,2.0706498242,-3.2478169169
H,0,-1.0805607571,2.9191725254,-2.0704431319
H,0,-0.4272412042,2.3985827969,-0.5226897502
H,0,-1.2450885706,0.5893010989,-2.8498734987
H,0,-2.0740218648,0.7419214782,-1.3055056849
H,0,-0.9829071056,-1.9355237396,-2.4764281866
H,0,-1.8269853596,-1.7753204041,-0.9266089492
H,0,-0.2195781068,-2.5147169118,-0.9939533955