SUPPORTING INFORMATION FOR

How an Enzyme Might Accelerate an Intramolecular Diels-Alder Reaction – Theozymes for the Formation of Salvileucalin B

Dean J. Tantillo*

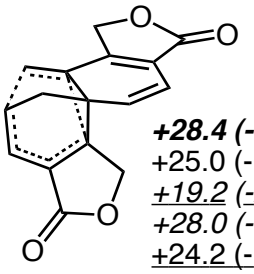
Department of Chemistry, University of California–Davis, 1 Shields Avenue, Davis, CA 95616

tantillo@chem.ucdavis.edu

Table of Contents

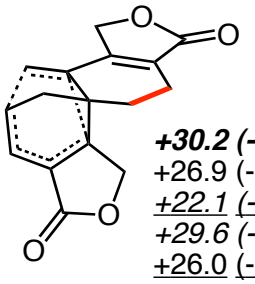
GAUSSIAN03, Revision D.01
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

A ‡



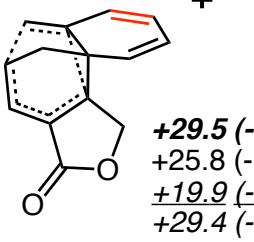
+28.4 (-6.0)
+25.0 (-18.0)
+19.2 *(-20.7)*
+28.0 (-8.2)
+24.2 (-18.3)

B ‡



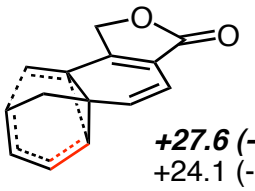
+30.2 (-1.2)
+26.9 (-12.7)
+22.1 *(-13.7)*
+29.6 (-3.1)
+26.0 (-12.8)

C ‡



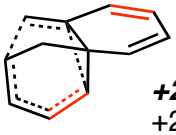
+29.5 (-5.5)
+25.8 (-17.7)
+19.9 *(-20.2)*
+29.4 (-7.6)
+25.3 (-17.8)

D ‡



+27.6 (-10.6)
+24.1 (-23.1)
+19.7 *(-24.4)*
+27.0 (-13.2)
+23.0 (-23.7)

E ‡

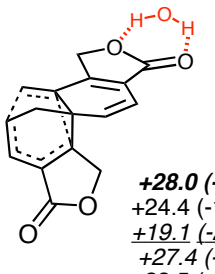


+29.3 (-9.7)
+25.8 (-22.1)
+21.3 *(-23.6)*
+29.6 (-11.7)
+25.6 (-22.2)

F ‡

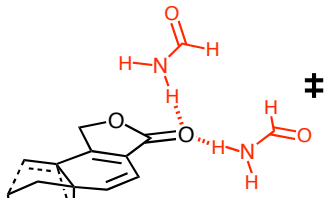
+29.9 (-8.1)
+25.5 (-20.9)
+22.4 *(-21.2)*
+29.8 (-10.1)
+25.3 (-20.5)

G



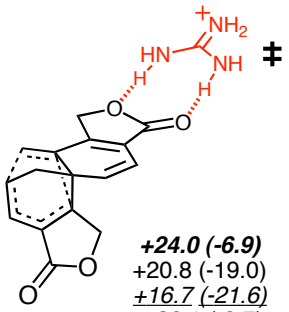
+28.0 (-6.1)
+24.4 (-18.1)
+19.1 (-20.8)
+27.4 (-8.3)
+23.5 (-18.5)

H



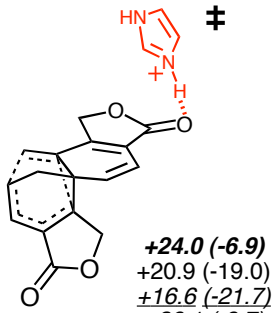
+27.2 (-6.2)
+23.9 (-17.7)
+18.8 (-20.1)
+26.9 (-7.8)
+23.1 (-18.1)

I



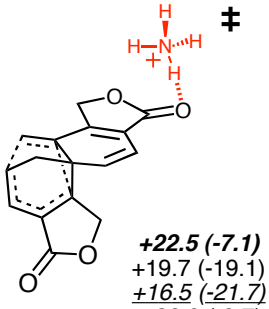
+24.0 (-6.9)
+20.8 (-19.0)
+16.7 (-21.6)
+26.1 (-8.7)
+22.4 (-19.0)

J



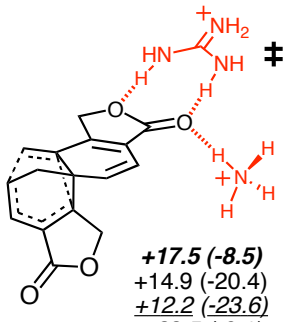
+24.0 (-6.9)
+20.9 (-19.0)
+16.6 (-21.7)
+26.1 (-8.7)
+22.5 (-18.9)

K



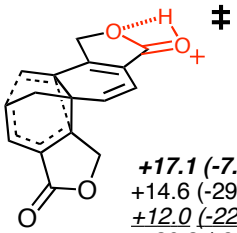
+22.5 (-7.1)
+19.7 (-19.1)
+16.5 (-21.7)
+26.0 (-8.7)
+22.4 (-18.9)

L



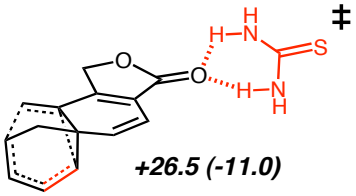
+17.5 (-8.5)
+14.9 (-20.4)
+12.2 (-23.6)
+23.5 (-9.1)
+20.3 (-19.4)

M



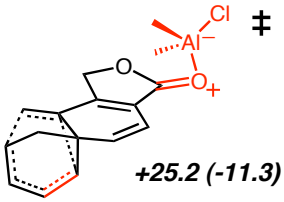
+17.1 (-7.9)
+14.6 (-29.6)
+12.0 (-22.5)
+20.3 (-9.4)
+17.3 (-19.5)

N



+26.5 (-11.0)

O



+25.2 (-11.3)

coordinates and energies for computed structures

A (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=-917.7660963
Zero-point correction= 0.245836 (Hartree/Particle)
Thermal correction to Energy= 0.261434
Thermal correction to Enthalpy= 0.262378
Thermal correction to Gibbs Free Energy= 0.202403
Sum of electronic and zero-point Energies= -917.520260
Sum of electronic and thermal Energies= -917.504662
Sum of electronic and thermal Enthalpies= -917.503718
Sum of electronic and thermal Free Energies= -917.563693

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.275707	0.181850	0.616962
2	6	0	0.488264	-0.789408	1.513537
3	6	0	1.805606	-1.028810	1.419924
4	6	0	2.554619	-0.382708	0.363764
5	6	0	1.974584	0.391832	-0.578928
6	6	0	0.545266	0.643349	-0.623573
7	1	0	-0.100495	-1.247169	2.305402
8	1	0	2.324017	-1.688003	2.109513
9	6	0	3.044665	0.858231	-1.529592
10	1	0	2.889813	0.508411	-2.557772
11	1	0	3.151841	1.949737	-1.551675
12	6	0	4.006261	-0.467424	0.096954
13	8	0	4.867161	-1.059299	0.697696
14	8	0	4.261688	0.285887	-1.030205
15	6	0	-0.627544	1.435968	1.517589
16	1	0	-0.752283	1.086617	2.554526
17	1	0	0.241312	2.102243	1.533334
18	6	0	-0.022738	1.273320	-1.669872
19	1	0	0.575983	1.636063	-2.500756
20	1	0	-1.090377	1.448304	-1.731909
21	6	0	-1.883163	2.191791	1.140957
22	1	0	-1.953154	3.229536	1.457942
23	6	0	-1.573227	-0.450259	0.157855
24	6	0	-2.913122	1.590175	0.525767
25	1	0	-3.849681	2.095313	0.311187
26	6	0	-2.746972	0.203742	0.118072
27	6	0	-3.772617	-0.694565	-0.464955
28	8	0	-4.939484	-0.488633	-0.683945
29	8	0	-3.157248	-1.894417	-0.752316
30	6	0	-1.767767	-1.829058	-0.403303
31	1	0	-1.546905	-2.627395	0.316364
32	1	0	-1.165468	-2.010106	-1.302952

single points:

mPW1PW91/6-31G(d) *HF=-917.5592438*
MP2/6-31G(d) *MP2=-915.0167279*
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-917.7779117*
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-917.5716611*

A (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=-917.7200213
Zero-point correction= *0.245016 (Hartree/Particle)*
Thermal correction to Energy= *0.259423*
Thermal correction to Enthalpy= *0.260368*
Thermal correction to Gibbs Free Energy= *0.204233*
Sum of electronic and zero-point Energies= *-917.475005*
Sum of electronic and thermal Energies= *-917.460598*
Sum of electronic and thermal Enthalpies= *-917.459654*
Sum of electronic and thermal Free Energies= *-917.515788*

1 imaginary frequency (-532.1837 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.405451	-1.131078	0.871546
2	6	0	-0.634995	-1.103786	1.961224
3	6	0	-1.823962	-0.506049	1.724167
4	6	0	-2.140356	-0.042201	0.389155
5	6	0	-1.372850	-0.356470	-0.702743
6	6	0	-0.193584	-1.134535	-0.540033
7	1	0	-0.402273	-1.540102	2.929249
8	1	0	-2.585017	-0.418388	2.494359
9	6	0	-2.124820	0.066461	-1.937710
10	1	0	-1.581791	0.813148	-2.530508
11	1	0	-2.379036	-0.773914	-2.594923
12	6	0	-3.389764	0.585208	-0.070643
13	8	0	-4.336192	0.985320	0.561739
14	8	0	-3.337118	0.658368	-1.452631
15	6	0	1.513349	-2.192174	0.877019
16	1	0	2.165628	-2.076175	1.752857
17	1	0	1.081906	-3.197982	0.916528
18	6	0	0.487485	-1.926064	-1.478125
19	1	0	0.568685	-2.994055	-1.300483
20	1	0	0.467839	-1.667736	-2.537763
21	6	0	2.336595	-2.003803	-0.409574
22	1	0	2.820945	-2.889985	-0.813177
23	6	0	1.094097	0.210372	0.632131
24	6	0	2.922886	-0.761395	-0.647431
25	1	0	3.742968	-0.622273	-1.344303
26	6	0	2.277340	0.334595	-0.058472
27	6	0	2.616106	1.776044	-0.158267
28	8	0	3.553920	2.308121	-0.695737
29	8	0	1.633989	2.477217	0.500925
30	6	0	0.645182	1.580880	1.037535
31	1	0	0.615048	1.699280	2.128543
32	1	0	-0.340666	1.859954	0.646590

---

single points:

mPW1PW91/6-31G(d)	*HF=-917.5193966*
MP2/6-31G(d)	*MP2=-914.9860941*
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d)	*HF=-917.733229*
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d)	*HF=-917.5331719*

A (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=-917.7784617

Zero-point correction=	*0.248771 (Hartree/Particle)*
Thermal correction to Energy=	*0.262907*
Thermal correction to Enthalpy=	*0.263852*
Thermal correction to Gibbs Free Energy=	*0.208093*
Sum of electronic and zero-point Energies=	*-917.529691*
Sum of electronic and thermal Energies=	*-917.515554*
Sum of electronic and thermal Enthalpies=	*-917.514610*
Sum of electronic and thermal Free Energies=	*-917.570369*

Center Number	*Atomic Number*	*Atomic Type*	*Coordinates (Angstroms) X*	*Y*	*Z*
1	6	0	-0.368819	0.884251	1.063214
2	6	0	0.626712	0.583695	2.110917
3	6	0	1.826483	0.032777	1.813364
4	6	0	2.207292	-0.133596	0.426560
5	6	0	1.431074	0.246328	-0.617086
6	6	0	0.058843	0.705376	-0.428960
7	1	0	0.380869	0.848754	3.136604
8	1	0	2.556386	-0.201028	2.582198
9	6	0	2.236328	0.129133	-1.880356
10	1	0	1.803043	-0.576147	-2.601484
11	1	0	2.378451	1.090256	-2.392119
12	6	0	3.535785	-0.531697	-0.090272
13	8	0	4.508505	-0.925077	0.501779
14	8	0	3.513697	-0.366766	-1.462055
15	6	0	-1.273584	2.113013	1.104447
16	1	0	-2.067974	2.047858	1.856170
17	1	0	-0.669669	3.002887	1.316802
18	6	0	-0.604373	1.825347	-1.224685
19	1	0	0.073991	2.684659	-1.285875
20	1	0	-0.893265	1.539032	-2.241945
21	6	0	-1.848950	2.186581	-0.347165
22	1	0	-2.256841	3.170258	-0.587686
23	6	0	-0.954961	-0.253511	0.222148
24	6	0	-2.860056	1.076620	-0.503612
25	1	0	-3.884121	1.238064	-0.825739
26	6	0	-2.358220	-0.128525	-0.206882
27	6	0	-2.967708	-1.476703	-0.222421
28	8	0	-4.089370	-1.807547	-0.513860
29	8	0	-2.008095	-2.375103	0.169252
30	6	0	-0.743789	-1.741974	0.471572
31	1	0	-0.490304	-1.965040	1.512306

32	1	0	0.019199	-2.186312	-0.174847

single points:

mPW1PW91/6-31G(d) HF=-917.587997

MP2/6-31G(d) MP2=-915.049749

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-917.7909862

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-917.6008626

B (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=-918.9955694

Zero-point correction= 0.269998 (Hartree/Particle)

Thermal correction to Energy= 0.285880

Thermal correction to Enthalpy= 0.286825

Thermal correction to Gibbs Free Energy= 0.226797

Sum of electronic and zero-point Energies= -918.725571

Sum of electronic and thermal Energies= -918.709689

Sum of electronic and thermal Enthalpies= -918.708745

Sum of electronic and thermal Free Energies= -918.768772

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.282781	0.266785	0.387452
2	6	0	-0.450772	1.638020	0.497371
3	6	0	-1.912709	1.520541	0.959930
4	6	0	-2.588865	0.445135	0.178208
5	6	0	-1.948918	-0.510218	-0.522249
6	6	0	-0.497649	-0.656188	-0.584153
7	1	0	0.112210	2.286228	1.178688
8	1	0	-2.438135	2.473490	0.825846
9	6	0	-2.984258	-1.378228	-1.192381
10	1	0	-2.916178	-1.359846	-2.286958
11	1	0	-2.940585	-2.423418	-0.863073
12	6	0	-4.047636	0.268485	0.014320
13	8	0	-4.955320	0.918066	0.470959
14	8	0	-4.247263	-0.823857	-0.803671
15	6	0	0.346935	-0.408894	1.804322
16	1	0	0.458853	0.387039	2.559454
17	1	0	-0.613356	-0.889692	2.019377
18	6	0	0.082934	-1.564819	-1.385114
19	1	0	-0.507472	-2.220236	-2.019586
20	1	0	1.158896	-1.689213	-1.433261
21	6	0	1.477318	-1.393434	2.012829
22	1	0	1.346219	-2.150095	2.782489
23	6	0	1.696256	0.475892	-0.103230
24	6	0	2.634425	-1.290771	1.341559
25	1	0	3.481943	-1.944985	1.520135
26	6	0	2.742193	-0.249212	0.332090
27	6	0	3.955285	0.159249	-0.414400
28	8	0	5.084720	-0.253213	-0.334836
29	8	0	3.583110	1.153745	-1.295030
30	6	0	2.179244	1.416600	-1.171845

31	1	0	2.045944	2.474877	-0.913384
32	1	0	1.699836	1.243234	-2.144109
33	1	0	-1.971014	1.300173	2.035262
34	1	0	-0.438527	2.120861	-0.488513

single points:

mPW1PW91/6-31G(d) *HF=-918.7919455*

MP2/6-31G(d) *MP2=-916.2172438*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-919.0078997*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-918.8047487*

B (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 918.9470379

Zero-point correction= 0.269510 (Hartree/Particle)

Thermal correction to Energy= 0.284197

Thermal correction to Enthalpy= 0.285141

Thermal correction to Gibbs Free Energy= 0.228533

Sum of electronic and zero-point Energies= -918.677528

Sum of electronic and thermal Energies= -918.662841

Sum of electronic and thermal Enthalpies= -918.661897

Sum of electronic and thermal Free Energies= -918.718505

1 imaginary frequency (-550.2767 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.432251	-1.110827	0.866470
2	6	0	-0.602754	-1.175285	1.997421
3	6	0	-1.786349	-0.187253	1.799780
4	6	0	-2.129104	0.007294	0.353168
5	6	0	-1.378780	-0.407988	-0.701818
6	6	0	-0.175051	-1.160939	-0.520314
7	1	0	-0.127105	-0.998194	2.969303
8	1	0	-1.556158	0.782919	2.261095
9	6	0	-2.126889	-0.080422	-1.970129
10	1	0	-1.577533	0.613673	-2.618417
11	1	0	-2.381868	-0.969931	-2.558524
12	6	0	-3.372367	0.607055	-0.155279
13	8	0	-4.305807	1.078218	0.449075
14	8	0	-3.337524	0.550538	-1.538318
15	6	0	1.549827	-2.162910	0.879440
16	1	0	2.211080	-2.027512	1.745348
17	1	0	1.122678	-3.169883	0.943415
18	6	0	0.506507	-1.960178	-1.455427
19	1	0	0.616009	-3.022577	-1.259292
20	1	0	0.430572	-1.737854	-2.521776
21	6	0	2.354262	-1.991825	-0.420658
22	1	0	2.843529	-2.878075	-0.818140
23	6	0	1.099871	0.231126	0.608490
24	6	0	2.947425	-0.748847	-0.649915
25	1	0	3.773581	-0.606801	-1.339004

26	6	0	2.301230	0.344581	-0.064570
27	6	0	2.640409	1.780762	-0.205970
28	8	0	3.590855	2.296728	-0.737309
29	8	0	1.641107	2.502514	0.401600
30	6	0	0.634713	1.624382	0.931310
31	1	0	0.555608	1.807115	2.011241
32	1	0	-0.329477	1.879873	0.474354
33	1	0	-2.670115	-0.548000	2.340020
34	1	0	-0.991051	-2.201097	2.018003

single points:

mPW1PW91/6-31G(d) HF=-918.7490397

MP2/6-31G(d) MP2=-916.1820864

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-918.960666

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-918.7632476

B (prod)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=-919.0003694

Zero-point correction= 0.272917 (Hartree/Particle)

Thermal correction to Energy= 0.287426

Thermal correction to Enthalpy= 0.288370

Thermal correction to Gibbs Free Energy= 0.231962

Sum of electronic and zero-point Energies= -918.727452

Sum of electronic and thermal Energies= -918.712944

Sum of electronic and thermal Enthalpies= -918.711999

Sum of electronic and thermal Free Energies= -918.768408

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.382745	0.928418	1.041274
2	6	0	0.656802	0.758112	2.142738
3	6	0	1.811320	-0.226958	1.810786
4	6	0	2.200331	-0.157431	0.368244
5	6	0	1.406916	0.273445	-0.629596
6	6	0	0.034905	0.735531	-0.412013
7	1	0	0.176683	0.455412	3.081271
8	1	0	1.519730	-1.255265	2.064089
9	6	0	2.170002	0.184825	-1.923855
10	1	0	1.708776	-0.504397	-2.643111
11	1	0	2.294966	1.156465	-2.418705
12	6	0	3.513289	-0.530876	-0.196047
13	8	0	4.502288	-0.941929	0.358605
14	8	0	3.460587	-0.316317	-1.560968
15	6	0	-1.309490	2.143001	1.058485
16	1	0	-2.089589	2.086869	1.826047
17	1	0	-0.716348	3.048040	1.239833
18	6	0	-0.650097	1.809417	-1.249039
19	1	0	0.007837	2.683143	-1.334409
20	1	0	-0.924720	1.485535	-2.259336
21	6	0	-1.902341	2.173194	-0.384363
22	1	0	-2.328995	3.142866	-0.648685

23	6	0	-0.979937	-0.241885	0.279536
24	6	0	-2.889657	1.041590	-0.522391
25	1	0	-3.901124	1.171063	-0.895374
26	6	0	-2.377320	-0.147914	-0.181407
27	6	0	-2.950921	-1.508418	-0.255313
28	8	0	-4.051311	-1.862765	-0.595866
29	8	0	-1.975178	-2.393930	0.131011
30	6	0	-0.761825	-1.730131	0.547036
31	1	0	-0.617561	-1.948608	1.610474
32	1	0	0.070811	-2.162211	-0.015397
33	1	0	2.681834	-0.012354	2.440896
34	1	0	1.091216	1.749443	2.325716

single points:

mPW1PW91/6-31G(d) HF=-918.8122407

MP2/6-31G(d) MP2=-916.2391546

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-919.0128124

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-918.825139

C (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 691.0905181

Zero-point correction= 0.224074 (Hartree/Particle)

Thermal correction to Energy= 0.236798

Thermal correction to Enthalpy= 0.237743

Thermal correction to Gibbs Free Energy= 0.184750

Sum of electronic and zero-point Energies= -690.866444

Sum of electronic and thermal Energies= -690.853720

Sum of electronic and thermal Enthalpies= -690.852776

Sum of electronic and thermal Free Energies= -690.905768

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.814299	0.195379	-0.348182
2	6	0	-1.626651	-0.618534	-1.344356
3	6	0	-2.903955	-0.976063	-1.141294
4	6	0	-3.587803	-0.656900	0.105116
5	6	0	-2.921187	-0.072064	1.122439
6	6	0	-1.502705	0.266217	1.040871
7	1	0	-1.129965	-0.845533	-2.285551
8	1	0	-3.449152	-1.511967	-1.914261
9	6	0	-0.678369	1.650411	-0.956617
10	1	0	-0.677707	1.561856	-2.054849
11	1	0	-1.584438	2.211321	-0.705187
12	6	0	-0.841280	0.668754	2.142958
13	1	0	-1.360420	0.768119	3.092749
14	1	0	0.215028	0.911750	2.137135
15	6	0	0.562682	2.422134	-0.564483
16	1	0	0.516881	3.506697	-0.630467
17	6	0	0.574023	-0.389167	-0.204602
18	6	0	1.706996	1.802849	-0.235771
19	1	0	2.626630	2.337304	-0.018664

20	6	0	1.695430	0.350589	-0.150413
21	6	0	2.849114	-0.549446	0.081387
22	8	0	4.019517	-0.286306	0.202987
23	8	0	2.362988	-1.838518	0.150273
24	6	0	0.936835	-1.831461	-0.006374
25	1	0	0.672727	-2.468162	-0.860245
26	1	0	0.476359	-2.262319	0.891899
27	1	0	-3.422292	0.132330	2.065963
28	1	0	-4.636678	-0.919003	0.211327

single points:

mPW1PW91/6-31G(d) *HF=-690.9331859*

MP2/6-31G(d) *MP2=-688.930899*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-691.0968601*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-690.9398915*

C (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 691.0427731

Zero-point correction= 0.223299 (Hartree/Particle)

Thermal correction to Energy= 0.234731

Thermal correction to Enthalpy= 0.235675

Thermal correction to Gibbs Free Energy= 0.186640

Sum of electronic and zero-point Energies= -690.819474

Sum of electronic and thermal Energies= -690.808043

Sum of electronic and thermal Enthalpies= -690.807098

Sum of electronic and thermal Free Energies= -690.856133

1 imaginary frequency (-547.9357 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.980976	0.448226	-0.667281
2	6	0	-2.071951	-0.347887	-1.323853
3	6	0	-2.728430	-1.275598	-0.590259
4	6	0	-2.509644	-1.425559	0.841949
5	6	0	-1.784574	-0.495015	1.535028
6	6	0	-1.209984	0.611240	0.829416
7	1	0	-2.301685	-0.185270	-2.374256
8	1	0	-3.484843	-1.900774	-1.059319
9	6	0	-0.567953	1.822961	-1.208571
10	1	0	-0.128619	1.734736	-2.211241
11	1	0	-1.438030	2.484231	-1.284176
12	6	0	-0.844485	1.863520	1.349948
13	1	0	-1.346640	2.750785	0.976432
14	1	0	-0.544685	1.949637	2.395924
15	6	0	0.472554	2.403275	-0.232222
16	1	0	0.517912	3.487806	-0.161188
17	6	0	0.315350	-0.323688	-0.428618
18	6	0	1.640031	1.674571	0.000280
19	1	0	2.540304	2.119907	0.410584
20	6	0	1.517025	0.287055	-0.147470

21	6	0	2.532425	-0.766331	0.092913
22	8	0	3.699307	-0.660660	0.378171
23	8	0	1.914175	-1.984817	-0.069538
24	6	0	0.525639	-1.804329	-0.403819
25	1	0	0.335537	-2.269270	-1.380282
26	1	0	-0.094039	-2.322155	0.339036
27	1	0	-1.761243	-0.503933	2.622873
28	1	0	-3.031975	-2.216529	1.371898

single points:

mPW1PW91/6-31G(d) *HF=-690.891992*

MP2/6-31G(d) *MP2=-688.8992644*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-691.050036*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-690.8995355*

C (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 691.1021661

Zero-point correction= 0.227033 (Hartree/Particle)

Thermal correction to Energy= 0.238232

Thermal correction to Enthalpy= 0.239176

Thermal correction to Gibbs Free Energy= 0.190447

Sum of electronic and zero-point Energies= -690.875134

Sum of electronic and thermal Energies= -690.863934

Sum of electronic and thermal Enthalpies= -690.862990

Sum of electronic and thermal Free Energies= -690.911719

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.913045	0.422072	-0.776538
2	6	0	-1.972395	-0.349946	-1.440985
3	6	0	-2.804687	-1.145021	-0.728021
4	6	0	-2.804314	-1.145204	0.728724
5	6	0	-1.971597	-0.350368	1.441493
6	6	0	-0.912580	0.421660	0.776655
7	1	0	-2.092011	-0.245759	-2.517357
8	1	0	-3.564436	-1.730235	-1.239660
9	6	0	-0.483134	1.818111	-1.218225
10	1	0	0.098965	1.829122	-2.146646
11	1	0	-1.371441	2.444995	-1.360011
12	6	0	-0.482296	1.817493	1.218739
13	1	0	-1.370556	2.444226	1.361458
14	1	0	0.100456	1.828049	2.146756
15	6	0	0.349548	2.336414	0.000093
16	1	0	0.461442	3.422717	0.000275
17	6	0	0.187354	-0.317143	-0.000607
18	6	0	1.673260	1.610030	-0.000306
19	1	0	2.635122	2.113461	-0.000002
20	6	0	1.532558	0.278234	-0.000560
21	6	0	2.530430	-0.813588	0.000007
22	8	0	3.735303	-0.754151	0.000361
23	8	0	1.850056	-2.004204	0.000287

24	6	0	0.413606	-1.821449	-0.001211
25	1	0	0.009973	-2.314617	-0.890805
26	1	0	0.007944	-2.315973	0.886672
27	1	0	-2.090833	-0.246347	2.517904
28	1	0	-3.563752	-1.730562	1.240684

single points:

mPW1PW91/6-31G(d) *HF=-690.9613303*

MP2/6-31G(d) *MP2=-688.9631572*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-691.1089321*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-690.9682398*

D (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 691.0891293

Zero-point correction= *0.224021 (Hartree/Particle)*

Thermal correction to Energy= *0.236726*

Thermal correction to Enthalpy= *0.237670*

Thermal correction to Gibbs Free Energy= *0.184737*

Sum of electronic and zero-point Energies= *-690.865108*

Sum of electronic and thermal Energies= *-690.852403*

Sum of electronic and thermal Enthalpies= *-690.851459*

Sum of electronic and thermal Free Energies= *-690.904393*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.129439	-0.503924	-0.164995
2	6	0	-0.277885	-1.762181	-0.306047
3	6	0	1.061654	-1.783451	-0.217038
4	6	0	1.762660	-0.527255	-0.057558
5	6	0	1.135950	0.669839	-0.095805
6	6	0	-0.295672	0.800685	-0.304209
7	1	0	-0.837304	-2.687942	-0.419984
8	1	0	1.632005	-2.706042	-0.266272
9	6	0	2.175075	1.749852	0.040945
10	1	0	2.232610	2.406018	-0.836490
11	1	0	2.026795	2.377727	0.928302
12	6	0	3.214200	-0.309557	0.108784
13	8	0	4.113446	-1.109806	0.181790
14	8	0	3.422847	1.053689	0.173167
15	6	0	-1.750879	-0.569098	1.281662
16	1	0	-1.944301	-1.625802	1.525929
17	1	0	-1.001408	-0.229011	2.004514
18	6	0	-0.855370	1.996453	-0.567834
19	1	0	-0.259245	2.904804	-0.595402
20	1	0	-1.914222	2.102137	-0.770269
21	6	0	-3.047740	0.184189	1.439271
22	1	0	-3.314369	0.542772	2.430805
23	6	0	-2.244842	-0.533301	-1.203940
24	6	0	-3.885016	0.330729	0.401384
25	1	0	-4.850782	0.814762	0.523290

26	6	0	-3.502744	-0.151643	-0.928092
27	1	0	-1.964887	-0.838652	-2.209444
28	1	0	-4.254925	-0.159854	-1.713802

single points:

mPW1PW91/6-31G(d) HF=-690.9319324

MP2/6-31G(d) MP2=-688.9290901

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-691.0968601

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-690.9398915

D (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 691.0445258

Zero-point correction= 0.223361 (Hartree/Particle)

Thermal correction to Energy= 0.234901

Thermal correction to Enthalpy= 0.235846

Thermal correction to Gibbs Free Energy= 0.186339

Sum of electronic and zero-point Energies= -690.821164

Sum of electronic and thermal Energies= -690.809624

Sum of electronic and thermal Enthalpies= -690.808680

Sum of electronic and thermal Free Energies= -690.858186

1 imaginary frequency (-543.6866 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.097799	0.910381	-0.174634
2	6	0	-0.138167	2.059279	-0.330217
3	6	0	1.185572	1.844929	-0.171831
4	6	0	1.674960	0.490364	-0.007733
5	6	0	0.878918	-0.607002	-0.192785
6	6	0	-0.498826	-0.445724	-0.540520
7	1	0	-0.530571	3.051513	-0.538977
8	1	0	1.909909	2.652554	-0.227268
9	6	0	1.756201	-1.829502	-0.170570
10	1	0	1.483180	-2.532749	0.626523
11	1	0	1.755273	-2.374963	-1.122434
12	6	0	3.065585	0.047970	0.159156
13	8	0	4.074228	0.689276	0.331039
14	8	0	3.078373	-1.337533	0.081914
15	6	0	-2.483273	0.986690	-0.811693
16	1	0	-3.067339	1.809828	-0.377673
17	1	0	-2.406328	1.167450	-1.889603
18	6	0	-1.367202	-1.326557	-1.200733
19	1	0	-1.793614	-1.024169	-2.152191
20	1	0	-1.243890	-2.406177	-1.104898
21	6	0	-3.178225	-0.347887	-0.526084
22	1	0	-3.924814	-0.680697	-1.243682
23	6	0	-1.250227	0.423194	1.272176
24	6	0	-3.310487	-0.738780	0.803766
25	1	0	-4.044233	-1.484795	1.095512
26	6	0	-2.334397	-0.298329	1.716098

27	1	0	-0.413112	0.622687	1.933034
28	1	0	-2.361068	-0.628584	2.751662

single points:

mPW1PW91/6-31G(d) *HF=-690.8935168*

MP2/6-31G(d) *MP2=-688.8976912*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-691.052768*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-690.9021148*

D (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 691.1092508

Zero-point correction= *0.227272 (Hartree/Particle)*

Thermal correction to Energy= *0.238397*

Thermal correction to Enthalpy= *0.239341*

Thermal correction to Gibbs Free Energy= *0.190613*

Sum of electronic and zero-point Energies= *-690.881979*

Sum of electronic and thermal Energies= *-690.870854*

Sum of electronic and thermal Enthalpies= *-690.869910*

Sum of electronic and thermal Free Energies= *-690.918637*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.090220	1.022417	-0.118126
2	6	0	-0.084305	2.102962	-0.180920
3	6	0	1.234585	1.855840	-0.017160
4	6	0	1.694787	0.483974	0.074550
5	6	0	0.873941	-0.589565	-0.014006
6	6	0	-0.578827	-0.449478	-0.034184
7	1	0	-0.433823	3.110462	-0.395812
8	1	0	1.975397	2.648851	-0.046959
9	6	0	1.715507	-1.830141	-0.102803
10	1	0	1.536801	-2.528079	0.725780
11	1	0	1.576774	-2.380494	-1.043081
12	6	0	3.094890	0.011757	0.069621
13	8	0	4.124756	0.636401	0.128836
14	8	0	3.069975	-1.367794	-0.031269
15	6	0	-2.329334	0.993434	-1.004701
16	1	0	-3.090321	1.727188	-0.715653
17	1	0	-2.041798	1.185681	-2.045592
18	6	0	-1.524495	-1.303657	-0.868292
19	1	0	-1.143793	-1.385012	-1.894002
20	1	0	-1.676503	-2.314361	-0.472958
21	6	0	-2.843483	-0.468919	-0.836395
22	1	0	-3.542029	-0.762101	-1.623551
23	6	0	-1.252732	0.221878	1.179683
24	6	0	-3.432863	-0.595537	0.548302
25	1	0	-4.447610	-0.949375	0.705438
26	6	0	-2.610944	-0.242551	1.545523
27	1	0	-0.580828	0.503302	1.984105
28	1	0	-2.889173	-0.279402	2.595190

single points:

mPW1PW91/6-31G(d)	*HF=-690.9687985*
MP2/6-31G(d)	*MP2=-688.9680522*
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d)	*HF=-691.1167996*
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d)	*HF=-690.9766015*

E (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 464.4113693

Zero-point correction=	*0.202187 (Hartree/Particle)*
Thermal correction to Energy=	*0.212025*
Thermal correction to Enthalpy=	*0.212970*
Thermal correction to Gibbs Free Energy=	*0.167162*
Sum of electronic and zero-point Energies=	*-464.209182*
Sum of electronic and thermal Energies=	*-464.199344*
Sum of electronic and thermal Enthalpies=	*-464.198400*
Sum of electronic and thermal Free Energies=	*-464.244207*

Center Number	*Atomic Number*	*Atomic Type*	*Coordinates (Angstroms) X*	*Y*	*Z*
1	6	0	0.024939	-0.355654	-0.156958
2	6	0	1.068643	-1.448000	-0.330903
3	6	0	2.380463	-1.258904	-0.118219
4	6	0	2.902792	0.058384	0.221393
5	6	0	2.093166	1.138662	0.211938
6	6	0	0.675403	1.049788	-0.132412
7	1	0	0.682550	-2.435254	-0.576353
8	1	0	3.074739	-2.091664	-0.201787
9	6	0	-0.669645	-0.635425	1.229351
10	1	0	-0.714794	-1.726681	1.377878
11	1	0	-0.026809	-0.251027	2.028359
12	6	0	-0.029352	2.172342	-0.367868
13	1	0	0.438565	3.149354	-0.272353
14	1	0	-1.071887	2.153035	-0.662422
15	6	0	-2.072682	-0.096096	1.346313
16	1	0	-2.452641	0.135972	2.338847
17	6	0	-1.005999	-0.455680	-1.274572
18	6	0	-2.855567	0.016676	0.262846
19	1	0	-3.888407	0.345819	0.348247
20	6	0	-2.322469	-0.288129	-1.067298
21	1	0	2.493775	2.130228	0.412671
22	1	0	3.960433	0.163325	0.448385
23	1	0	-0.619795	-0.625041	-2.277202
24	1	0	-3.013888	-0.335845	-1.905936

single points:

mPW1PW91/6-31G(d)	*HF=-464.3036296*
MP2/6-31G(d)	*MP2=-462.841102*
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d)	*HF=-464.4126948*
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d)	*HF=-464.3053464*

E (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 464.3638415
Zero-point correction= 0.201374 (Hartree/Particle)
Thermal correction to Energy= 0.210022
Thermal correction to Enthalpy= 0.210966
Thermal correction to Gibbs Free Energy= 0.168477
Sum of electronic and zero-point Energies= -464.162468
Sum of electronic and thermal Energies= -464.153819
Sum of electronic and thermal Enthalpies= -464.152875
Sum of electronic and thermal Free Energies= -464.195365

1 imaginary frequency (-560.8656 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.153120	-0.657381	-0.209106
2	6	0	-1.446844	-1.401364	-0.356072
3	6	0	-2.598716	-0.776797	-0.026857
4	6	0	-2.633031	0.635253	0.333851
5	6	0	-1.531788	1.421939	0.164857
6	6	0	-0.319377	0.841847	-0.359158
7	1	0	-1.437071	-2.432407	-0.702752
8	1	0	-3.543231	-1.314204	-0.079278
9	6	0	1.070578	-1.078631	-1.019704
10	1	0	1.394889	-2.090266	-0.738757
11	1	0	0.841083	-1.088992	-2.091421
12	6	0	0.720448	1.485651	-1.046906
13	1	0	0.929669	1.190538	-2.070706
14	1	0	0.938855	2.536450	-0.847264
15	6	0	2.179577	-0.068664	-0.704491
16	1	0	2.920629	0.105902	-1.481789
17	6	0	0.283054	-0.421866	1.244588
18	6	0	2.564483	0.068853	0.627807
19	1	0	3.525046	0.502759	0.891121
20	6	0	1.582271	-0.148999	1.609770
21	1	0	-1.593982	2.502169	0.282706
22	1	0	-3.576543	1.074920	0.644336
23	1	0	-0.511832	-0.410785	1.982548
24	1	0	1.807283	0.024862	2.659788

<u>single points:</u>
mPW1PW91/6-31G(d) HF=-464.2625482
MP2/6-31G(d) MP2=-462.8071252
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-464.36549
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-464.2645892

E (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 464.4298283
Zero-point correction= 0.205298 (Hartree/Particle)
Thermal correction to Energy= 0.213566
Thermal correction to Enthalpy= 0.214510
Thermal correction to Gibbs Free Energy= 0.172729
Sum of electronic and zero-point Energies= -464.224531
Sum of electronic and thermal Energies= -464.216262
Sum of electronic and thermal Enthalpies= -464.215318
Sum of electronic and thermal Free Energies= -464.257099

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.191964	0.776018	-0.067354
2	6	0	1.504386	1.441163	-0.066376
3	6	0	2.644035	0.729267	0.085652
4	6	0	2.643912	-0.729662	0.085391
5	6	0	1.504136	-1.441134	-0.067518
6	6	0	0.191983	-0.775716	-0.068600
7	1	0	1.539476	2.517590	-0.223553
8	1	0	3.603396	1.240324	0.111976
9	6	0	-0.967507	1.218207	-0.951212
10	1	0	-1.448779	2.144875	-0.617210
11	1	0	-0.611651	1.364197	-1.978724
12	6	0	-0.967331	-1.216792	-0.953021
13	1	0	-0.611572	-1.361044	-1.980832
14	1	0	-1.448436	-2.144116	-0.620576
15	6	0	-1.940440	0.000589	-0.875057
16	1	0	-2.679217	0.001120	-1.680425
17	6	0	-0.254748	-0.000492	1.182095
18	6	0	-2.569386	-0.000506	0.498271
19	1	0	-3.647425	-0.000946	0.632091
20	6	0	-1.697150	-0.001009	1.515457
21	1	0	1.538590	-2.517557	-0.224618
22	1	0	3.603147	-1.240807	0.112244
23	1	0	0.455499	-0.001349	2.002685
24	1	0	-1.996139	-0.001883	2.560583

<u>single points:</u>
mPW1PW91/6-31G(d) HF=-464.3388385
MP2/6-31G(d) MP2=-462.8786493
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-464.4313547
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-464.3407067

F (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 310.8084137
Zero-point correction= 0.155968 (Hartree/Particle)
Thermal correction to Energy= 0.163329
Thermal correction to Enthalpy= 0.164273
Thermal correction to Gibbs Free Energy= 0.124341
Sum of electronic and zero-point Energies= -310.652446

Sum of electronic and thermal Energies= -310.645085
Sum of electronic and thermal Enthalpies= -310.644141
Sum of electronic and thermal Free Energies= -310.684073

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.573615	0.396831	0.825345
2	6	0	1.778869	0.435822	-0.101708
3	6	0	-0.508615	1.427688	0.396546
4	1	0	-1.099446	1.713704	1.282530
5	1	0	-0.024892	2.348102	0.046482
6	6	0	2.205676	-0.537757	-0.905392
7	1	0	3.081058	-0.405000	-1.535596
8	1	0	1.696852	-1.495734	-0.966208
9	6	0	-1.453515	0.887832	-0.649314
10	1	0	-1.941054	1.590601	-1.321355
11	6	0	-0.024279	-0.988560	0.955772
12	6	0	-1.735249	-0.423466	-0.700207
13	1	0	-2.452916	-0.813027	-1.418431
14	6	0	-1.088550	-1.359581	0.224754
15	1	0	0.475286	-1.698469	1.611293
16	1	0	-1.481249	-2.371706	0.297093
17	1	0	2.321755	1.383399	-0.084325
18	1	0	0.936886	0.715279	1.813752

single points:
mPW1PW91/6-31G(d) *HF=-310.7335099*
MP2/6-31G(d) *MP2=-309.7221402*
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-310.8090596*
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-310.7351753*

F (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 310.7608456
Zero-point correction= 0.155845 (Hartree/Particle)
Thermal correction to Energy= 0.161754
Thermal correction to Enthalpy= 0.162699
Thermal correction to Gibbs Free Energy= 0.126398
Sum of electronic and zero-point Energies= -310.605000
Sum of electronic and thermal Energies= -310.599091
Sum of electronic and thermal Enthalpies= -310.598147
Sum of electronic and thermal Free Energies= -310.63444

1 imaginary frequency (-579.0593 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.675962	0.889687	0.722592
2	6	0	-1.238804	0.686736	-0.652066
3	6	0	-0.436184	-0.492090	1.329762

4	1	0	0.223731	-0.420608	2.204598
5	1	0	-1.378946	-0.943924	1.659012
6	6	0	-1.289102	-0.647701	-1.069690
7	1	0	-1.888510	-1.352468	-0.498428
8	1	0	-1.249641	-0.886795	-2.133443
9	6	0	0.226374	-1.332396	0.231613
10	1	0	0.072932	-2.409041	0.274827
11	6	0	0.586698	1.381345	0.057551
12	6	0	1.441262	-0.852971	-0.271945
13	1	0	2.146167	-1.519477	-0.761538
14	6	0	1.617693	0.533663	-0.322583
15	1	0	0.647301	2.444092	-0.163509
16	1	0	2.500433	0.958726	-0.794993
17	1	0	-1.149431	1.606566	1.398731
18	1	0	-1.315883	1.525302	-1.336651

single points:

mPW1PW91/6-31G(d) *HF=-310.6928677*

MP2/6-31G(d) *MP2=-309.6863852*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-310.7624253*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-310.6947782*

F (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 310.8252183

Zero-point correction= 0.159639 (Hartree/Particle)

Thermal correction to Energy= 0.165115

Thermal correction to Enthalpy= 0.166059

Thermal correction to Gibbs Free Energy= 0.130604

Sum of electronic and zero-point Energies= -310.665579

Sum of electronic and thermal Energies= -310.660104

Sum of electronic and thermal Enthalpies= -310.659160

Sum of electronic and thermal Free Energies= -310.694614

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.108851	0.419438	-0.753051
2	6	0	1.108915	0.419564	0.752886
3	6	0	0.425086	-0.858922	-1.208679
4	1	0	-0.136656	-0.749239	-2.143433
5	1	0	1.169929	-1.653930	-1.345046
6	6	0	0.425196	-0.858726	1.208781
7	1	0	1.170052	-1.653711	1.345215
8	1	0	-0.136463	-0.748889	2.143567
9	6	0	-0.506630	-1.184030	0.000120
10	1	0	-0.858255	-2.219044	0.000220
11	6	0	0.189611	1.390416	-0.000124
12	6	0	-1.637400	-0.183206	0.000089
13	1	0	-2.675856	-0.503479	0.000159
14	6	0	-1.265460	1.105004	-0.000035
15	1	0	0.497846	2.432150	-0.000229
16	1	0	-1.975589	1.928353	-0.000076

17	1	0	1.928051	0.835392	1.332768
18	1	0	1.927937	0.835169	-1.333071

---

single points:

mPW1PW91/6-31G(d) *HF=-310.7668404*

MP2/6-31G(d) *MP2=-309.7559829*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-310.825974*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-310.7678079*

G (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 994.1852721

Zero-point correction= *0.269481 (Hartree/Particle)*

Thermal correction to Energy= *0.288866*

Thermal correction to Enthalpy= *0.289810*

Thermal correction to Gibbs Free Energy= *0.219624*

Sum of electronic and zero-point Energies= *-993.915791*

Sum of electronic and thermal Energies= *-993.896406*

Sum of electronic and thermal Enthalpies= *-993.895462*

Sum of electronic and thermal Free Energies= *-993.965648*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.786989	0.201812	0.633769
2	6	0	-0.037047	-0.729108	1.582674
3	6	0	1.288777	-0.935156	1.550969
4	6	0	2.063285	-0.293393	0.510348
5	6	0	1.501923	0.439080	-0.478222
6	6	0	0.069510	0.646940	-0.587878
7	1	0	-0.645705	-1.185059	2.360205
8	1	0	1.794154	-1.563904	2.277343
9	6	0	2.594737	0.912556	-1.397563
10	1	0	2.499340	0.527447	-2.419659
11	1	0	2.675500	2.004871	-1.444905
12	6	0	3.521134	-0.339547	0.304464
13	8	0	4.377274	-0.891329	0.957017
14	8	0	3.807312	0.389420	-0.827379
15	6	0	-1.191469	1.472571	1.487756
16	1	0	-1.355587	1.146480	2.526729
17	1	0	-0.332556	2.150852	1.523568
18	6	0	-0.470721	1.228266	-1.676254
19	1	0	0.151313	1.583110	-2.493327
20	1	0	-1.539265	1.369489	-1.787367
21	6	0	-2.439732	2.201104	1.039132
22	1	0	-2.534731	3.246564	1.322090
23	6	0	-2.057453	-0.464610	0.148078
24	6	0	-3.436403	1.567548	0.401358
25	1	0	-4.370005	2.052973	0.134809
26	6	0	-3.236735	0.171823	0.043645
27	6	0	-4.228519	-0.759026	-0.548368
28	8	0	-5.388121	-0.575444	-0.817961
29	8	0	-3.587357	-1.958686	-0.773044

30	6	0	-2.213625	-1.863926	-0.373608
31	1	0	-2.011855	-2.634968	0.380686
32	1	0	-1.574859	-2.067856	-1.242771
33	1	0	6.341752	0.183205	-1.127632
34	1	0	6.276463	-0.651040	0.124088
35	8	0	6.913643	-0.326930	-0.535590

single points:

mPW1PW91/6-31G(d) *HF=-993.9570415*

MP2/6-31G(d) *MP2=-991.2247512*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-994.1997913*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-993.9720388*

G (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 994.1401024

Zero-point correction= *0.268904 (Hartree/Particle)*

Thermal correction to Energy= *0.287002*

Thermal correction to Enthalpy= *0.287946*

Thermal correction to Gibbs Free Energy= *0.221871*

Sum of electronic and zero-point Energies= *-993.871199*

Sum of electronic and thermal Energies= *-993.853101*

Sum of electronic and thermal Enthalpies= *-993.852156*

Sum of electronic and thermal Free Energies= *-993.918232*

1 imaginary frequency (-524.3309 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.048790	-1.217515	0.753136
2	6	0	0.121622	-1.432709	1.921797
3	6	0	-1.144400	-0.964347	1.856142
4	6	0	-1.639001	-0.408621	0.613125
5	6	0	-0.950054	-0.517128	-0.570350
6	6	0	0.317802	-1.155913	-0.595442
7	1	0	0.493634	-1.936258	2.810251
8	1	0	-1.831671	-1.051606	2.692656
9	6	0	-1.860138	-0.071734	-1.684304
10	1	0	-1.469999	0.792595	-2.234995
11	1	0	-2.086406	-0.867444	-2.403233
12	6	0	-2.983966	0.098797	0.330636
13	8	0	-3.910019	0.314940	1.081439
14	8	0	-3.079898	0.317168	-1.030909
15	6	0	2.266912	-2.127191	0.545322
16	1	0	2.983669	-2.020964	1.370531
17	1	0	1.960139	-3.177702	0.506710
18	6	0	0.991225	-1.754221	-1.671715
19	1	0	1.215574	-2.815334	-1.624660
20	1	0	0.841982	-1.391211	-2.689397
21	6	0	2.933765	-1.706449	-0.775652
22	1	0	3.476757	-2.477750	-1.316825
23	6	0	1.552417	0.216512	0.614714

24	6	0	3.339923	-0.381606	-0.924716
25	1	0	4.064088	-0.070034	-1.670454
26	6	0	2.636373	0.559135	-0.158975
27	6	0	2.797550	2.034321	-0.120269
28	8	0	3.608879	2.731225	-0.673787
29	8	0	1.814287	2.534028	0.700843
30	6	0	0.994927	1.470556	1.215879
31	1	0	1.064214	1.467792	2.311483
32	1	0	-0.051369	1.664967	0.951313
33	1	0	-5.652724	0.754340	0.046489
34	1	0	-5.506932	0.926140	-1.440433
35	8	0	-6.188676	0.896530	-0.753261

single points:

mPW1PW91/6-31G(d) HF=-993.9180938

MP2/6-31G(d) MP2=-991.1943837

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-994.1560869

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-993.9345996

G (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 994.1977877

Zero-point correction= 0.272395 (Hartree/Particle)

Thermal correction to Energy= 0.290314

Thermal correction to Enthalpy= 0.291258

Thermal correction to Gibbs Free Energy= 0.225180

Sum of electronic and zero-point Energies= -993.925393

Sum of electronic and thermal Energies= -993.907474

Sum of electronic and thermal Enthalpies= -993.906530

Sum of electronic and thermal Free Energies= -993.972608

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.989002	-1.050064	0.940431
2	6	0	0.073866	-1.009866	2.097433
3	6	0	-1.191295	-0.541921	1.989032
4	6	0	-1.714962	-0.214228	0.679513
5	6	0	-1.011628	-0.361768	-0.471447
6	6	0	0.405886	-0.700175	-0.469299
7	1	0	0.436526	-1.399912	3.045507
8	1	0	-1.861548	-0.498810	2.841689
9	6	0	-1.938790	-0.150995	-1.634009
10	1	0	-1.645675	0.691713	-2.272596
11	1	0	-2.048398	-1.038826	-2.269680
12	6	0	-3.111351	0.112998	0.335836
13	8	0	-4.059205	0.319055	1.058140
14	8	0	-3.210820	0.148869	-1.038032
15	6	0	1.998813	-2.172935	0.717125
16	1	0	2.852717	-2.135280	1.402369
17	1	0	1.500611	-3.141640	0.839343
18	6	0	1.086634	-1.619344	-1.478861
19	1	0	0.484108	-2.525034	-1.616405

20	1	0	1.251605	-1.159913	-2.459604
21	6	0	2.436143	-1.974940	-0.770361
22	1	0	2.905323	-2.865951	-1.191783
23	6	0	1.387323	0.251020	0.241940
24	6	0	3.323504	-0.755642	-0.837090
25	1	0	4.320947	-0.761569	-1.265536
26	6	0	2.747527	0.335149	-0.317269
27	6	0	3.228571	1.727592	-0.177464
28	8	0	4.281240	2.211020	-0.508524
29	8	0	2.234637	2.455742	0.426030
30	6	0	1.070010	1.658260	0.735548
31	1	0	0.904593	1.699611	1.816313
32	1	0	0.208477	2.110192	0.234575
33	1	0	-5.649911	0.752084	-1.509827
34	1	0	-5.793353	0.763081	-0.011451
35	8	0	-6.313543	0.904238	-0.821272

single points:

mPW1PW91/6-31G(d) *HF=-993.9859012*

MP2/6-31G(d) *MP2=-991.2578599*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-994.2130082*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-994.0015564*

H (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1257.564214

Zero-point correction= *0.340169 (Hartree/Particle)*

Thermal correction to Energy= *0.366792*

Thermal correction to Enthalpy= *0.367736*

Thermal correction to Gibbs Free Energy= *0.274334*

Sum of electronic and zero-point Energies= *-1257.224045*

Sum of electronic and thermal Energies= *-1257.197422*

Sum of electronic and thermal Enthalpies= *-1257.196478*

Sum of electronic and thermal Free Energies= *-1257.289880*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.003654	0.139480	0.430817
2	6	0	1.041032	1.244054	0.008219
3	6	0	-0.279070	1.077344	-0.169883
4	6	0	-0.829837	-0.255795	-0.026161
5	6	0	-0.058992	-1.348321	0.194227
6	6	0	1.386001	-1.283480	0.307728
7	1	0	1.481382	2.234764	-0.077338
8	1	0	-0.935416	1.907622	-0.413375
9	6	0	-0.948805	-2.558366	0.242784
10	1	0	-0.741419	-3.286381	-0.549618
11	1	0	-0.924342	-3.077129	1.207746
12	6	0	-2.231830	-0.689532	-0.122433
13	8	0	-3.245255	-0.039513	-0.312160
14	8	0	-2.278199	-2.042021	0.040937
15	6	0	2.368161	0.427695	1.944563

16	1	0	2.365695	1.518967	2.091481
17	1	0	1.559445	0.041940	2.574065
18	6	0	2.131780	-2.404866	0.342437
19	6	0	3.712343	-0.090256	2.407030
20	1	0	3.835696	-0.277655	3.470765
21	6	0	3.281032	0.213979	-0.380261
22	6	0	4.745091	-0.222214	1.559767
23	1	0	5.738314	-0.520423	1.880372
24	6	0	4.504073	0.037417	0.148990
25	6	0	5.506052	0.081982	-0.944596
26	8	0	6.702087	-0.049377	-0.895001
27	8	0	4.823424	0.303282	-2.121768
28	6	0	3.415841	0.390763	-1.865592
29	1	0	3.052037	1.362286	-2.223517
30	1	0	2.900692	-0.392863	-2.436469
31	1	0	-4.999255	-1.145487	-0.312262
32	7	0	-5.812567	-1.752200	-0.301285
33	1	0	-3.474437	1.972308	-0.542967
34	7	0	-3.407076	2.983832	-0.613264
35	6	0	-3.483850	3.768671	0.499659
36	1	0	-3.598989	3.420482	-1.506309
37	8	0	-3.596792	4.980453	0.501118
38	1	0	-3.402169	3.171965	1.430957
39	1	0	-5.675074	-2.753594	-0.283641
40	6	0	-7.081852	-1.273471	-0.269854
41	1	0	-7.104985	-0.164385	-0.280385
42	8	0	-8.094168	-1.952357	-0.236359
43	1	0	3.213348	-2.378573	0.399442
44	1	0	1.673269	-3.389514	0.314108

single points:

mPW1PW91/6-31G(d) *HF=-1257.2672984*

MP2/6-31G(d) *MP2=-1253.8299538*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-1257.5861869*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-1257.2889169*

H (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1257.520134

Zero-point correction= 0.339470 (Hartree/Particle)

Thermal correction to Energy= 0.364840

Thermal correction to Enthalpy= 0.365784

Thermal correction to Gibbs Free Energy= 0.276775

Sum of electronic and zero-point Energies= -1257.180664

Sum of electronic and thermal Energies= -1257.155294

Sum of electronic and thermal Enthalpies= -1257.154350

Sum of electronic and thermal Free Energies= -1257.243359

1 imaginary frequency (-515.4470 cm^{-1})

Standard orientation:

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

1	6	0	-2.211452	1.127307	-0.638882
2	6	0	-1.087230	2.079964	-0.323534
3	6	0	0.156761	1.595383	-0.114084
4	6	0	0.425921	0.190313	-0.356957
5	6	0	-0.478811	-0.634462	-0.989345
6	6	0	-1.742409	-0.130121	-1.386238
7	1	0	-1.298594	3.142626	-0.238918
8	1	0	0.978896	2.245395	0.172686
9	6	0	0.213415	-1.931313	-1.309550
10	1	0	-0.250349	-2.797888	-0.824143
11	1	0	0.289349	-2.133100	-2.383592
12	6	0	1.693777	-0.525669	-0.245156
13	8	0	2.767026	-0.174473	0.221574
14	8	0	1.543674	-1.776197	-0.782015
15	6	0	-3.470936	1.618343	-1.364392
16	1	0	-4.017481	2.349928	-0.754466
17	1	0	-3.205986	2.107121	-2.307645
18	6	0	-2.620376	-0.610477	-2.370076
19	1	0	-2.865714	0.028774	-3.212361
20	1	0	-2.656179	-1.673487	-2.611672
21	6	0	-4.362163	0.391129	-1.618489
22	1	0	-5.019299	0.432340	-2.483897
23	6	0	-2.691835	0.318295	0.562150
24	6	0	-4.744414	-0.393918	-0.532682
25	1	0	-5.583756	-1.080724	-0.572411
26	6	0	-3.886478	-0.360972	0.576889
27	6	0	-3.996163	-1.098936	1.860762
28	8	0	-4.872040	-1.824850	2.254367
29	8	0	-2.867529	-0.815728	2.594111
30	6	0	-2.000872	0.072188	1.868698
31	1	0	-1.874286	0.997175	2.446315
32	1	0	-1.013109	-0.393801	1.769799
33	1	0	4.239676	-1.600068	0.067662
34	7	0	4.903847	-2.359145	-0.049818
35	1	0	3.345384	1.647181	0.856096
36	7	0	3.499888	2.627180	1.079985
37	6	0	4.045145	3.478814	0.165791
38	1	0	3.536560	2.902445	2.053515
39	8	0	4.425151	4.612313	0.396690
40	1	0	4.082825	3.027411	-0.846412
41	1	0	4.565222	-3.257875	-0.365410
42	6	0	6.233229	-2.211388	0.173776
43	1	0	6.483554	-1.183439	0.507704
44	8	0	7.077028	-3.081457	0.035762

single points:

mPW1PW91/6-31G(d)	*HF=-1257.2292659*
MP2/6-31G(d)	*MP2=-1253.8000369*
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d)	*HF=-1257.5432488*
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d)	*HF=-1257.2521825*

H (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1257.5768864
Zero-point correction= 0.343072 (Hartree/Particle)
Thermal correction to Energy= 0.368260
Thermal correction to Enthalpy= 0.369204
Thermal correction to Gibbs Free Energy= 0.279923
Sum of electronic and zero-point Energies= -1257.233814
Sum of electronic and thermal Energies= -1257.208626
Sum of electronic and thermal Enthalpies= -1257.207682
Sum of electronic and thermal Free Energies= -1257.296963

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.130195	1.026424	-0.702780
2	6	0	-1.027142	1.940658	-0.350925
3	6	0	0.203849	1.486127	-0.019649
4	6	0	0.495334	0.073004	-0.162791
5	6	0	-0.402132	-0.837404	-0.625886
6	6	0	-1.798418	-0.496497	-0.855721
7	1	0	-1.220985	3.009734	-0.393623
8	1	0	1.005468	2.164810	0.255774
9	6	0	0.304882	-2.139868	-0.856841
10	1	0	-0.087256	-2.961316	-0.245174
11	1	0	0.301673	-2.460939	-1.905679
12	6	0	1.803000	-0.594394	-0.056652
13	8	0	2.882313	-0.159766	0.305765
14	8	0	1.665502	-1.890834	-0.461129
15	6	0	-3.168103	1.345099	-1.775354
16	1	0	-3.889703	2.110445	-1.469819
17	1	0	-2.661201	1.691432	-2.683298
18	6	0	-2.649554	-1.030959	-2.003359
19	1	0	-2.085996	-0.966359	-2.941685
20	1	0	-2.980787	-2.066324	-1.867914
21	6	0	-3.856254	-0.034744	-2.032973
22	1	0	-4.395967	-0.063861	-2.981209
23	6	0	-2.635435	0.021104	0.331087
24	6	0	-4.735118	-0.345963	-0.845672
25	1	0	-5.791863	-0.581010	-0.926140
26	6	0	-4.071693	-0.308325	0.316238
27	6	0	-4.513290	-0.550721	1.707719
28	8	0	-5.603718	-0.846930	2.124218
29	8	0	-3.425326	-0.383107	2.527718
30	6	0	-2.230469	-0.023774	1.800754
31	1	0	-1.881381	0.944710	2.171393
32	1	0	-1.465140	-0.775440	2.017619
33	1	0	4.429385	-1.534605	0.200140
34	7	0	5.124845	-2.268677	0.114446
35	6	0	6.451694	-2.044528	0.288045
36	1	0	4.821362	-3.202786	-0.124917
37	8	0	7.330878	-2.883512	0.187144
38	1	0	6.661723	-0.984888	0.540514
39	1	0	3.437477	1.743512	0.775407
40	7	0	3.555410	2.744060	0.907904
41	6	0	3.979102	3.541088	-0.114318
42	1	0	3.652712	3.100705	1.850339
43	8	0	4.313801	4.706427	-0.007086
44	1	0	3.960725	3.008319	-1.086754

---

single points:

mPW1PW91/6-31G(d) *HF=-1257.9254989*

MP2/6-31G(d) *MP2=-1253.8619992*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-1257.5985548*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-1257.3178123*

I (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1123.5670591

Zero-point correction= 0.335916 (Hartree/Particle)

Thermal correction to Energy= 0.358461

Thermal correction to Enthalpy= 0.359405

Thermal correction to Gibbs Free Energy= 0.282258

Sum of electronic and zero-point Energies= -1123.231143

Sum of electronic and thermal Energies= -1123.208598

Sum of electronic and thermal Enthalpies= -1123.207654

Sum of electronic and thermal Free Energies= -1123.284801

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.878836	-0.093146	0.691860
2	6	0	-1.143357	-1.327538	1.198546
3	6	0	0.185961	-1.504916	1.139533
4	6	0	0.985560	-0.487806	0.488889
5	6	0	0.443700	0.595422	-0.125607
6	6	0	-0.984272	0.830387	-0.185521
7	1	0	-1.769015	-2.069502	1.688597
8	1	0	0.670954	-2.380161	1.559107
9	6	0	1.548460	1.413707	-0.732303
10	1	0	1.493513	1.485590	-1.823682
11	1	0	1.626419	2.422188	-0.312725
12	6	0	2.433439	-0.440461	0.329256
13	8	0	3.299175	-1.205488	0.716665
14	8	0	2.758395	0.688711	-0.390761
15	6	0	-2.353823	0.697893	1.979480
16	1	0	-2.589031	-0.040026	2.761917
17	1	0	-1.507546	1.277991	2.362520
18	6	0	-1.490453	1.823647	-0.944060
19	1	0	-2.556093	1.997551	-1.030644
20	1	0	-0.846560	2.496427	-1.504345
21	6	0	-3.575268	1.572079	1.796755
22	1	0	-3.694912	2.409885	2.478700
23	6	0	-3.114196	-0.499701	-0.088191
24	6	0	-4.525955	1.271627	0.897667
25	1	0	-5.447258	1.837016	0.800142
26	6	0	-4.291346	0.140354	0.014516
27	6	0	-5.241832	-0.454796	-0.961007
28	8	0	-6.382323	-0.155664	-1.195980
29	8	0	-4.575990	-1.469037	-1.616959
30	6	0	-3.230448	-1.567554	-1.139319
31	1	0	-3.067914	-2.581045	-0.750555

32	1	0	-2.541464	-1.415974	-1.980998
33	7	0	5.732131	0.809088	-0.964813
34	1	0	6.045498	1.315710	-1.780139
35	6	0	6.570259	-0.007768	-0.313879
36	7	0	6.091837	-0.913590	0.532190
37	7	0	7.893839	0.100998	-0.524968
38	1	0	5.075647	-1.067424	0.618156
39	1	0	6.707037	-1.406731	1.163709
40	1	0	8.285295	0.899136	-1.003541
41	1	0	8.542363	-0.569808	-0.139344
42	1	0	4.728796	0.776970	-0.787147

single points:

mPW1PW91/6-31G(d) HF=-1123.3094436

MP2/6-31G(d) MP2=-1120.1802122

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=-1123.630404

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=-1123.3734017

I (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1123.5280221

Zero-point correction= 0.335145 (Hartree/Particle)

Thermal correction to Energy= 0.356453

Thermal correction to Enthalpy= 0.357397

Thermal correction to Gibbs Free Energy= 0.283955

Sum of electronic and zero-point Energies= -1123.192877

Sum of electronic and thermal Energies= -1123.171569

Sum of electronic and thermal Enthalpies= -1123.170625

Sum of electronic and thermal Free Energies= -1123.244067

1 imaginary frequency (-487.6012 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.249018	-1.273277	-0.472753
2	6	0	-1.452488	-1.901403	-1.588972
3	6	0	-0.125865	-1.661591	-1.672370
4	6	0	0.540314	-0.954178	-0.595413
5	6	0	-0.079495	-0.709699	0.618387
6	6	0	-1.421985	-1.093167	0.816915
7	1	0	-1.962383	-2.513911	-2.327426
8	1	0	0.473276	-2.048136	-2.491318
9	6	0	0.959930	-0.224020	1.592627
10	1	0	0.756253	0.783056	1.972878
11	1	0	1.118644	-0.898491	2.440100
12	6	0	1.942205	-0.637884	-0.470482
13	8	0	2.860436	-0.718026	-1.274071
14	8	0	2.183328	-0.175269	0.816581
15	6	0	-3.592741	-1.876425	-0.042873
16	1	0	-4.332491	-1.809524	-0.851760
17	1	0	-3.478825	-2.935050	0.211415
18	6	0	-2.113078	-1.309417	2.018490

19	1	0	-2.546517	-2.285203	2.212604
20	1	0	-1.842800	-0.767686	2.925478
21	6	0	-4.088708	-1.075490	1.170309
22	1	0	-4.728063	-1.595492	1.879286
23	6	0	-2.484040	0.222156	-0.653857
24	6	0	-4.199948	0.307800	1.066701
25	1	0	-4.788544	0.899750	1.760546
26	6	0	-3.406969	0.921473	0.081805
27	6	0	-3.296233	2.363635	-0.261589
28	8	0	-3.895666	3.304347	0.185468
29	8	0	-2.325381	2.476569	-1.231808
30	6	0	-1.775293	1.190471	-1.551788
31	1	0	-1.960873	0.973909	-2.612029
32	1	0	-0.688727	1.219447	-1.405739
33	7	0	4.968247	0.866843	1.150393
34	1	0	5.131536	1.631507	1.789330
35	6	0	5.893142	0.545275	0.236744
36	7	0	5.558354	-0.191449	-0.815672
37	7	0	7.157944	0.974970	0.401929
38	1	0	4.565524	-0.406105	-1.014686
39	1	0	6.268096	-0.593243	-1.411565
40	1	0	7.476507	1.332538	1.290652
41	1	0	7.852540	0.844028	-0.318761
42	1	0	4.014915	0.509543	1.073803

single points:

mPW1PW91/6-31G(d) *HF=-1123.2762271*

MP2/6-31G(d) *MP2=-1120.1536746*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-1123.5887571*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-1123.3376581*

I (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1123.5808366

Zero-point correction= 0.338709 (Hartree/Particle)

Thermal correction to Energy= 0.359831

Thermal correction to Enthalpy= 0.360775

Thermal correction to Gibbs Free Energy= 0.287531

Sum of electronic and zero-point Energies= -1123.242127

Sum of electronic and thermal Energies= -1123.221006

Sum of electronic and thermal Enthalpies= -1123.220062

Sum of electronic and thermal Free Energies= -1123.293306

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.150092	-1.263463	-0.595441
2	6	0	-1.319083	-1.673370	-1.742912
3	6	0	-0.013019	-1.333249	-1.842948
4	6	0	0.636051	-0.698059	-0.714240
5	6	0	0.009280	-0.435671	0.468158
6	6	0	-1.423013	-0.588919	0.629909
7	1	0	-1.782444	-2.290608	-2.508619

8	1	0	0.587506	-1.618415	-2.700379
9	6	0	1.028865	-0.010322	1.482307
10	1	0	0.865919	1.004272	1.863237
11	1	0	1.118372	-0.694861	2.333647
12	6	0	2.060692	-0.437915	-0.543703
13	8	0	2.986145	-0.540132	-1.329693
14	8	0	2.282488	-0.023644	0.754051
15	6	0	-3.246309	-2.142789	0.000775
16	1	0	-4.140631	-2.203602	-0.628231
17	1	0	-2.862451	-3.157711	0.153698
18	6	0	-2.119079	-1.083071	1.894176
19	1	0	-1.607066	-1.975139	2.273958
20	1	0	-2.165531	-0.339418	2.697014
21	6	0	-3.546561	-1.464473	1.375724
22	1	0	-4.072853	-2.128160	2.063399
23	6	0	-2.353743	0.215771	-0.309128
24	6	0	-4.289781	-0.176653	1.115129
25	1	0	-5.239336	0.071936	1.578706
26	6	0	-3.644668	0.634359	0.268619
27	6	0	-3.967046	1.989511	-0.233648
28	8	0	-4.915639	2.687724	0.005962
29	8	0	-2.945433	2.379875	-1.067935
30	6	0	-1.933670	1.366563	-1.219954
31	1	0	-1.895673	1.070347	-2.272897
32	1	0	-0.969655	1.808439	-0.949255
33	7	0	5.154009	0.823458	1.186637
34	1	0	5.348654	1.525771	1.885601
35	6	0	6.077062	0.512314	0.267473
36	7	0	5.722817	-0.136473	-0.836192
37	7	0	7.358919	0.860957	0.477055
38	1	0	4.727250	-0.296283	-1.056055
39	1	0	6.420443	-0.537433	-1.446896
40	1	0	7.678879	1.160725	1.386509
41	1	0	8.056870	0.747257	-0.243497
42	1	0	4.185741	0.523318	1.076711

---

single points:

mPW1PW91/6-31G(d) *HF=-1123.3397131*

MP2/6-31G(d) *MP2=-1120.2146733*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-1123.6443248*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-1123.4036849*

J (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)
(this structure only converged using the GDIIS procedure)

HF=- 1144.3997205
Zero-point correction= 0.331991 (Hartree/Particle)
Thermal correction to Energy= 0.353118
Thermal correction to Enthalpy= 0.354063
Thermal correction to Gibbs Free Energy= 0.278267
Sum of electronic and zero-point Energies= -1144.067729
Sum of electronic and thermal Energies= -1144.046602
Sum of electronic and thermal Enthalpies= -1144.045658
Sum of electronic and thermal Free Energies= -1144.121453

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.097309	0.026930	0.700756
2	6	0	-1.322188	-1.099351	1.373848
3	6	0	0.011280	-1.247077	1.327494
4	6	0	0.777683	-0.311194	0.531313
5	6	0	0.202354	0.662943	-0.220868
6	6	0	-1.231553	0.851250	-0.296561
7	1	0	-1.923994	-1.780916	1.970024
8	1	0	0.523048	-2.039963	1.862981
9	6	0	1.284676	1.412278	-0.945029
10	1	0	1.220902	1.332761	-2.035392
11	1	0	1.343214	2.470711	-0.669966
12	6	0	2.220233	-0.245965	0.340423
13	8	0	3.106555	-0.941912	0.823691
14	8	0	2.514832	0.770322	-0.522525
15	6	0	-2.608364	0.970623	1.866079
16	1	0	-2.814104	0.341109	2.745586
17	1	0	-1.787703	1.633303	2.160793
18	6	0	-1.768378	1.723307	-1.173920
19	1	0	-1.145101	2.331266	-1.824153
20	1	0	-2.838649	1.859388	-1.270810
21	6	0	-3.864850	1.759429	1.567880
22	1	0	-4.022446	2.675549	2.131067
23	6	0	-3.311280	-0.528747	-0.018861
24	6	0	-4.798120	1.301075	0.718529
25	1	0	-5.741663	1.809370	0.547098
26	6	0	-4.513061	0.072194	-0.004617
27	6	0	-5.433057	-0.685518	-0.892489
28	8	0	-6.582888	-0.466127	-1.166772
29	8	0	-4.723956	-1.751513	-1.405584
30	6	0	-3.378716	-1.731807	-0.917180
31	1	0	-3.179213	-2.676723	-0.395586
32	1	0	-2.690926	-1.667615	-1.770941
33	1	0	4.670108	-0.654376	0.411369
34	7	0	5.653795	-0.419227	0.108514
35	6	0	6.817837	-1.062975	0.473917
36	6	0	5.943061	0.584277	-0.713651
37	6	0	7.846136	-0.420882	-0.153098
38	1	0	6.817931	-1.911600	1.139723
39	1	0	5.224892	1.257208	-1.156321
40	1	0	8.910199	-0.596639	-0.142854
41	1	0	7.772876	1.265075	-1.467095
42	7	0	7.272775	0.602256	-0.887055

single points:

mPW1PW91/6-31G(d) *HF=-1144.1395404*

MP2/6-31G(d) *MP2=-1140.9508418*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-1144.4593134*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-1144.1997016*

J (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1144.3606385
Zero-point correction= 0.331135 (Hartree/Particle)
Thermal correction to Energy= 0.351036
Thermal correction to Enthalpy= 0.351980
Thermal correction to Gibbs Free Energy= 0.280327
Sum of electronic and zero-point Energies= -1144.029503
Sum of electronic and thermal Energies= -1144.009602
Sum of electronic and thermal Enthalpies= -1144.008658
Sum of electronic and thermal Free Energies= -1144.080311

1 imaginary frequency (-487.7723 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.449037	-1.228582	-0.564916
2	6	0	-1.627618	-1.780669	-1.703372
3	6	0	-0.298563	-1.541923	-1.737932
4	6	0	0.342731	-0.915939	-0.597390
5	6	0	-0.305727	-0.755272	0.616064
6	6	0	-1.653717	-1.145179	0.754250
7	1	0	-2.121442	-2.336437	-2.495688
8	1	0	0.318834	-1.872621	-2.567678
9	6	0	0.715386	-0.342235	1.641279
10	1	0	0.507519	0.637278	2.085894
11	1	0	0.854419	-1.072951	2.444574
12	6	0	1.738186	-0.608752	-0.407705
13	8	0	2.674340	-0.633078	-1.207060
14	8	0	1.956719	-0.244966	0.900108
15	6	0	-3.806927	-1.850693	-0.211548
16	1	0	-4.525918	-1.720706	-1.031399
17	1	0	-3.706007	-2.925605	-0.030526
18	6	0	-2.375369	-1.440972	1.920251
19	1	0	-2.818594	-2.424948	2.034306
20	1	0	-2.124223	-0.966692	2.869517
21	6	0	-4.327708	-1.133587	1.042749
22	1	0	-4.987355	-1.697347	1.697662
23	6	0	-2.672319	0.277585	-0.646604
24	6	0	-4.428715	0.254275	1.034438
25	1	0	-5.031162	0.800020	1.753786
26	6	0	-3.608936	0.929992	0.114200
27	6	0	-3.484921	2.391675	-0.126899
28	8	0	-4.091145	3.302690	0.369734
29	8	0	-2.491929	2.565409	-1.065204
30	6	0	-1.939659	1.301331	-1.459992
31	1	0	-2.102792	1.158527	-2.536350
32	1	0	-0.856441	1.314920	-1.289048
33	7	0	5.065631	0.107047	-0.281328
34	6	0	5.219332	0.507252	0.976007
35	6	0	6.278595	0.174912	-0.934044
36	1	0	4.131297	-0.204007	-0.682099
37	1	0	4.434146	0.556676	1.714576
38	6	0	7.196627	0.633067	-0.033778
39	1	0	6.386937	-0.104043	-1.970321
40	1	0	6.909960	1.171909	2.016186

41	1	0	8.252680	0.830812	-0.127467
42	7	0	6.509285	0.832533	1.150344

---

single points:

mPW1PW91/6-31G(d) *HF=-1144.106304*

MP2/6-31G(d) *MP2=-1140.9243487*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-1144.4176427*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-1144.1639114*

J (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1144.4135392

Zero-point correction= *0.334816 (Hartree/Particle)*

Thermal correction to Energy= *0.354513*

Thermal correction to Enthalpy= *0.355457*

Thermal correction to Gibbs Free Energy= *0.283908*

Sum of electronic and zero-point Energies= *-1144.078724*

Sum of electronic and thermal Energies= *-1144.059026*

Sum of electronic and thermal Enthalpies= *-1144.058082*

Sum of electronic and thermal Free Energies= *-1144.129631*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.352287	-1.166607	0.752762
2	6	0	1.490689	-1.429590	1.920362
3	6	0	0.181204	-1.088451	1.939203
4	6	0	-0.436923	-0.610946	0.719282
5	6	0	0.222395	-0.499693	-0.469856
6	6	0	1.659302	-0.662269	-0.570462
7	1	0	1.934481	-1.938397	2.772495
8	1	0	-0.442301	-1.264207	2.809522
9	6	0	-0.774208	-0.216964	-1.553821
10	1	0	-0.607241	0.740651	-2.059919
11	1	0	-0.838467	-1.006122	-2.311828
12	6	0	-1.854018	-0.381997	0.467629
13	8	0	-2.799745	-0.386319	1.248169
14	8	0	-2.046947	-0.145092	-0.864734
15	6	0	3.468857	-2.108098	0.308710
16	1	0	4.344569	-2.078255	0.965543
17	1	0	3.093906	-3.137402	0.280199
18	6	0	2.393989	-1.311924	-1.738837
19	1	0	1.895561	-2.248709	-2.015028
20	1	0	2.462762	-0.678460	-2.629744
21	6	0	3.806462	-1.613304	-1.134181
22	1	0	4.354673	-2.357297	-1.714123
23	6	0	2.559605	0.264080	0.281162
24	6	0	4.538467	-0.297773	-1.021846
25	1	0	5.501557	-0.106166	-1.484590
26	6	0	3.866709	0.612431	-0.307013
27	6	0	4.172934	2.021715	0.028438
28	8	0	5.128286	2.687903	-0.268735
29	8	0	3.126713	2.509939	0.776200

30	6	0	2.108922	1.521016	1.021186
31	1	0	2.032854	1.362972	2.101416
32	1	0	1.155887	1.921483	0.661323
33	7	0	-5.247906	0.157084	0.266475
34	6	0	-5.425423	0.440977	-1.019721
35	6	0	-6.460137	0.220653	0.921629
36	1	0	-4.304863	-0.071162	0.684873
37	1	0	-4.648057	0.466101	-1.767810
38	6	0	-7.402348	0.555339	-0.007392
39	1	0	-6.550458	0.025828	1.978681
40	1	0	-7.150883	0.930918	-2.097888
41	1	0	-8.466555	0.708473	0.077629
42	7	0	-6.730161	0.686735	-1.209523

single points:

mPW1PW91/6-31G(d) *HF=-1144.1697736*

MP2/6-31G(d) *MP2=-1140.9853522*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-1144.4731458*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-1144.2298848*

K (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

Zero-point correction= *0.296427 (Hartree/Particle)*
Thermal correction to Energy= *0.315493*
Thermal correction to Enthalpy= *0.316437*
Thermal correction to Gibbs Free Energy= *0.247395*
Sum of electronic and zero-point Energies= *-974.419445*
Sum of electronic and thermal Energies= *-974.400379*
Sum of electronic and thermal Enthalpies= *-974.399435*
Sum of electronic and thermal Free Energies= *-974.468477*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.824406	0.186938	0.636215
2	6	0	-0.006966	-0.755653	1.510262
3	6	0	1.321983	-0.924658	1.423276
4	6	0	2.035117	-0.214772	0.381530
5	6	0	1.409159	0.553385	-0.552438
6	6	0	-0.026928	0.727555	-0.585998
7	1	0	-0.568960	-1.268497	2.286864
8	1	0	1.866504	-1.571946	2.102712
9	6	0	2.442726	1.094960	-1.497950
10	1	0	2.324416	0.752162	-2.530737
11	1	0	2.516744	2.187113	-1.492467
12	6	0	3.456013	-0.200882	0.089097
13	8	0	4.381128	-0.769920	0.681601
14	8	0	3.699470	0.563206	-0.998936
15	6	0	-1.248982	1.396665	1.567188
16	1	0	-1.403694	1.002828	2.583519
17	1	0	-0.405060	2.090672	1.642146
18	6	0	-0.621042	1.358626	-1.619785
19	1	0	-0.043085	1.782969	-2.436440

20	1	0	-1.696411	1.471871	-1.684227
21	6	0	-2.514621	2.120370	1.161553
22	1	0	-2.624962	3.151277	1.487474
23	6	0	-2.088913	-0.501483	0.159032
24	6	0	-3.507010	1.490095	0.512876
25	1	0	-4.455156	1.964025	0.279652
26	6	0	-3.282300	0.113498	0.102353
27	6	0	-4.268416	-0.819392	-0.504254
28	8	0	-5.432765	-0.646868	-0.747158
29	8	0	-3.604218	-1.996420	-0.779820
30	6	0	-2.228096	-1.888835	-0.402976
31	1	0	-1.999183	-2.678695	0.324042
32	1	0	-1.601882	-2.056781	-1.289468
33	1	0	6.986882	-0.019759	-0.919250
34	7	0	6.864901	-0.585491	-0.074250
35	1	0	7.219173	-1.530480	-0.250905
36	1	0	7.406271	-0.167439	0.688523
37	1	0	5.791263	-0.629359	0.202909

single points:

mPW1PW91/6-31G(d) HF=- 974.4934459

MP2/6-31G(d) MP2=- 971.7681543

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=- 974.7823289

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=- 974.5603426

K (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 974.6785754

Zero-point correction= 0.294916 (Hartree/Particle)

Thermal correction to Energy= 0.312758

Thermal correction to Enthalpy= 0.313702

Thermal correction to Gibbs Free Energy= 0.248649

Sum of electronic and zero-point Energies= -974.383659

Sum of electronic and thermal Energies= -974.365817

Sum of electronic and thermal Enthalpies= -974.364873

Sum of electronic and thermal Free Energies= -974.42992

1 imaginary frequency (-474.9844 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.112855	-1.169790	0.811023
2	6	0	0.138798	-1.379937	1.944065
3	6	0	-1.138453	-0.963943	1.806856
4	6	0	-1.597236	-0.490482	0.514220
5	6	0	-0.844848	-0.658033	-0.643176
6	6	0	0.433467	-1.241229	-0.574592
7	1	0	0.486910	-1.833712	2.867807
8	1	0	-1.854026	-1.044558	2.619438
9	6	0	-1.719636	-0.320946	-1.820270
10	1	0	-1.344697	0.520597	-2.412272
11	1	0	-1.915544	-1.165286	-2.487974

12	6	0	-2.902475	-0.047484	0.125375
13	8	0	-3.898172	0.212533	0.826286
14	8	0	-2.982790	0.080609	-1.227619
15	6	0	2.384009	-2.024582	0.712659
16	1	0	3.051102	-1.838740	1.565073
17	1	0	2.136281	-3.090776	0.716842
18	6	0	1.183092	-1.845191	-1.594789
19	1	0	1.491269	-2.880013	-1.487588
20	1	0	1.076573	-1.528563	-2.632681
21	6	0	3.100093	-1.636390	-0.587715
22	1	0	3.714688	-2.396465	-1.063370
23	6	0	1.552935	0.281079	0.650520
24	6	0	3.395401	-0.298657	-0.825676
25	1	0	4.119416	0.014599	-1.571459
26	6	0	2.624732	0.645215	-0.122265
27	6	0	2.707574	2.129674	-0.156513
28	8	0	3.475928	2.838415	-0.747965
29	8	0	1.691702	2.609479	0.640411
30	6	0	0.930000	1.530063	1.198144
31	1	0	0.996020	1.570605	2.293386
32	1	0	-0.124548	1.658922	0.925986
33	1	0	-5.078256	0.647083	0.145088
34	7	0	-6.033142	1.004956	-0.356139
35	1	0	-6.804869	0.363127	-0.155062
36	1	0	-6.284351	1.937908	-0.017605
37	1	0	-5.889158	1.046087	-1.368742

single points:

mPW1PW91/6-31G(d) *HF=- 974.4620027*

MP2/6-31G(d) *MP2=- 971.7417868*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=- 974.7409119*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=- 974.524657*

K (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 974.7298842

Zero-point correction= 0.299142 (Hartree/Particle)

Thermal correction to Energy= 0.316797

Thermal correction to Enthalpy= 0.317741

Thermal correction to Gibbs Free Energy= 0.252649

Sum of electronic and zero-point Energies= -974.430742

Sum of electronic and thermal Energies= -974.413087

Sum of electronic and thermal Enthalpies= -974.412143

Sum of electronic and thermal Free Energies= -974.477235

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.020949	-0.991432	1.011434
2	6	0	0.036026	-0.902706	2.105186
3	6	0	-1.223814	-0.450347	1.906002
4	6	0	-1.677015	-0.215138	0.550282
5	6	0	-0.907616	-0.444883	-0.557057

6	6	0	0.503414	-0.748923	-0.461793
7	1	0	0.343830	-1.241460	3.091293
8	1	0	-1.934938	-0.365861	2.720918
9	6	0	-1.771474	-0.340446	-1.777320
10	1	0	-1.465578	0.455784	-2.464618
11	1	0	-1.863181	-1.274947	-2.341822
12	6	0	-3.024377	0.066753	0.090824
13	8	0	-4.036506	0.330521	0.752448
14	8	0	-3.084019	0.000421	-1.259056
15	6	0	2.060536	-2.104594	0.908679
16	1	0	2.873388	-2.001781	1.635122
17	1	0	1.578327	-3.076044	1.064907
18	6	0	1.262903	-1.710090	-1.370344
19	1	0	0.691846	-2.638803	-1.487066
20	1	0	1.478116	-1.305998	-2.365303
21	6	0	2.575432	-1.985171	-0.561417
22	1	0	3.087685	-2.886978	-0.899723
23	6	0	1.421893	0.267354	0.264218
24	6	0	3.432381	-0.746788	-0.663410
25	1	0	4.445905	-0.749495	-1.052177
26	6	0	2.803742	0.357681	-0.244572
27	6	0	3.228800	1.775626	-0.202079
28	8	0	4.271051	2.270870	-0.536665
29	8	0	2.179903	2.511020	0.300482
30	6	0	1.048752	1.695663	0.655930
31	1	0	0.872366	1.797528	1.731311
32	1	0	0.173903	2.080846	0.122767
33	1	0	-6.304491	0.827313	-1.366018
34	7	0	-6.338390	0.834518	-0.342482
35	1	0	-6.643532	1.759589	-0.025079
36	1	0	-7.018292	0.136581	-0.026156
37	1	0	-5.333248	0.604105	0.073974

---

single points:

mPW1PW91/6-31G(d) *HF=- 974.523886*

MP2/6-31G(d) *MP2=- 971.8027607*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=- 974.7961314*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=- 974.5905092*

L (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

Zero-point correction= 0.387124 (Hartree/Particle)
Thermal correction to Energy= 0.413268
Thermal correction to Enthalpy= 0.414212
Thermal correction to Gibbs Free Energy= 0.327690
Sum of electronic and zero-point Energies= -1180.025636
Sum of electronic and thermal Energies= -1179.999492
Sum of electronic and thermal Enthalpies= -1179.998547
Sum of electronic and thermal Free Energies= -1180.085070

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

1	6	0	2.062272	0.151464	0.689247
2	6	0	1.343674	1.480728	0.846817
3	6	0	0.024162	1.671883	0.682330
4	6	0	-0.800129	0.552029	0.271254
5	6	0	-0.264675	-0.681490	0.013823
6	6	0	1.145799	-0.963282	0.108822
7	1	0	1.972554	2.308661	1.164185
8	1	0	-0.423740	2.642855	0.873607
9	6	0	-1.370569	-1.606124	-0.399058
10	1	0	-1.277226	-1.986347	-1.420893
11	1	0	-1.519716	-2.445816	0.286796
12	6	0	-2.222878	0.482250	0.038198
13	8	0	-3.120850	1.340705	0.135820
14	8	0	-2.566504	-0.773490	-0.348052
15	6	0	2.556173	-0.258900	2.139043
16	1	0	2.836083	0.661902	2.673177
17	1	0	1.709878	-0.681500	2.690989
18	6	0	1.631543	-2.162936	-0.283471
19	1	0	0.980239	-2.958377	-0.636249
20	1	0	2.690720	-2.388480	-0.261399
21	6	0	3.751690	-1.186205	2.177997
22	1	0	3.865870	-1.813419	3.057779
23	6	0	3.290325	0.315282	-0.190070
24	6	0	4.689465	-1.160198	1.216125
25	1	0	5.598335	-1.751781	1.260349
26	6	0	4.456111	-0.301730	0.067552
27	6	0	5.400580	-0.014464	-1.048769
28	8	0	6.525873	-0.396381	-1.208332
29	8	0	4.738373	0.804479	-1.942049
30	6	0	3.408327	1.060759	-1.491842
31	1	0	3.275803	2.145684	-1.386166
32	1	0	2.699608	0.707897	-2.253984
33	7	0	-5.459250	-1.485216	-1.123423
34	1	0	-5.778998	-2.086354	-1.870612
35	6	0	-6.314797	-0.946654	-0.250045
36	7	0	-5.900124	0.045724	0.547834
37	7	0	-7.576703	-1.383983	-0.180279
38	1	0	-4.981289	0.470077	0.418940
39	1	0	-6.418139	0.277978	1.384208
40	1	0	-7.867169	-2.237119	-0.639240
41	1	0	-8.287228	-0.871453	0.324630
42	1	0	-4.463498	-1.302320	-1.039784
43	1	0	-2.987155	2.994504	0.086816
44	1	0	-3.027001	4.494816	0.934945
45	1	0	-2.235541	4.416604	-0.532582
46	1	0	-3.898493	4.337171	-0.479358
47	7	0	-3.035560	4.061737	0.004018

---

single points:

mPW1PW91/6-31G(d) *HF=- 1180.1391704*

MP2/6-31G(d) *MP2=- 1176.829123*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=- 1180.6044767*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=- 1180.3315809*

L (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1180.383804
Zero-point correction= 0.386035 (Hartree/Particle)
Thermal correction to Energy= 0.410953
Thermal correction to Enthalpy= 0.411897
Thermal correction to Gibbs Free Energy= 0.329224
Sum of electronic and zero-point Energies= -1179.997769
Sum of electronic and thermal Energies= -1179.972851
Sum of electronic and thermal Enthalpies= -1179.971907
Sum of electronic and thermal Free Energies= -1180.054580

1 imaginary frequency (-412.5244cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.335546	0.427417	-1.270168
2	6	0	-1.525883	1.612505	-1.738225
3	6	0	-0.228034	1.715383	-1.379933
4	6	0	0.425767	0.604986	-0.706922
5	6	0	-0.178921	-0.660660	-0.658464
6	6	0	-1.466033	-0.854483	-1.167082
7	1	0	-2.001644	2.372820	-2.351363
8	1	0	0.365757	2.568625	-1.699850
9	6	0	0.864076	-1.652599	-0.223491
10	1	0	0.614410	-2.163480	0.712153
11	1	0	1.118237	-2.396240	-0.984056
12	6	0	1.778615	0.462364	-0.296078
13	8	0	2.719610	1.289081	-0.186749
14	8	0	2.049143	-0.840627	0.019069
15	6	0	-3.611869	0.031449	-2.028521
16	1	0	-4.373844	0.819808	-1.957267
17	1	0	-3.402573	-0.122141	-3.091644
18	6	0	-2.081173	-2.057684	-1.540673
19	1	0	-2.477352	-2.173998	-2.543467
20	1	0	-1.828668	-2.999750	-1.054384
21	6	0	-4.154976	-1.248284	-1.389110
22	1	0	-4.730951	-1.921820	-2.018370
23	6	0	-2.708210	0.491599	0.205000
24	6	0	-4.318953	-1.314973	-0.013592
25	1	0	-4.907553	-2.093254	0.463064
26	6	0	-3.630239	-0.351646	0.756759
27	6	0	-3.660215	-0.136604	2.230352
28	8	0	-4.292720	-0.706367	3.072663
29	8	0	-2.768339	0.884078	2.502218
30	6	0	-2.143975	1.344404	1.302576
31	1	0	-2.385281	2.405581	1.152772
32	1	0	-1.055221	1.257464	1.409173
33	7	0	4.774955	-1.634342	1.080189
34	1	0	4.989065	-2.302926	1.807191
35	6	0	5.743644	-1.029376	0.387231
36	7	0	5.445872	0.036782	-0.364124
37	7	0	7.003357	-1.477820	0.452940
38	1	0	4.515467	0.461039	-0.325383
39	1	0	6.079034	0.338983	-1.091632
40	1	0	7.224849	-2.373780	0.865725
41	1	0	7.777472	-0.932053	0.099728

42	1	0	3.799530	-1.426100	0.880474
43	1	0	2.540876	2.841701	0.071920
44	1	0	3.004208	4.441522	-0.417376
45	1	0	1.567032	4.241880	0.401410
46	1	0	3.013762	4.062255	1.206071
47	7	0	2.530588	3.901346	0.315215

single points:

mPW1PW91/6-31G(d) HF=- 1180.115473

MP2/6-31G(d) MP2=- 1176.8096632

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=- 1180.5669811

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=- 1180.2992587

L (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1180.4287887

Zero-point correction= 0.389678 (Hartree/Particle)

Thermal correction to Energy= 0.414471

Thermal correction to Enthalpy= 0.415415

Thermal correction to Gibbs Free Energy= 0.332792

Sum of electronic and zero-point Energies= -1180.039111

Sum of electronic and thermal Energies= -1180.014318

Sum of electronic and thermal Enthalpies= -1180.013374

Sum of electronic and thermal Free Energies= -1180.095996

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.269642	0.406551	-1.320259
2	6	0	-1.431176	1.540203	-1.739031
3	6	0	-0.161995	1.707414	-1.294942
4	6	0	0.477583	0.640130	-0.550029
5	6	0	-0.136507	-0.571217	-0.317931
6	6	0	-1.535185	-0.787934	-0.550137
7	1	0	-1.849008	2.235366	-2.463050
8	1	0	0.431908	2.550212	-1.637646
9	6	0	0.891466	-1.548437	0.159373
10	1	0	0.692130	-1.942814	1.161344
11	1	0	1.061212	-2.385528	-0.526387
12	6	0	1.867010	0.502758	-0.185600
13	8	0	2.807480	1.321305	-0.202319
14	8	0	2.119001	-0.765587	0.229989
15	6	0	-3.289165	-0.268128	-2.235124
16	1	0	-4.196108	0.329972	-2.371275
17	1	0	-2.845153	-0.451534	-3.219401
18	6	0	-2.174093	-2.087163	-1.026542
19	6	0	-3.588527	-1.619393	-1.512311
20	1	0	-4.058475	-2.348914	-2.172628
21	6	0	-2.543000	0.183190	0.144187
22	6	0	-4.405551	-1.329379	-0.276784
23	1	0	-5.346348	-1.822230	-0.051695
24	6	0	-3.831528	-0.427565	0.528480
25	6	0	-4.225345	0.101517	1.855517
26	8	0	-5.187448	-0.150359	2.523241

27	8	0	-3.241056	0.983363	2.260278
28	6	0	-2.214176	1.155272	1.277211
29	1	0	-2.228118	2.195204	0.932865
30	1	0	-1.249134	0.958936	1.755862
31	7	0	4.928573	-1.596864	1.188115
32	1	0	5.165802	-2.226069	1.942867
33	6	0	5.871994	-1.060007	0.408884
34	7	0	5.556721	-0.036119	-0.393701
35	7	0	7.122804	-1.533144	0.437726
36	1	0	4.643557	0.415904	-0.332498
37	1	0	6.158466	0.209714	-1.167741
38	1	0	7.347831	-2.406512	0.895239
39	1	0	7.888840	-1.029654	0.011066
40	1	0	3.949259	-1.379567	1.027983
41	1	0	2.655762	2.964386	-0.064121
42	1	0	3.046853	4.508058	-0.725040
43	1	0	1.701311	4.364762	0.250732
44	1	0	3.226261	4.258754	0.915407
45	7	0	2.657263	4.025493	0.093171
46	1	0	-1.603096	-2.495435	-1.868535
47	1	0	-2.248083	-2.855229	-0.249801

single points:

mPW1PW91/6-31G(d) HF=- 1180.1716936

MP2/6-31G(d) MP2=- 1176.8666696

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) HF=- 1180.6189541

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) HF=- 1180.3624903

M (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 918.1098238

Zero-point correction= 0.258315 (Hartree/Particle)

Thermal correction to Energy= 0.274056

Thermal correction to Enthalpy= 0.275000

Thermal correction to Gibbs Free Energy= 0.215183

Sum of electronic and zero-point Energies= -917.851509

Sum of electronic and thermal Energies= -917.835768

Sum of electronic and thermal Enthalpies= -917.834824

Sum of electronic and thermal Free Energies= -917.894641

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.310859	0.113852	0.655634
2	6	0	0.479815	-0.904204	1.461567
3	6	0	1.799451	-1.125915	1.352001
4	6	0	2.526276	-0.388568	0.338325
5	6	0	1.913255	0.469409	-0.550653
6	6	0	0.495318	0.704304	-0.536398
7	1	0	-0.091292	-1.440271	2.215119
8	1	0	2.320527	-1.833076	1.987953
9	6	0	2.952422	1.008478	-1.489287

10	1	0	2.821134	0.720699	-2.536001
11	1	0	3.106348	2.089238	-1.422628
12	6	0	3.898609	-0.393835	-0.015527
13	8	0	4.832510	-1.078419	0.568129
14	8	0	4.195481	0.377954	-1.035017
15	6	0	-0.685360	1.280390	1.661174
16	1	0	-0.894962	0.823956	2.640405
17	1	0	0.195636	1.914139	1.808224
18	6	0	-0.085255	1.436191	-1.516751
19	1	0	0.498314	1.901389	-2.307014
20	1	0	-1.156387	1.589670	-1.559490
21	6	0	-1.893026	2.102298	1.270331
22	1	0	-1.944414	3.122539	1.640539
23	6	0	-1.606983	-0.492340	0.148232
24	6	0	-2.912438	1.561079	0.581161
25	1	0	-3.828045	2.100097	0.359435
26	6	0	-2.763282	0.193094	0.115178
27	6	0	-3.799741	-0.657199	-0.533246
28	8	0	-4.948090	-0.403262	-0.773788
29	8	0	-3.201876	-1.858070	-0.850659
30	6	0	-1.825449	-1.849310	-0.464129
31	1	0	-1.651513	-2.676466	0.236159
32	1	0	-1.205086	-2.026875	-1.353034
33	1	0	5.709021	-0.937010	0.155356

single points:

mPW1PW91/6-31G(d) *HF=-917.9027436*

MP2/6-31G(d) *MP2=-915.3493718*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-918.1754909*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-917.9688024*

M (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 918.0818831

Zero-point correction= 0.257558 (Hartree/Particle)

Thermal correction to Energy= 0.272289

Thermal correction to Enthalpy= 0.273233

Thermal correction to Gibbs Free Energy= 0.216530

Sum of electronic and zero-point Energies= -917.824325

Sum of electronic and thermal Energies= -917.809594

Sum of electronic and thermal Enthalpies= -917.808650

Sum of electronic and thermal Free Energies= -917.865354

1 imaginary frequency (-399.5005 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.458150	-1.076723	0.909560
2	6	0	-0.576930	-1.003449	2.006801
3	6	0	-1.766520	-0.416410	1.767644
4	6	0	-2.102426	-0.037157	0.404951

5	6	0	-1.339730	-0.468830	-0.701390
6	6	0	-0.181926	-1.219400	-0.497165
7	1	0	-0.331670	-1.390211	2.991856
8	1	0	-2.509128	-0.293781	2.549625
9	6	0	-2.122274	-0.155485	-1.948770
10	1	0	-1.618056	0.545018	-2.621112
11	1	0	-2.458092	-1.027407	-2.515608
12	6	0	-3.262801	0.527926	-0.129990
13	8	0	-4.259879	1.042186	0.537948
14	8	0	-3.323454	0.517030	-1.453756
15	6	0	1.573830	-2.129995	0.990266
16	1	0	2.212029	-1.958623	1.868249
17	1	0	1.153096	-3.135651	1.087818
18	6	0	0.486650	-2.037745	-1.417886
19	1	0	0.670390	-3.079977	-1.182148
20	1	0	0.472904	-1.820322	-2.485683
21	6	0	2.423379	-2.012663	-0.275744
22	1	0	2.930310	-2.905957	-0.631255
23	6	0	1.141141	0.262950	0.653829
24	6	0	2.891129	-0.772299	-0.678022
25	1	0	3.670542	-0.661469	-1.426174
26	6	0	2.269690	0.362109	-0.107795
27	6	0	2.613279	1.801182	-0.277740
28	8	0	3.501867	2.300744	-0.909554
29	8	0	1.684570	2.519347	0.441766
30	6	0	0.735294	1.648243	1.066542
31	1	0	0.787145	1.778632	2.155518
32	1	0	-0.273915	1.933730	0.746976
33	1	0	-4.970001	1.348035	-0.059825

single points:

mPW1PW91/6-31G(d)	HF=-917.8795254
MP2/6-31G(d)	MP2=-915.3303095
CPCM(CHCl3,UAKS)-B3LYP/6-31G(d)	HF=-918.1432046
CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d)	HF=-917.9412108

M (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 918.1248674

Zero-point correction=	0.260831 (Hartree/Particle)
Thermal correction to Energy=	0.275269
Thermal correction to Enthalpy=	0.276214
Thermal correction to Gibbs Free Energy=	0.219993
Sum of electronic and zero-point Energies=	-917.864037
Sum of electronic and thermal Energies=	-917.849598
Sum of electronic and thermal Enthalpies=	-917.848654
Sum of electronic and thermal Free Energies=	-917.904875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.421667	0.912436	1.079268

2	6	0	0.605594	0.654565	2.107068
3	6	0	1.792499	0.073172	1.820976
4	6	0	2.152590	-0.118015	0.429040
5	6	0	1.357768	0.294298	-0.632181
6	6	0	0.011331	0.731781	-0.447112
7	1	0	0.387603	0.967785	3.124884
8	1	0	2.523520	-0.139298	2.593354
9	6	0	2.158467	0.209299	-1.894352
10	1	0	1.757998	-0.494239	-2.630847
11	1	0	2.356727	1.169076	-2.381835
12	6	0	3.393203	-0.476126	-0.150731
13	8	0	4.435926	-0.911426	0.487342
14	8	0	3.449556	-0.323055	-1.454956
15	6	0	-1.335959	2.135622	1.090420
16	1	0	-2.118542	2.068316	1.853437
17	1	0	-0.746814	3.039571	1.278580
18	6	0	-0.695806	1.813886	-1.253465
19	1	0	-0.042469	2.688682	-1.350933
20	1	0	-1.002841	1.493804	-2.254376
21	6	0	-1.929998	2.162164	-0.352625
22	1	0	-2.364006	3.129694	-0.607153
23	6	0	-0.980595	-0.242128	0.300067
24	6	0	-2.907215	1.021024	-0.491976
25	1	0	-3.924493	1.143527	-0.850806
26	6	0	-2.375709	-0.165102	-0.171416
27	6	0	-2.925913	-1.540710	-0.235174
28	8	0	-4.014742	-1.907225	-0.579618
29	8	0	-1.933166	-2.404842	0.168065
30	6	0	-0.738720	-1.725583	0.583593
31	1	0	-0.582450	-1.911253	1.651122
32	1	0	0.102170	-2.153731	0.030359
33	1	0	5.193791	-1.073047	-0.110843

---

single points:

mPW1PW91/6-31G(d) *HF=-917.9340131*

MP2/6-31G(d) *MP2=-915.3852546*

CPCM(CHCl3,UAKS)-B3LYP/6-31G(d) *HF=-918.190428*

CPCM(CHCl3,UAKS)- mPW1PW91/6-31G(d) *HF=-917.999918*

N (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1239.3216881

Zero-point correction= 0.286627 (Hartree/Particle)

Thermal correction to Energy= 0.306391

Thermal correction to Enthalpy= 0.307335

Thermal correction to Gibbs Free Energy= 0.233475

Sum of electronic and zero-point Energies= -1239.035061

Sum of electronic and thermal Energies= -1239.015297

Sum of electronic and thermal Enthalpies= -1239.014353

Sum of electronic and thermal Free Energies= -1239.088213

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

1	6	0	-3.060934	-0.611454	-0.213321
2	6	0	-1.921160	-1.533952	-0.631662
3	6	0	-0.625400	-1.183161	-0.648611
4	6	0	-0.279396	0.184618	-0.324708
5	6	0	-1.209889	1.143776	-0.102710
6	6	0	-2.636027	0.883056	-0.170590
7	1	0	-2.216160	-2.553967	-0.866169
8	1	0	0.160766	-1.887183	-0.902681
9	6	0	-0.497366	2.444971	0.141392
10	1	0	-0.720836	3.212027	-0.608975
11	1	0	-0.689075	2.865352	1.135278
12	6	0	1.054179	0.794074	-0.231308
13	8	0	2.151386	0.287647	-0.368099
14	8	0	0.903251	2.121465	0.049661
15	6	0	-3.476580	-1.075684	1.234520
16	1	0	-3.348491	-2.168014	1.295232
17	1	0	-2.772102	-0.652728	1.958897
18	6	0	-3.527483	1.892518	-0.164115
19	1	0	-3.210818	2.927828	-0.068673
20	1	0	-4.591745	1.716497	-0.260992
21	6	0	-4.902875	-0.757320	1.605214
22	1	0	-5.144407	-0.646281	2.659604
23	6	0	-4.234135	-0.800262	-1.169631
24	6	0	-5.858305	-0.699203	0.665204
25	1	0	-6.899282	-0.536661	0.932380
26	6	0	-5.509428	-0.842701	-0.750284
27	1	0	-3.994720	-0.855921	-2.228892
28	1	0	-6.313168	-0.946525	-1.475600
29	1	0	4.072012	1.023509	-0.001052
30	7	0	5.059156	0.846072	0.154144
31	6	0	5.568259	-0.407542	0.116637
32	1	0	5.710460	1.612112	0.208228
33	7	0	4.649159	-1.399099	-0.008222
34	1	0	4.997926	-2.335549	-0.134002
35	1	0	3.677928	-1.193368	-0.209812
36	16	0	7.224103	-0.723327	0.247320

N (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1239.2788203
Zero-point correction= 0.286056 (Hartree/Particle)
Thermal correction to Energy= 0.304634
Thermal correction to Enthalpy= 0.305578
Thermal correction to Gibbs Free Energy= 0.235237
Sum of electronic and zero-point Energies= -1238.992764
Sum of electronic and thermal Energies= -1238.974187
Sum of electronic and thermal Enthalpies= -1238.973242
Sum of electronic and thermal Free Energies= -1239.043583

1 imaginary frequency (-531.2562 cm^{-1})

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.989580	-0.994498	-0.246066
2	6	0	1.847149	-1.887473	-0.650981
3	6	0	0.581770	-1.422856	-0.578293
4	6	0	0.352678	-0.025669	-0.265555
5	6	0	1.369755	0.896754	-0.230655
6	6	0	2.713894	0.492277	-0.478594
7	1	0	2.057985	-2.905110	-0.969493
8	1	0	-0.272164	-2.050365	-0.816344
9	6	0	0.754266	2.264354	-0.119337
10	1	0	1.059278	2.798550	0.788314
11	1	0	0.959847	2.905280	-0.984142
12	6	0	-0.916731	0.683954	-0.160699
13	8	0	-2.058457	0.257030	-0.163276
14	8	0	-0.663076	2.028228	-0.052325
15	6	0	4.396964	-1.283517	-0.763002
16	1	0	4.755283	-2.255825	-0.398256
17	1	0	4.411475	-1.314745	-1.857892
18	6	0	3.809221	1.245152	-0.923883
19	1	0	4.280437	0.976881	-1.864157
20	1	0	3.893439	2.305552	-0.682847
21	6	0	5.301205	-0.168194	-0.232106
22	1	0	6.178089	0.084999	-0.823452
23	6	0	3.064035	-0.738029	1.263823
24	6	0	5.343606	0.035910	1.144044
25	1	0	6.166867	0.577269	1.601275
26	6	0	4.204448	-0.304700	1.897860
27	1	0	2.135104	-0.846775	1.814248
28	1	0	4.176713	-0.114768	2.967846
29	1	0	-3.937804	1.117784	-0.037652
30	7	0	-4.944042	0.997724	0.026994
31	6	0	-5.505713	-0.232717	0.074940
32	1	0	-5.540884	1.789194	0.203754
33	7	0	-4.645897	-1.265437	-0.113241
34	1	0	-3.643949	-1.116035	-0.145209
35	1	0	-5.012828	-2.196437	-0.000950
36	16	0	-7.162613	-0.470500	0.321533

N (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1239.3423299
Zero-point correction= 0.289851 (Hartree/Particle)
Thermal correction to Energy= 0.308034
Thermal correction to Enthalpy= 0.308978
Thermal correction to Gibbs Free Energy= 0.239405
Sum of electronic and zero-point Energies= -1239.052479
Sum of electronic and thermal Energies= -1239.034296
Sum of electronic and thermal Enthalpies= -1239.033352
Sum of electronic and thermal Free Energies= -1239.102925

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.975814	-1.110690	-0.176236

2	6	0	1.789095	-1.965955	-0.377993
3	6	0	0.532758	-1.484527	-0.248201
4	6	0	0.336595	-0.060046	-0.061777
5	6	0	1.352035	0.840788	-0.028418
6	6	0	2.748178	0.427206	0.008021
7	1	0	1.953513	-3.001164	-0.668123
8	1	0	-0.338021	-2.118702	-0.380642
9	6	0	0.768423	2.222284	-0.060070
10	1	0	1.016513	2.816873	0.827683
11	1	0	1.054664	2.798464	-0.948754
12	6	0	-0.931911	0.680935	-0.091885
13	8	0	-2.074976	0.266751	-0.126824
14	8	0	-0.655557	2.019932	-0.085500
15	6	0	4.248691	-1.254456	-1.000504
16	1	0	4.837065	-2.141546	-0.740732
17	1	0	3.994170	-1.307509	-2.065871
18	6	0	3.890129	1.141064	-0.702845
19	6	0	5.019775	0.063073	-0.682188
20	6	0	3.202789	-0.456978	1.188366
21	6	0	5.533721	-0.032528	0.734887
22	1	0	6.584938	0.105542	0.969656
23	6	0	4.598823	-0.291696	1.658249
24	1	0	2.440873	-0.662490	1.933478
25	1	0	4.810219	-0.387076	2.719550
26	1	0	-3.976721	1.128532	-0.153403
27	7	0	-4.983910	1.008168	-0.119223
28	6	0	-5.545026	-0.216554	0.016895
29	1	0	-5.586742	1.808992	-0.022489
30	7	0	-4.678185	-1.258421	-0.056499
31	1	0	-3.675977	-1.109209	-0.061142
32	1	0	-5.047274	-2.177253	0.127237
33	16	0	-7.207707	-0.438945	0.230482
34	1	0	5.809168	0.273103	-1.407187
35	1	0	3.598844	1.375601	-1.734218
36	1	0	4.207674	2.067741	-0.211902

O (reactant)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1473.6709943
Zero-point correction= 0.299202 (Hartree/Particle)
Thermal correction to Energy= 0.320650
Thermal correction to Enthalpy= 0.321594
Thermal correction to Gibbs Free Energy= 0.246364
Sum of electronic and zero-point Energies= -1473.371793
Sum of electronic and thermal Energies= -1473.350344
Sum of electronic and thermal Enthalpies= -1473.349400
Sum of electronic and thermal Free Energies= -1473.424631

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.996705	-0.584030	-0.170120

2	6	0	-1.955848	-1.680445	-0.367215
3	6	0	-0.627563	-1.491423	-0.320562
4	6	0	-0.139296	-0.139453	-0.149048
5	6	0	-0.955171	0.946747	-0.130198
6	6	0	-2.392683	0.843571	-0.282175
7	1	0	-2.360179	-2.681935	-0.492071
8	1	0	0.081144	-2.307912	-0.413030
9	6	0	-0.101834	2.175950	-0.001820
10	1	0	-0.164776	2.852283	-0.860636
11	1	0	-0.286724	2.748293	0.913223
12	6	0	1.233604	0.331709	-0.034427
13	8	0	2.265159	-0.344335	-0.022657
14	8	0	1.253048	1.672460	0.059460
15	6	0	-3.567543	-0.791897	1.284417
16	1	0	-3.594959	-1.873329	1.490817
17	1	0	-2.862031	-0.368412	2.007513
18	6	0	-3.147459	1.941864	-0.480887
19	1	0	-2.710697	2.937063	-0.491286
20	1	0	-4.215683	1.878111	-0.646876
21	6	0	-4.958088	-0.246631	1.488248
22	1	0	-5.251908	0.042311	2.494423
23	6	0	-4.116665	-0.765993	-1.190125
24	6	0	-5.831554	-0.202887	0.470666
25	1	0	-6.856355	0.124889	0.624326
26	6	0	-5.411359	-0.590941	-0.877886
27	1	0	-3.816280	-1.004746	-2.207481
28	1	0	-6.171632	-0.700821	-1.647709
29	13	0	4.200323	0.120754	0.086711
30	6	0	4.358842	0.911013	1.889834
31	1	0	5.407428	1.135270	2.128130
32	1	0	3.802320	1.853571	1.986949
33	1	0	3.998443	0.231801	2.673521
34	6	0	4.485626	1.183138	-1.554111
35	1	0	3.936537	2.134931	-1.540979
36	1	0	5.548382	1.431176	-1.679182
37	1	0	4.183413	0.638859	-2.458527
38	17	0	5.019170	-1.900468	-0.044138

O (TS)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

HF=- 1473.6301737
Zero-point correction= 0.298494 (Hartree/Particle)
Thermal correction to Energy= 0.318834
Thermal correction to Enthalpy= 0.319778
Thermal correction to Gibbs Free Energy= 0.247679
Sum of electronic and zero-point Energies= -1473.331680
Sum of electronic and thermal Energies= -1473.311340
Sum of electronic and thermal Enthalpies= -1473.310395
Sum of electronic and thermal Free Energies= -1473.382495

1 imaginary frequency (-517.4280 cm^{-1})

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

1	6	0	-2.948143	0.968866	-0.206176
2	6	0	-1.912302	2.022135	-0.501087
3	6	0	-0.601996	1.711972	-0.413469
4	6	0	-0.217072	0.329401	-0.201552
5	6	0	-1.117436	-0.713102	-0.285453
6	6	0	-2.487461	-0.451495	-0.553002
7	1	0	-2.237670	3.028990	-0.748898
8	1	0	0.177416	2.452372	-0.565533
9	6	0	-0.340221	-1.999135	-0.261034
10	1	0	-0.593912	-2.643920	0.587280
11	1	0	-0.419230	-2.582161	-1.184124
12	6	0	1.103276	-0.239700	-0.099172
13	8	0	2.187637	0.352511	-0.013671
14	8	0	1.036723	-1.589713	-0.110015
15	6	0	-4.366926	1.129748	-0.746710
16	1	0	-4.848709	2.019929	-0.319906
17	1	0	-4.359353	1.247808	-1.835534
18	6	0	-3.471410	-1.293838	-1.088008
19	1	0	-3.955645	-1.009744	-2.016758
20	1	0	-3.434888	-2.371892	-0.927489
21	6	0	-5.142103	-0.122924	-0.333415
22	1	0	-5.968864	-0.431635	-0.968737
23	6	0	-3.026487	0.593883	1.277802
24	6	0	-5.181394	-0.451289	1.017764
25	1	0	-5.939015	-1.127810	1.402837
26	6	0	-4.114420	-0.031335	1.837059
27	1	0	-2.134627	0.780323	1.867562
28	1	0	-4.090832	-0.301131	2.889630
29	13	0	4.057375	-0.267819	0.114823
30	6	0	4.121287	-1.152373	1.881471
31	1	0	3.468398	-2.035042	1.933215
32	1	0	5.138540	-1.495790	2.113990
33	1	0	3.825891	-0.475354	2.693860
34	6	0	4.333213	-1.275391	-1.563196
35	1	0	4.109770	-0.669909	-2.451639
36	1	0	5.378895	-1.597956	-1.659830
37	1	0	3.713961	-2.181633	-1.616548
38	17	0	5.049806	1.683605	0.101912

O (product)

B3LYP/6-31G(d)// B3LYP/6-31G(d)

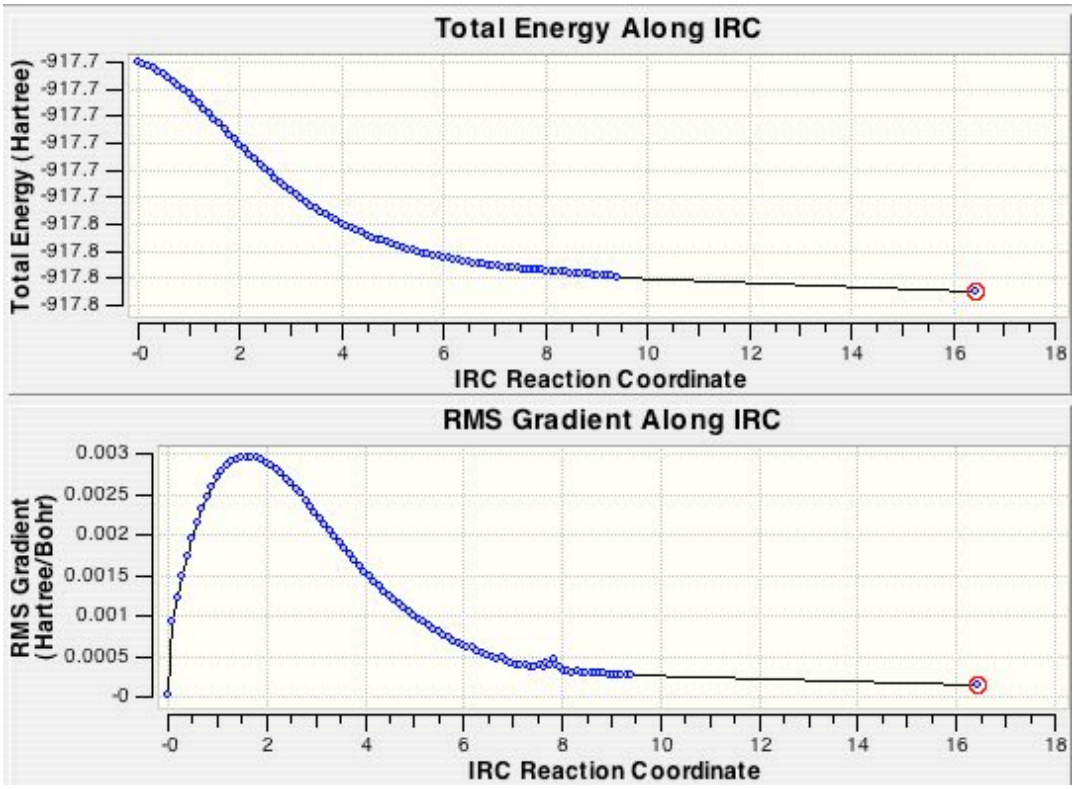
HF=- 1473.69205
Zero-point correction= 0.302310 (Hartree/Particle)
Thermal correction to Energy= 0.322273
Thermal correction to Enthalpy= 0.323217
Thermal correction to Gibbs Free Energy= 0.251570
Sum of electronic and zero-point Energies= -1473.389740
Sum of electronic and thermal Energies= -1473.369777
Sum of electronic and thermal Enthalpies= -1473.368833
Sum of electronic and thermal Free Energies= -1473.440480

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

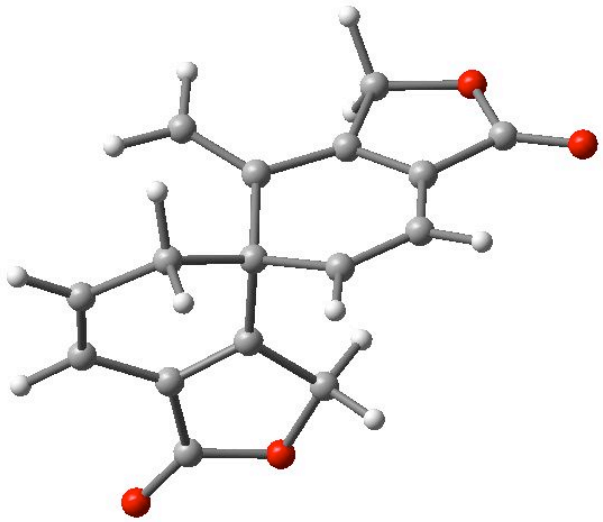
1	6	0	-2.943872	1.087050	-0.115676
2	6	0	-1.861522	2.088894	-0.198725
3	6	0	-0.561650	1.754035	-0.042645
4	6	0	-0.206759	0.350764	0.047536
5	6	0	-1.107376	-0.667778	-0.038679
6	6	0	-2.540160	-0.425736	-0.039937
7	1	0	-2.139006	3.116450	-0.421290
8	1	0	0.232683	2.491976	-0.084091
9	6	0	-0.358998	-1.961592	-0.142308
10	1	0	-0.557455	-2.649871	0.686925
11	1	0	-0.518923	-2.496214	-1.085630
12	6	0	1.122825	-0.241526	0.023595
13	8	0	2.210456	0.339183	0.074255
14	8	0	1.033137	-1.580713	-0.077153
15	6	0	-4.193681	1.144229	-0.985232
16	1	0	-4.892846	1.932903	-0.686179
17	1	0	-3.909027	1.311945	-2.030779
18	6	0	-3.560462	-1.209165	-0.854410
19	6	0	-4.811472	-0.275372	-0.802087
20	6	0	-3.139369	0.307577	1.182815
21	6	0	-5.382050	-0.357055	0.593850
22	1	0	-6.415322	-0.640280	0.770512
23	6	0	-4.519459	-0.063782	1.575418
24	1	0	-2.434247	0.539139	1.974640
25	1	0	-4.776785	-0.082317	2.630534
26	13	0	4.098657	-0.286804	0.030224
27	6	0	4.281509	-1.221747	1.760538
28	1	0	3.647863	-2.117445	1.825312
29	1	0	5.316424	-1.553128	1.920935
30	1	0	4.025395	-0.573783	2.609065
31	6	0	4.218729	-1.240869	-1.695431
32	1	0	3.944227	-0.600655	-2.544214
33	1	0	5.244975	-1.584943	-1.882774
34	1	0	3.573815	-2.129834	-1.728662
35	17	0	5.078842	1.666612	-0.001313
36	1	0	-3.205595	-1.321510	-1.886263
37	1	0	-3.781993	-2.203710	-0.451637
38	1	0	-5.543189	-0.518003	-1.575531

IRC results for A (TS)

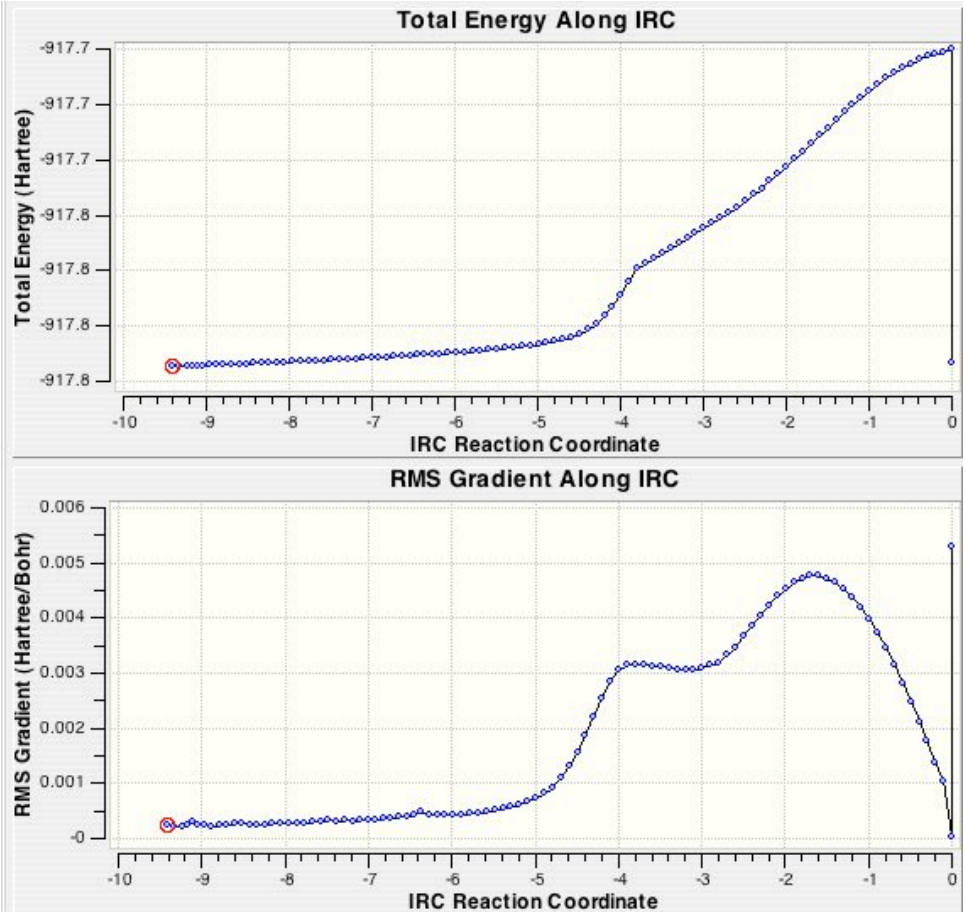
towards reactant:



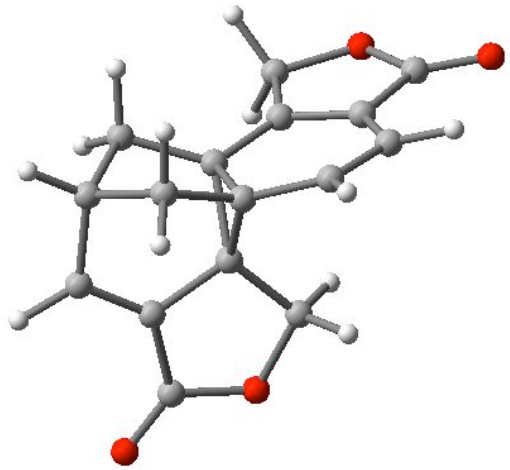
last point:



towards product:

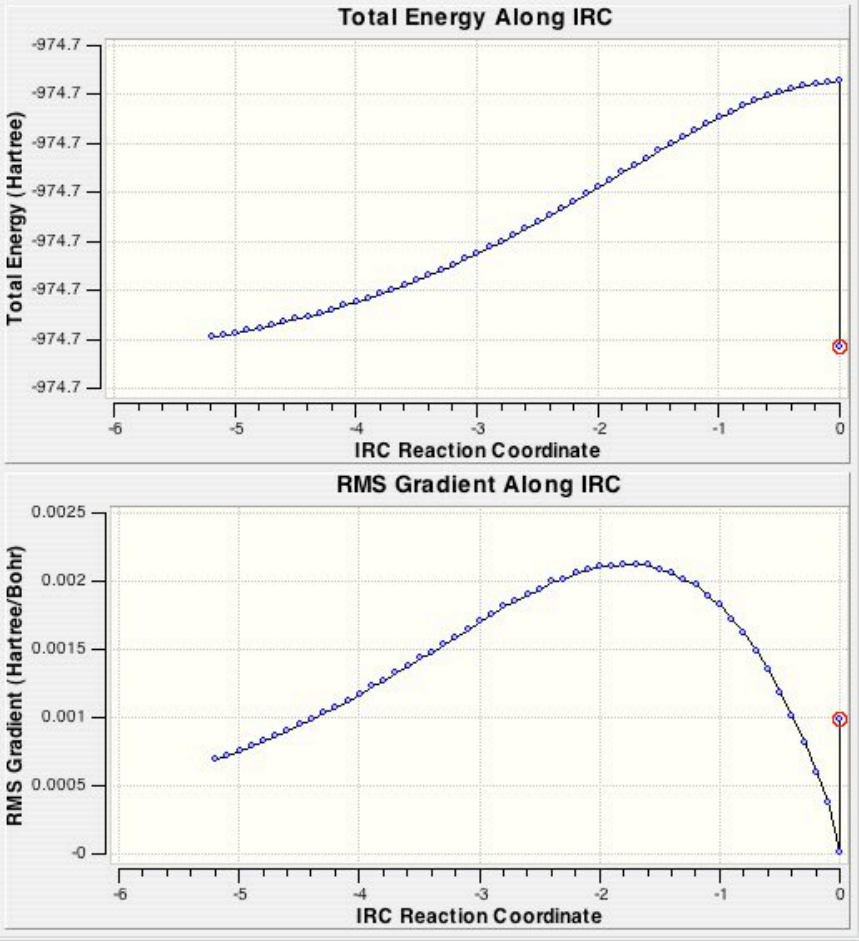


last point:

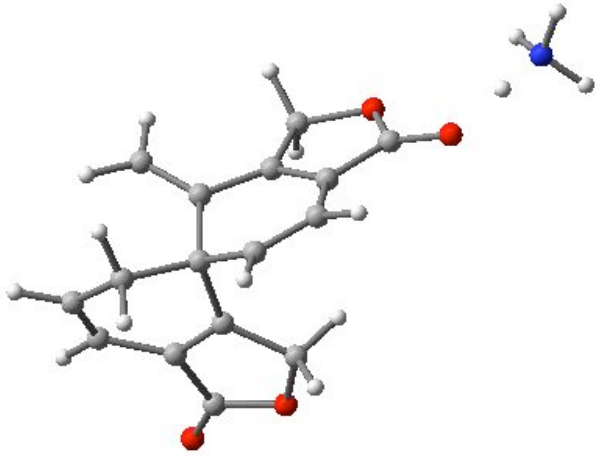


IRC results for K (TS)

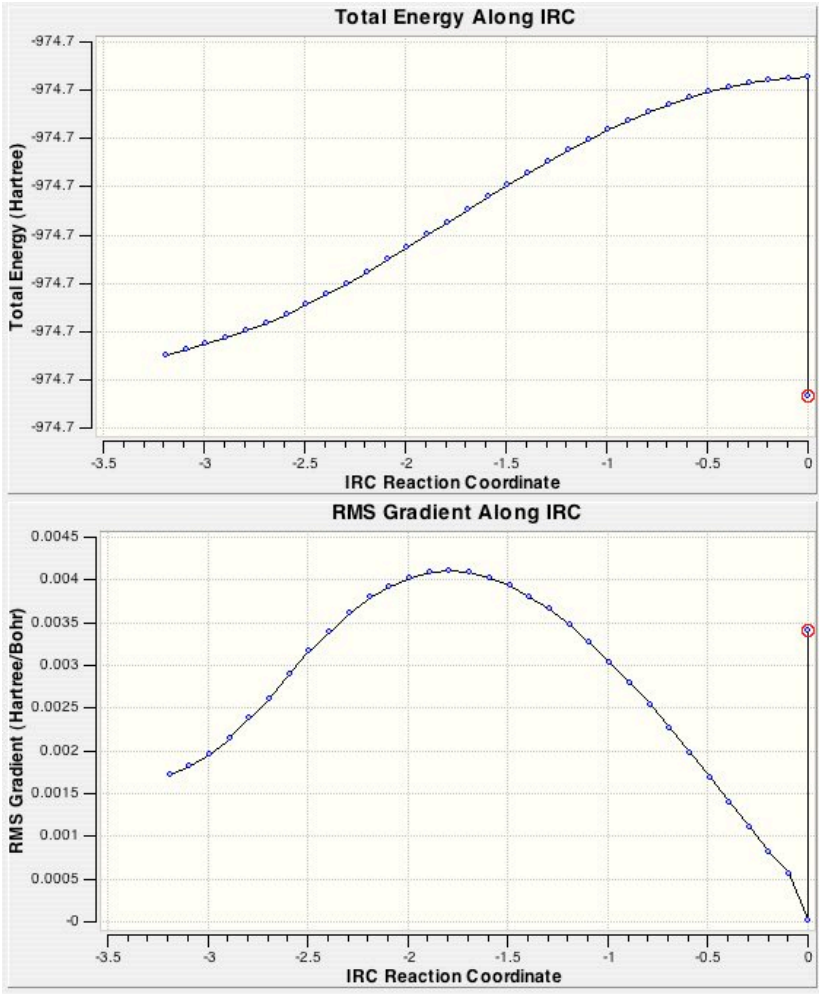
towards reactant:



last point:



towards product:



final structure: