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SUPPORTING INFORMATION

Title: Mechanisms of Brønsted Acid Catalyzed Additions of Phenols and Protected Amines to Olefins: A DFT Study
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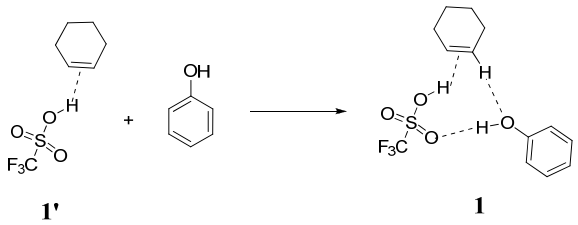
Ref. No.: O200800337

1. Complexes of TfOH, alkene and phenol

The trifluoromethanesulfonic acid (TfOH) can coordinate the olefin to form a complex **1′** which is also a relatively stable species in the system, but the phenol can further form hydrogen bond with **1′**, leading to the formation of a true reactive intermediate **1** for the intermolecular addition of phenol to olefin. Moreover, there are 0.042 e charge transfer between olefin and TfOH in **1′** and 0.049 e charge transfer between olefin and TfOH/phenol in **1**, which means that TfOH has activated the olefin in the first intermediate.



1′ **1**

2. The comparison of the intermolecular addition of phenol to olefin catalyzed by TfOH and its analog $(CH_3)_3CSO_3H$

The comparison of reaction energy profiles of intermolecular addition of phenol to olefin catalyzed by TfOH and its analog $(CH_3)_3CSO_3H$ is shown in Figure S1. Clearly, the activation energy of the reaction catalyzed by TfOH is lower than that by $(CH_3)_3CSO_3H$.

From the natural population analysis, the natural charge of the transferred hydrogen from TfOH in the transition state **TS2** is 0.011 e more positive than that of the transferred hydrogen from $(CH_3)_3CSO_3H$ in the transition state **TS2(CH$_3$)**, indicating that TfOH is a much stronger acid than $(CH_3)_3CSO_3H$.

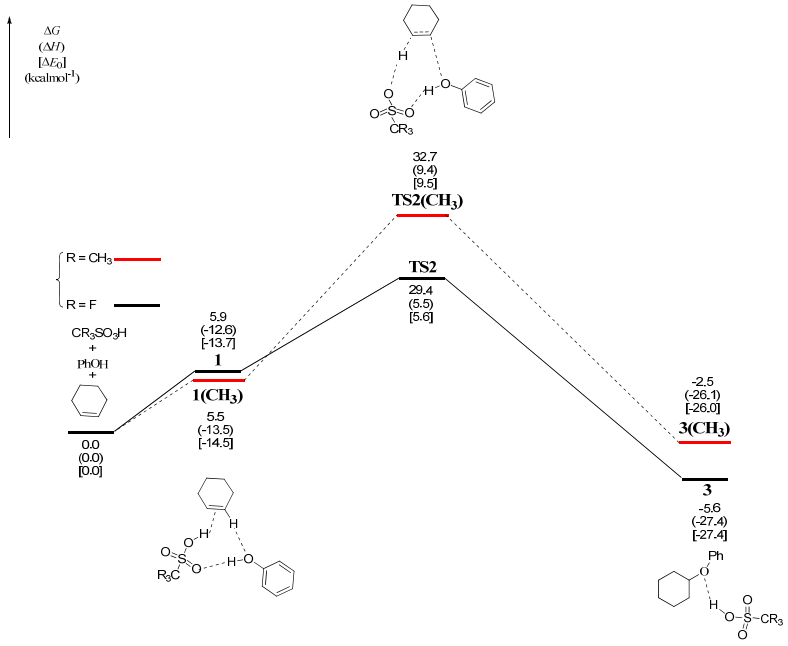


Figure S1. Comparison of reaction energy profiles of intermolecular addition of phenol to olefin catalyzed by TfOH and its analog $(CH_3)_3CSO_3H$.

3. Regioselectivity of the addition of *p*-methoxyphenol to the terminal olefin

The computed potential surface for TfOH catalyzed intermolecular addition is shown in Figure S2. In the terminal olefin, there are two sites (site 1 and site 2) that can be attacked by the nucleophilic *p*-methoxyphenol. On the basis of the different activation energy barriers, the addition reaction occurring at site 2 (the internal carbon of the alkene) is much more favored than that at site 1(the terminal carbon of the alkene).

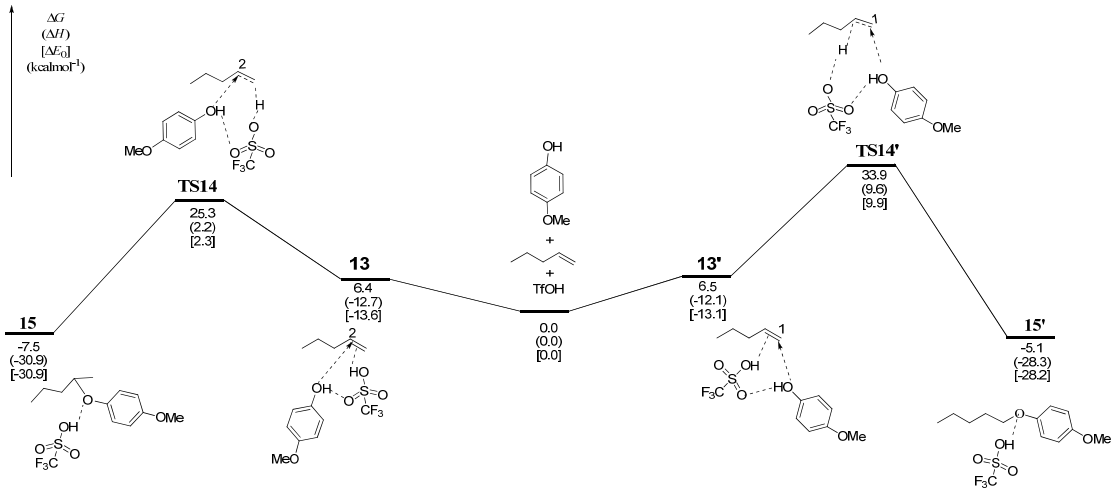


Figure S2. The potential energy surface for TfOH catalyzed intermolecular addition of *p*-methoxyphenol to terminal olefin.

4. Energy differences between precursor complexes and transition states in gas phase and solution

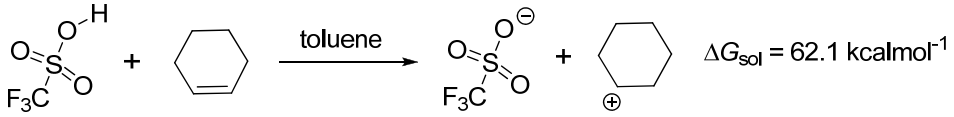
Table S1. Energy differences (in kcalmol^{-1}) between the precursor complexes and the transition states in gas phase and solution.

Structures	$\Delta E_0^{\neq}$	$\Delta H^{\neq}$	$\Delta G^{\neq}$	$\Delta G_{sol}^{\neq}$
1↔TS2	19.3	18.1	23.5	20.6[a]
4↔TS5	23.1	22.1	26.3	23.1[a]
7↔TS8	14.7	13.5	18.4	12.3[b]
10↔ TS11	25.9	24.7	28.4	20.9[b]
13↔TS14	15.9	14.9	18.9	14.3[a]
13′↔TS14′	23.0	21.7	27.4	24.7[a]
16↔TS17	18.6	17.6	21.6	16.9[a]
19↔TS20	22.7	22.0	23.0	18.6[a]
22↔TS23	22.6	21.7	24.6	20.9[a]

[a] In toluene. [b] In dichloroethane.

5. Discussions of possible stepwise mechanism of addition in solution

Attempts to locate the zwitterionic intermediate derived from the stepwise pathway in the toluene solution were unsuccessful. The final addition product was directly obtained instead. The additional calculations show that the formation of the assumed stepwise products, protonated cyclohexane and TfO^- is highly endogonic by 117.4 and 62.1 kcalmol^{-1} in gas phase and toluene, respectively. Therefore, a stepwise mechanism can be ruled out.



6. Effects of basis sets.

Table S2. Effects of basis sets for the reaction shown in Figure 1.

ΔE (kcalmol^{-1})	B3LYP/6-31G(d)	B3LYP/6-31G+(d)	B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)
reactants	0.0	0.0	0.0
1	-15.3	-12.2	-12.2
TS2	4.8	7.3	10.1
3	-31.2	-25.6	-20.8

7. Cartesian coordinates and energies of all species

Cyclohexene: B3LYP\6-31G(d) = -234.6482949

Sum of electronic and zero-point Energies = -234.501308

Sum of electronic and thermal Energies = -234.495818

Sum of electronic and thermal Enthalpies = -234.494874

Sum of electronic and thermal Free Energies = -234.529945

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.666040	1.306032	-0.057363
2	6	0	-1.498960	0.047885	-0.110674
3	6	0	-0.698344	-1.192241	0.318667
4	6	0	0.698334	-1.192246	-0.318668
5	6	0	1.498960	0.047873	0.110677
6	6	0	0.666051	1.306026	0.057361
7	1	0	-1.199385	2.254656	-0.113130
8	1	0	1.199404	2.254647	0.113129
9	1	0	-2.386109	0.164153	0.527539
10	1	0	-1.889947	-0.090114	-1.131658
11	1	0	-1.244613	-2.105968	0.053955

12	1	0	-0.593179	-1.192684	1.412638
13	1	0	1.244596	-2.105978	-0.053959
14	1	0	0.593170	-1.192685	-1.412640
15	1	0	2.386112	0.164134	-0.527533
16	1	0	1.889942	-0.090130	1.131662

PhOH: B3LYP\6-31G(d) = -307.4648701

Sum of electronic and zero-point Energies = -307.360064

Sum of electronic and thermal Energies = -307.354563

Sum of electronic and thermal Enthalpies = -307.353619

Sum of electronic and thermal Free Energies = -307.389036

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.205966	0.231957	0.000000
2	6	0	-1.189086	-1.163546	0.000000
3	6	0	0.021359	-1.857615	0.000000
4	6	0	1.220879	-1.139873	0.000000
5	6	0	1.218133	0.253245	0.000000
6	6	0	0.000000	0.941476	0.000000
7	8	0	0.050335	2.309478	0.000000
8	1	0	-2.152676	0.770157	0.000000
9	1	0	-2.130544	-1.706710	0.000000
10	1	0	0.030835	-2.943561	0.000000
11	1	0	2.170448	-1.668783	0.000000
12	1	0	2.142477	0.822501	0.000000
13	1	0	-0.855135	2.656703	0.000000

TfOH: B3LYP\6-31G(d) = -961.9991175

Sum of electronic and zero-point Energies = -961.960578

Sum of electronic and thermal Energies = -961.952711

Sum of electronic and thermal Enthalpies = -961.951767

Sum of electronic and thermal Free Energies = -961.993767

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	1.424844	-0.154107	-1.252697
2	6	0	1.008536	0.009426	-0.001931
3	9	0	1.542844	-0.924295	0.780074

4	9	0	1.361222	1.219634	0.436150
5	16	0	-0.852884	-0.148451	0.075890
6	8	0	-1.216041	-1.372516	-0.605693
7	8	0	-1.256960	1.097713	-0.898198
8	8	0	-1.260729	0.173692	1.435901
9	1	0	-1.495420	1.856465	-0.330470

$TsNH_2$: B3LYP\6-31G(d) = -875.4893073
Sum of electronic and zero-point Energies = -875.334266
Sum of electronic and thermal Energies = -875.323134
Sum of electronic and thermal Enthalpies = -875.322190
Sum of electronic and thermal Free Energies = -875.373168

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.899488	0.018744	-0.139896
2	8	0	-2.320793	1.355410	-0.573309
3	6	0	-0.110836	0.010537	-0.072485
4	6	0	0.569845	-1.208465	-0.064698
5	6	0	0.581432	1.220564	-0.048979
6	6	0	1.960949	-1.206051	-0.017001
7	6	0	1.974755	1.202864	-0.001702
8	6	0	2.684929	-0.004605	0.021307
9	6	0	4.192923	-0.016363	0.099982
10	7	0	-2.359679	-0.174677	1.487194
11	8	0	-2.335322	-1.200382	-0.828377
12	1	0	0.015885	-2.139903	-0.114949
13	1	0	0.035152	2.156913	-0.087351
14	1	0	2.495644	-2.152813	-0.018207
15	1	0	2.519019	2.143960	0.009142
16	1	0	4.621858	0.916318	-0.279675
17	1	0	4.531347	-0.134251	1.137970
18	1	0	4.617914	-0.845876	-0.475067
19	1	0	-2.776004	0.689991	1.827911
20	1	0	-3.026320	-0.942614	1.543142

Cyclohexa-1,3-diene: B3LYP\6-31G(d) = -233.4189362
Sum of electronic and zero-point Energies = -233.296106
Sum of electronic and thermal Energies = -233.290934
Sum of electronic and thermal Enthalpies = -233.289989
Sum of electronic and thermal Free Energies = -233.324355

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192884	-0.735261	0.240000
2	6	0	-1.197557	0.727963	-0.239976
3	6	0	0.118031	-1.424647	-0.064478
4	6	0	0.109202	1.425309	0.064301
5	6	0	1.262435	-0.722357	-0.104263
6	6	0	1.257921	0.730054	0.104247
7	1	0	-1.358265	-0.765965	1.330772
8	1	0	-2.033174	-1.278645	-0.207904
9	1	0	-2.041045	1.265877	0.208577
10	1	0	-1.363639	0.758111	-1.330607
11	1	0	0.123400	-2.505849	-0.184899
12	1	0	0.108035	2.506562	0.184638
13	1	0	2.214744	-1.220352	-0.272549
14	1	0	2.207062	1.233895	0.272988

CbzNH$_2$: B3LYP\6-31G(d) = -515.4909521
Sum of electronic and zero-point Energies = -515.329309
Sum of electronic and thermal Energies = -515.319465
Sum of electronic and thermal Enthalpies = -515.318521
Sum of electronic and thermal Free Energies = -515.366120

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.162697	0.596060	0.506079
2	6	0	-2.170793	1.475650	0.065286
3	6	0	-2.935271	-0.780425	0.469766
4	6	0	-0.956668	0.982524	-0.411697
5	6	0	-1.718662	-1.272564	-0.005230
6	6	0	-0.719455	-0.399154	-0.450130
7	6	0	0.595849	-0.937772	-0.958054
8	8	0	1.621702	-0.928566	0.068483
9	6	0	2.418386	0.171920	0.106066
10	8	0	2.361357	1.111709	-0.666288
11	7	0	3.283426	0.081609	1.161217
12	1	0	-4.109757	0.982342	0.873888
13	1	0	-2.345084	2.548209	0.089354
14	1	0	-3.703659	-1.470192	0.809022

15	1	0	-0.179515	1.661699	-0.749621
16	1	0	-1.543437	-2.345980	-0.033631
17	1	0	0.503806	-1.989774	-1.238372
18	1	0	0.960549	-0.361643	-1.810766
19	1	0	4.054344	0.731592	1.165135
20	1	0	3.410177	-0.810099	1.616398

1-pentene: B3LYP\6-31G(d) = -196.5349802
Sum of electronic and zero-point Energies = -196.397289
Sum of electronic and thermal Energies = -196.390749
Sum of electronic and thermal Enthalpies = -196.389805
Sum of electronic and thermal Free Energies = -196.427078

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.484929	-0.216538	-0.304338
2	6	0	1.419444	0.341285	0.271897
3	6	0	0.074418	-0.312810	0.433695
4	6	0	-1.057197	0.448652	-0.283108
5	6	0	-2.431408	-0.196516	-0.079318
6	1	0	2.453695	-1.229022	-0.702836
7	1	0	3.430041	0.312008	-0.397712
8	1	0	1.499106	1.360847	0.654930
9	1	0	0.117626	-1.345040	0.060905
10	1	0	-0.173797	-0.377566	1.504924
11	1	0	-0.825994	0.503823	-1.354975
12	1	0	-1.080350	1.486216	0.078599
13	1	0	-2.698485	-0.233994	0.984101
14	1	0	-3.216145	0.363342	-0.600601
15	1	0	-2.446806	-1.225054	-0.460303

(*E*)-2-pentene: B3LYP\6-31G(d) = -196.5404425
Sum of electronic and zero-point Energies = -196.403061
Sum of electronic and thermal Energies = -196.396357
Sum of electronic and thermal Enthalpies = -196.395413
Sum of electronic and thermal Free Energies = -196.432863

Standard orientation:

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

1	6	0	2.534186	-0.269132	0.054173
2	6	0	1.171715	0.336303	0.239506
3	6	0	0.065351	-0.036870	-0.409088
4	6	0	-1.302232	0.561836	-0.217706
5	6	0	-2.340123	-0.462909	0.271236
6	1	0	2.519020	-1.073229	-0.689577
7	1	0	3.264480	0.482787	-0.275154
8	1	0	2.917852	-0.685693	0.995681
9	1	0	1.103050	1.148188	0.966828
10	1	0	0.130923	-0.851691	-1.134787
11	1	0	-1.651978	0.988375	-1.170138
12	1	0	-1.242453	1.396793	0.492332
13	1	0	-2.055193	-0.873579	1.246287
14	1	0	-3.331278	-0.005230	0.369395
15	1	0	-2.427806	-1.302083	-0.429589

(*Z*)-2-pentene: B3LYP\6-31G(d) = -196.5381217
Sum of electronic and zero-point Energies = -196.400482
Sum of electronic and thermal Energies = -196.393816
Sum of electronic and thermal Enthalpies = -196.392872
Sum of electronic and thermal Free Energies = -196.430651

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.076708	-0.674079	-0.083057
2	6	0	-1.305726	0.615320	-0.146202
3	6	0	-0.012404	0.817927	0.133384
4	6	0	1.017664	-0.190451	0.569579
5	6	0	2.199818	-0.283286	-0.411008
6	1	0	-1.459067	-1.526883	0.211547
7	1	0	-2.906048	-0.598639	0.633586
8	1	0	-2.527409	-0.906818	-1.057447
9	1	0	-1.891914	1.481465	-0.456529
10	1	0	0.369424	1.835176	0.025992
11	1	0	0.568542	-1.181544	0.696282
12	1	0	1.404139	0.099236	1.558509
13	1	0	2.683074	0.692677	-0.540879
14	1	0	2.958667	-0.986594	-0.049102
15	1	0	1.864716	-0.620664	-1.398137

1: B3LYP\6-31G(d) = -1504.1366357

Sum of electronic and zero-point Energies = -1503.843800
Sum of electronic and thermal Energies = -1503.821341
Sum of electronic and thermal Enthalpies = -1503.820396
Sum of electronic and thermal Free Energies = -1503.903352

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.649808	4.168762	0.575658
2	6	0	0.436325	3.254453	0.339976
3	6	0	2.956650	3.362872	0.601304
4	6	0	0.693473	2.224771	-0.733599
5	6	0	3.177506	2.629317	-0.732029
6	6	0	1.918359	1.952876	-1.221518
7	1	0	1.703919	4.911741	-0.232126
8	1	0	1.523670	4.728150	1.509816
9	1	0	-0.444143	3.846128	0.057619
10	1	0	0.148027	2.740295	1.269176
11	1	0	3.810279	4.016384	0.815375
12	1	0	2.913245	2.626505	1.416287
13	1	0	-0.177825	1.701644	-1.123318
14	1	0	3.982552	1.888546	-0.634132
15	1	0	3.520868	3.336405	-1.503205
16	1	0	2.022173	1.229149	-2.030204
17	1	0	1.532383	0.530682	0.291210
18	9	0	2.075354	-3.473509	-0.874210
19	6	0	2.475544	-2.294457	-0.408625
20	9	0	3.586107	-2.441542	0.305439
21	9	0	2.707310	-1.463018	-1.429862
22	16	0	1.122953	-1.578608	0.663887
23	8	0	1.063661	-2.349587	1.887299
24	8	0	-0.036479	-1.421437	-0.219266
25	8	0	1.752425	-0.145525	1.002610
26	1	0	-1.521176	-0.200710	-0.047413
27	8	0	-2.089147	0.591806	-0.021610
28	6	0	-3.403922	0.220129	-0.062339
29	6	0	-3.801470	-1.121316	-0.114155
30	6	0	-4.367268	1.235537	-0.048392
31	6	0	-5.160027	-1.438119	-0.150398
32	6	0	-5.720050	0.904719	-0.085431
33	6	0	-6.126637	-0.431551	-0.136555
34	1	0	-3.049459	-1.907080	-0.123868
35	1	0	-4.038544	2.269655	-0.007539
36	1	0	-5.460397	-2.482134	-0.189255

37	1	0	-6.462495	1.698741	-0.073831
38	1	0	-7.182693	-0.683783	-0.164740

TS2: B3LYP\6-31G(d) = -1504.1045947, imaginary frequency = -53 cm^{-1}

Sum of electronic and zero-point Energies = -1503.813020

Sum of electronic and thermal Energies = -1503.792445

Sum of electronic and thermal Enthalpies = -1503.791501

Sum of electronic and thermal Free Energies = -1503.865943

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.579363	3.093579	0.329858
2	6	0	-2.339248	2.144782	-0.861390
3	6	0	-1.557703	2.854921	1.448666
4	6	0	-0.922135	1.906784	-1.191228
5	6	0	-0.131015	3.067574	0.930364
6	6	0	0.160172	2.181557	-0.293891
7	1	0	-2.507293	4.133271	-0.015647
8	1	0	-3.602395	2.954091	0.694448
9	1	0	-2.872529	2.455637	-1.770370
10	1	0	-2.770319	1.147695	-0.636264
11	1	0	-1.755302	3.531086	2.288052
12	1	0	-1.660131	1.831532	1.834501
13	1	0	-0.689568	1.568957	-2.195649
14	1	0	0.604270	2.836204	1.706604
15	1	0	0.011602	4.121247	0.655217
16	1	0	1.082936	2.425580	-0.833568
17	1	0	0.452665	1.150370	0.132243
18	9	0	4.292469	-0.890967	-0.977668
19	6	0	3.490457	-0.106620	-0.255141
20	9	0	4.185410	0.406608	0.764776
21	9	0	3.080276	0.915228	-1.039909
22	16	0	2.019231	-1.062515	0.369244
23	8	0	2.572789	-2.136760	1.190038
24	8	0	1.326360	-1.468001	-0.892211
25	8	0	1.228120	-0.024927	1.119539
26	1	0	-0.202039	-0.933322	-1.147513
27	8	0	-1.109650	-0.583808	-1.406518
28	6	0	-2.098137	-1.161313	-0.662758
29	6	0	-1.877672	-1.635773	0.640891
30	6	0	-3.381662	-1.225725	-1.227690
31	6	0	-2.936413	-2.199669	1.348948

32	6	0	-4.433711	-1.783003	-0.499252
33	6	0	-4.215686	-2.276126	0.787858
34	1	0	-0.891682	-1.551887	1.085027
35	1	0	-3.524072	-0.870490	-2.244204
36	1	0	-2.759689	-2.577919	2.352094
37	1	0	-5.422416	-1.840654	-0.946526
38	1	0	-5.033366	-2.716831	1.350660

3: B3LYP\6-31G(d) = -1504.1620469

Sum of electronic and zero-point Energies = -1503.865606

Sum of electronic and thermal Energies = -1503.844859

Sum of electronic and thermal Enthalpies = -1503.843914

Sum of electronic and thermal Free Energies = -1503.921696

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.536664	3.372397	1.266870
2	6	0	-1.405589	1.841687	1.168664
3	6	0	-0.428157	4.081400	0.473455
4	6	0	-1.384703	1.400524	-0.294882
5	6	0	-0.401099	3.610417	-0.989264
6	6	0	-0.271997	2.079694	-1.087980
7	1	0	-2.518385	3.681673	0.878367
8	1	0	-1.509912	3.676535	2.319944
9	1	0	-2.232195	1.347885	1.694096
10	1	0	-0.471014	1.516599	1.642576
11	1	0	-0.567796	5.168679	0.516835
12	1	0	0.543353	3.867929	0.940604
13	1	0	0.427933	4.082665	-1.529530
14	1	0	-1.324517	3.932804	-1.492898
15	1	0	-0.311149	1.749441	-2.132949
16	1	0	0.697362	1.768619	-0.681563
17	9	0	3.453904	-1.923960	-1.244099
18	6	0	3.219928	-0.717545	-0.735203
19	9	0	4.376399	-0.112712	-0.467068
20	9	0	2.533671	0.012497	-1.622794
21	16	0	2.232688	-0.860521	0.842538
22	8	0	2.910314	-1.826513	1.685080
23	8	0	0.902319	-1.536302	0.271115
24	8	0	1.961032	0.505879	1.282081
25	1	0	0.196408	-0.852575	0.035291
26	8	0	-1.196349	-0.049740	-0.399739

27	6	0	-2.333902	-0.844879	-0.271271
28	6	0	-2.445363	-1.698723	0.826441
29	6	0	-3.317493	-0.823432	-1.263125
30	6	0	-3.557182	-2.536864	0.930994
31	6	0	-4.430144	-1.655845	-1.141638
32	6	0	-4.553443	-2.513730	-0.046124
33	1	0	-1.663346	-1.709830	1.578836
34	1	0	-3.199414	-0.173076	-2.124707
35	1	0	-3.643055	-3.205520	1.782914
36	1	0	-5.195651	-1.642081	-1.912600
37	1	0	-5.418478	-3.164712	0.041451
38	1	0	-2.352616	1.623664	-0.761545

4: B3LYP\6-31G(d) = -2072.1584094

Sum of electronic and zero-point Energies = -2071.815308

Sum of electronic and thermal Energies = -2071.787334

Sum of electronic and thermal Enthalpies = -2071.786390

Sum of electronic and thermal Free Energies = -2071.881649

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.364327	4.239959	-0.741765
2	6	0	0.195530	3.246189	-0.848678
3	6	0	2.665602	3.525801	-0.349356
4	6	0	0.585989	1.975521	-1.565225
5	6	0	3.049933	2.468452	-1.397487
6	6	0	1.863019	1.636887	-1.823133
7	1	0	1.506563	4.734748	-1.712418
8	1	0	1.123515	5.028195	-0.018946
9	1	0	-0.651160	3.705452	-1.376154
10	1	0	-0.191127	2.992880	0.150426
11	1	0	3.481507	4.247378	-0.226104
12	1	0	2.529809	3.035125	0.625006
13	1	0	-0.219244	1.319231	-1.895893
14	1	0	3.838476	1.810055	-1.009660
15	1	0	3.481274	2.953042	-2.287157
16	1	0	2.067765	0.726261	-2.386478
17	9	0	3.623915	-2.969297	0.177223
18	6	0	3.360244	-1.695657	0.452814
19	9	0	3.923006	-1.356060	1.607736
20	9	0	3.841817	-0.918213	-0.524530
21	16	0	1.508001	-1.471909	0.554153

22	8	0	1.049388	-2.141479	1.754871
23	8	0	0.989338	-1.797658	-0.773362
24	8	0	1.434178	0.110695	0.801794
25	1	0	1.331383	0.602342	-0.067744
26	7	0	-1.606852	-0.941178	-2.230054
27	16	0	-3.036606	-1.344770	-1.395720
28	8	0	-3.016018	-2.751127	-0.978345
29	6	0	-2.876427	-0.339074	0.076598
30	8	0	-4.123630	-0.820927	-2.228186
31	6	0	-3.361160	0.968759	0.069148
32	6	0	-2.264712	-0.875873	1.211078
33	6	0	-3.218081	1.748754	1.215785
34	6	0	-2.120561	-0.077304	2.343525
35	6	0	-2.595883	1.242188	2.366129
36	6	0	-2.462991	2.084226	3.612865
37	1	0	-1.758298	-1.153279	-3.216744
38	1	0	-0.817799	-1.479834	-1.864152
39	1	0	-3.851388	1.358278	-0.816984
40	1	0	-1.911267	-1.901448	1.207713
41	1	0	-3.601897	2.766109	1.219844
42	1	0	-1.631563	-0.489304	3.222395
43	1	0	-3.194885	1.780148	4.372377
44	1	0	-1.469588	1.977812	4.062687
45	1	0	-2.630073	3.145035	3.401602

TS5: B3LYP\6-31G(d) = -2072.120453, imaginary frequency = -142 cm^{-1}

Sum of electronic and zero-point Energies = -2071.778488

Sum of electronic and thermal Energies = -2071.752165

Sum of electronic and thermal Enthalpies = -2071.751221

Sum of electronic and thermal Free Energies = -2071.839793

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.016794	3.325349	2.239043
2	6	0	-0.691594	2.854107	0.925027
3	6	0	1.326364	2.620153	2.458626
4	6	0	0.235810	2.885596	-0.225886
5	6	0	2.279560	2.845152	1.280160
6	6	0	1.602625	2.523708	-0.080428
7	1	0	0.127307	4.413125	2.196484
8	1	0	-0.702732	3.130997	3.070071
9	1	0	-1.615703	3.388539	0.689694

10	1	0	-0.973255	1.793343	1.038995
11	1	0	1.793021	2.989433	3.379728
12	1	0	1.164480	1.543929	2.584706
13	1	0	-0.150078	3.215375	-1.183158
14	1	0	3.165802	2.211450	1.372094
15	1	0	2.623223	3.887728	1.252432
16	1	0	2.220844	2.732300	-0.956666
17	1	0	1.482903	1.364681	-0.006463
18	9	0	3.992748	-2.071225	-1.255309
19	6	0	3.522493	-1.156344	-0.405275
20	9	0	4.164550	-1.276144	0.762230
21	9	0	3.788635	0.069836	-0.905064
22	16	0	1.686457	-1.347745	-0.166389
23	8	0	1.500455	-2.633222	0.508293
24	8	0	1.144242	-1.224463	-1.546631
25	8	0	1.355005	-0.145264	0.684684
26	7	0	-0.667901	0.952384	-1.876439
27	16	0	-2.367576	0.707989	-1.849327
28	8	0	-2.784058	0.035874	-3.084955
29	6	0	-2.546523	-0.400363	-0.458906
30	8	0	-2.949503	2.013094	-1.501884
31	6	0	-3.279993	0.026511	0.648004
32	6	0	-1.998221	-1.685684	-0.514007
33	6	0	-3.446673	-0.846013	1.723842
34	6	0	-2.157564	-2.531097	0.578391
35	6	0	-2.882888	-2.127920	1.711180
36	6	0	-3.036006	-3.060243	2.888045
37	1	0	-0.447090	1.283346	-2.820143
38	1	0	-0.136325	0.072267	-1.730191
39	1	0	-3.717661	1.019103	0.654298
40	1	0	-1.435362	-2.017261	-1.379840
41	1	0	-4.022391	-0.522853	2.587491
42	1	0	-1.698687	-3.515251	0.553792
43	1	0	-3.468425	-4.019601	2.580410
44	1	0	-2.061765	-3.277920	3.342399
45	1	0	-3.681010	-2.631152	3.660736

6: B3LYP\6-31G(d) = -2072.1870453

Sum of electronic and zero-point Energies = -2071.839771

Sum of electronic and thermal Energies = -2071.813937

Sum of electronic and thermal Enthalpies = -2071.812993

Sum of electronic and thermal Free Energies = -2071.901097

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.396716	-2.142482	2.213880
2	6	0	-1.253335	-1.642185	1.314805
3	6	0	-3.768677	-1.710676	1.676276
4	6	0	-1.453964	-2.115346	-0.130074
5	6	0	-3.964339	-2.176407	0.226311
6	6	0	-2.824326	-1.681783	-0.678113
7	7	0	-0.407798	-1.559809	-1.051476
8	16	0	1.177423	-2.332650	-1.028964
9	8	0	1.528507	-2.404964	-2.450746
10	6	0	2.239712	-1.140245	-0.235655
11	8	0	1.098176	-3.530322	-0.189011
12	6	0	2.611953	-1.325606	1.094657
13	6	0	2.707936	-0.050981	-0.977468
14	6	0	3.447474	-0.385250	1.695805
15	6	0	3.536312	0.876873	-0.356681
16	6	0	3.911560	0.730597	0.988810
17	6	0	4.791119	1.763047	1.649842
18	1	0	-2.359097	-3.239641	2.278532
19	1	0	-2.248928	-1.765207	3.232659
20	1	0	-0.293438	-2.005457	1.696027
21	1	0	-1.213938	-0.546770	1.339611
22	1	0	-4.569461	-2.108373	2.311711
23	1	0	-3.846464	-0.614676	1.718068
24	1	0	-1.392412	-3.210832	-0.154157
25	1	0	-4.923374	-1.819913	-0.168272
26	1	0	-4.001699	-3.274763	0.196134
27	1	0	-2.958233	-2.067762	-1.698579
28	1	0	-2.855665	-0.586589	-0.741404
29	1	0	-0.701752	-1.726770	-2.019435
30	1	0	2.264745	-2.195871	1.640648
31	1	0	2.433302	0.061906	-2.020705
32	1	0	3.741809	-0.522129	2.732871
33	1	0	3.894535	1.731672	-0.924041
34	1	0	5.700869	1.944039	1.065548
35	1	0	4.265700	2.722145	1.735381
36	1	0	5.089508	1.453251	2.655637
37	9	0	-2.409021	3.272479	-1.330732
38	6	0	-1.979022	2.799676	-0.163891
39	9	0	-2.033280	3.761019	0.756586
40	9	0	-2.768697	1.783818	0.218123
41	16	0	-0.216476	2.203765	-0.308842
42	8	0	0.554591	3.312596	-0.842847

43	8	0	-0.408124	1.105347	-1.448325
44	8	0	0.112362	1.575614	0.966903
45	1	0	-0.365807	0.135160	-1.105612

7: B3LYP\6-31G(d) = -1710.9324933

Sum of electronic and zero-point Energies = -1710.606916

Sum of electronic and thermal Energies = -1710.580492

Sum of electronic and thermal Enthalpies = -1710.579548

Sum of electronic and thermal Free Energies = -1710.670398

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.360438	2.790344	2.017441
2	6	0	-0.886220	3.004379	1.563718
3	6	0	1.473696	2.409070	1.071742
4	6	0	-1.176765	2.916471	0.128877
5	6	0	1.262520	2.981400	-0.341692
6	6	0	-0.179437	2.877433	-0.782181
7	1	0	0.571712	2.812714	3.083838
8	1	0	-1.705472	3.217490	2.244976
9	1	0	1.516316	1.309744	1.022077
10	1	0	2.445254	2.729950	1.463467
11	1	0	-2.216880	2.913933	-0.191234
12	1	0	1.925315	2.473514	-1.050252
13	1	0	1.544187	4.048001	-0.363735
14	1	0	-0.404008	2.880436	-1.847719
15	1	0	-0.980357	0.821826	-0.697576
16	9	0	-4.789095	-1.028020	-0.078279
17	6	0	-3.848250	-0.414240	-0.792102
18	9	0	-3.954205	-0.762459	-2.070972
19	9	0	-3.997258	0.910503	-0.678258
20	16	0	-2.172177	-0.909459	-0.131055
21	8	0	-1.986648	-2.311867	-0.445962
22	8	0	-2.111358	-0.383514	1.230968
23	8	0	-1.236454	-0.048402	-1.113765
24	6	0	4.781303	0.384948	-1.923914
25	6	0	5.003647	-0.225961	-0.686952
26	6	0	3.565669	0.193228	-2.583562
27	6	0	4.017465	-1.027721	-0.112572
28	6	0	2.576819	-0.605954	-2.005092
29	6	0	2.793138	-1.224859	-0.767710
30	6	0	1.719060	-2.083104	-0.145566

31	8	0	0.950457	-1.347114	0.840474
32	6	0	1.305537	-1.522750	2.147132
33	8	0	2.250467	-2.189869	2.527555
34	7	0	0.467104	-0.801948	2.949624
35	1	0	5.553917	1.003232	-2.373631
36	1	0	5.950087	-0.082494	-0.172081
37	1	0	3.389660	0.659013	-3.549949
38	1	0	4.183172	-1.503008	0.850165
39	1	0	1.628853	-0.754657	-2.517407
40	1	0	0.981342	-2.392401	-0.888273
41	1	0	2.144505	-2.962622	0.341122
42	1	0	0.513086	-1.030180	3.931681
43	1	0	-0.433999	-0.529725	2.572073

TS8: B3LYP\6-31G(d) = -1710.9103081, imaginary frequency = -70 cm^{-1}

Sum of electronic and zero-point Energies = -1710.583493

Sum of electronic and thermal Energies = -1710.559067

Sum of electronic and thermal Enthalpies = -1710.558123

Sum of electronic and thermal Free Energies = -1710.641051

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.969961	3.034443	-0.797232
2	6	0	0.658825	3.337236	-0.536509
3	6	0	2.394120	1.776527	-1.472386
4	6	0	-0.326283	2.355204	-0.755053
5	6	0	1.263146	1.150107	-2.301563
6	6	0	-0.077657	1.143675	-1.553616
7	1	0	2.741678	3.731679	-0.478313
8	1	0	0.401861	4.255442	-0.017277
9	1	0	2.741968	1.088063	-0.685043
10	1	0	3.279170	1.971329	-2.090598
11	1	0	-1.351028	2.535708	-0.445250
12	1	0	1.535132	0.131133	-2.587636
13	1	0	1.149641	1.729247	-3.227153
14	1	0	-0.928358	1.018880	-2.237329
15	1	0	-0.216937	0.269392	-0.882236
16	9	0	-4.932521	-0.042031	-0.241111
17	6	0	-3.707096	-0.320575	-0.694432
18	9	0	-3.810324	-1.185504	-1.710239
19	9	0	-3.186543	0.835963	-1.198822
20	16	0	-2.608957	-0.985079	0.655991

21	8	0	-3.297970	-2.180829	1.144435
22	8	0	-2.558837	0.173349	1.601349
23	8	0	-1.320264	-1.213579	-0.058206
24	6	0	3.772322	-2.450102	-1.599578
25	6	0	4.662893	-1.777475	-0.761725
26	6	0	2.423199	-2.546213	-1.244189
27	6	0	4.203565	-1.203503	0.426340
28	6	0	1.961861	-1.980586	-0.054324
29	6	0	2.855179	-1.304259	0.790872
30	6	0	2.387856	-0.737870	2.112197
31	8	0	1.089329	-0.114552	1.995098
32	6	0	1.043278	1.225806	1.901164
33	8	0	2.004703	1.982053	1.951047
34	7	0	-0.247313	1.649428	1.673141
35	1	0	4.126729	-2.898965	-2.523837
36	1	0	5.712673	-1.695764	-1.031145
37	1	0	1.724953	-3.071994	-1.890052
38	1	0	4.899268	-0.678206	1.077419
39	1	0	0.908834	-2.047955	0.207242
40	1	0	2.234330	-1.533233	2.847626
41	1	0	3.100532	-0.012905	2.511007
42	1	0	-0.428677	2.584564	2.016438
43	1	0	-1.039481	0.976969	1.750262

9: B3LYP\6-31G(d) = -1710.949141
Sum of electronic and zero-point Energies = -1710.619717
Sum of electronic and thermal Energies = -1710.595193
Sum of electronic and thermal Enthalpies = -1710.594248
Sum of electronic and thermal Free Energies = -1710.680031

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.792841	3.180218	-0.689001
2	6	0	1.831853	3.230142	0.237626
3	6	0	2.579676	2.648660	-2.083258
4	6	0	0.417299	2.750975	-0.006803
5	6	0	1.086591	2.517062	-2.422946
6	6	0	0.308502	1.876712	-1.265249
7	6	0	3.535915	-3.391997	-1.176576
8	6	0	4.375659	-2.681023	-0.318902
9	6	0	2.148977	-3.272699	-1.049586
10	6	0	3.828699	-1.849890	0.660928

11	6	0	1.603677	-2.448667	-0.066541
12	6	0	2.442122	-1.728201	0.796457
13	6	0	1.848582	-0.838195	1.853049
14	8	0	1.261042	0.318948	1.184963
15	6	0	0.515343	1.107931	1.961613
16	8	0	0.369630	1.002823	3.159453
17	7	0	-0.177967	2.091351	1.205362
18	1	0	3.790126	3.539793	-0.438834
19	1	0	2.042099	3.644083	1.223675
20	1	0	3.077172	1.670610	-2.173705
21	1	0	3.079748	3.303279	-2.809694
22	1	0	-0.230640	3.628497	-0.147307
23	1	0	0.955095	1.921888	-3.333721
24	1	0	0.675280	3.513622	-2.636322
25	1	0	-0.745361	1.746063	-1.531838
26	1	0	0.717741	0.885465	-1.052000
27	1	0	3.959116	-4.039954	-1.939624
28	1	0	5.454655	-2.771343	-0.411559
29	1	0	1.492205	-3.828741	-1.713305
30	1	0	4.483994	-1.293224	1.327108
31	1	0	0.525807	-2.355685	0.037812
32	1	0	1.051540	-1.332867	2.413027
33	1	0	2.602275	-0.482417	2.560816
34	1	0	-0.505334	2.781977	1.878470
35	1	0	-1.670873	1.372217	0.806807
36	9	0	-4.246258	-0.153428	-1.534063
37	6	0	-3.169523	-0.820006	-1.125126
38	9	0	-3.366638	-2.129137	-1.281829
39	9	0	-2.112784	-0.446011	-1.856076
40	16	0	-2.845055	-0.480115	0.680393
41	8	0	-4.075086	-0.785492	1.386724
42	8	0	-2.642106	1.101404	0.615840
43	8	0	-1.580249	-1.136412	1.006768

10: B3LYP\6-31G(d) = -1710.9322752
Sum of electronic and zero-point Energies = -1710.606546
Sum of electronic and thermal Energies = -1710.580144
Sum of electronic and thermal Enthalpies = -1710.579200
Sum of electronic and thermal Free Energies = -1710.669865

Standard orientation:

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

1	6	0	2.169520	3.033494	1.278049
2	6	0	1.600417	1.635370	1.588227
3	6	0	1.262579	3.838532	0.375556
4	6	0	0.104993	1.658614	1.807516
5	6	0	-0.064855	3.635422	0.365542
6	6	0	-0.664914	2.595027	1.212208
7	1	0	2.313360	3.600293	2.213437
8	1	0	3.164723	2.931442	0.831350
9	1	0	2.101368	1.208051	2.463647
10	1	0	1.819595	0.947796	0.757984
11	1	0	1.702342	4.633411	-0.223174
12	1	0	-0.338053	0.885527	2.430282
13	1	0	-0.720688	4.249102	-0.246908
14	1	0	-1.743482	2.601761	1.359948
15	9	0	-4.934073	-0.537269	-0.229952
16	6	0	-3.892398	0.183880	-0.637688
17	9	0	-3.995098	0.427968	-1.940450
18	9	0	-3.862520	1.341345	0.031829
19	16	0	-2.326941	-0.773730	-0.287699
20	8	0	-2.300406	-1.904483	-1.193638
21	8	0	-2.273623	-0.920286	1.166963
22	8	0	-1.242127	0.299158	-0.785196
23	1	0	-0.893557	0.830083	-0.014017
24	6	0	4.503669	0.732827	-1.666185
25	6	0	4.765580	-0.290313	-0.750777
26	6	0	3.263154	0.792618	-2.304160
27	6	0	3.792597	-1.251073	-0.475086
28	6	0	2.289431	-0.168930	-2.027293
29	6	0	2.544146	-1.198626	-1.112354
30	6	0	1.481199	-2.225651	-0.806076
31	8	0	0.710828	-1.873296	0.372641
32	6	0	1.109587	-2.429490	1.551386
33	8	0	2.101271	-3.120413	1.696364
34	7	0	0.247397	-2.057853	2.548329
35	1	0	5.265676	1.476470	-1.885403
36	1	0	5.731260	-0.342316	-0.254591
37	1	0	3.054433	1.583956	-3.019361
38	1	0	3.984912	-2.042465	0.243383
39	1	0	1.321739	-0.120025	-2.521060
40	1	0	0.737820	-2.272726	-1.604121
41	1	0	1.916911	-3.213776	-0.646996
42	1	0	0.335864	-2.588226	3.402976
43	1	0	-0.685496	-1.767756	2.274389

TS11: B3LYP\6-31G(d) = -1710.8894086, imaginary frequency = -193 cm^{-1}

Sum of electronic and zero-point Energies = -1710.565320

Sum of electronic and thermal Energies = -1710.540803

Sum of electronic and thermal Enthalpies = -1710.539859

Sum of electronic and thermal Free Energies = -1710.624598

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.162117	3.168457	0.826958
2	6	0	1.747714	1.870560	1.573911
3	6	0	1.321682	3.364204	-0.410274
4	6	0	0.270790	1.840475	1.735560
5	6	0	0.098075	2.840241	-0.522601
6	6	0	-0.559436	2.089916	0.609064
7	1	0	2.092862	4.049210	1.484285
8	1	0	3.220942	3.067786	0.564795
9	1	0	2.269262	1.744430	2.524681
10	1	0	2.036079	1.035675	0.920602
11	1	0	1.738031	3.959480	-1.219701
12	1	0	-0.162896	1.845140	2.728490
13	1	0	-0.496501	2.959173	-1.423459
14	1	0	-1.560961	2.449532	0.871384
15	1	0	-0.839426	1.031230	0.128962
16	9	0	-5.066361	-0.417603	-0.148214
17	6	0	-3.951136	0.117144	-0.651585
18	9	0	-4.079022	0.222232	-1.977677
19	9	0	-3.806110	1.358487	-0.141857
20	16	0	-2.469150	-0.919992	-0.211854
21	8	0	-2.672857	-2.211205	-0.863631
22	8	0	-2.466127	-0.879338	1.273853
23	8	0	-1.327784	-0.107460	-0.798486
24	6	0	4.202142	0.254177	-2.307012
25	6	0	4.879384	-0.548633	-1.388213
26	6	0	2.810538	0.170310	-2.410100
27	6	0	4.166164	-1.432716	-0.575748
28	6	0	2.097183	-0.720044	-1.607157
29	6	0	2.774987	-1.531385	-0.684434
30	6	0	2.008412	-2.516491	0.165792
31	8	0	0.905876	-1.879472	0.858436
32	6	0	1.194458	-1.279215	2.026090
33	8	0	2.265983	-1.303825	2.599583
34	7	0	0.092314	-0.552539	2.468580
35	1	0	4.755313	0.942202	-2.941253

36	1	0	5.960583	-0.484412	-1.298363
37	1	0	2.278461	0.794375	-3.123041
38	1	0	4.692076	-2.048245	0.149965
39	1	0	1.014092	-0.778363	-1.682306
40	1	0	1.515833	-3.276131	-0.445775
41	1	0	2.658682	-3.000603	0.897301
42	1	0	0.096651	-0.437508	3.476312
43	1	0	-0.824616	-0.804968	2.066912

12: B3LYP\6-31G(d) = -1710.9512554
Sum of electronic and zero-point Energies = -1710.621721
Sum of electronic and thermal Energies = -1710.597191
Sum of electronic and thermal Enthalpies = -1710.596247
Sum of electronic and thermal Free Energies = -1710.681554

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.947754	3.919082	0.224390
2	6	0	2.078288	2.895585	0.973945
3	6	0	3.026030	3.619918	-1.252094
4	6	0	0.788989	2.614387	0.188318
5	6	0	2.209135	2.765873	-1.875772
6	6	0	1.093884	2.012676	-1.192287
7	1	0	2.551921	4.935927	0.375589
8	1	0	3.956693	3.931934	0.657873
9	1	0	1.836246	3.265706	1.978553
10	1	0	2.631745	1.958104	1.093649
11	1	0	3.797126	4.137506	-1.820621
12	1	0	2.331467	2.584119	-2.942086
13	1	0	0.188778	2.044134	-1.812759
14	1	0	1.360507	0.953896	-1.092506
15	9	0	-3.362476	-0.316661	1.488652
16	6	0	-3.868312	-0.622098	0.293198
17	9	0	-4.183112	-1.916701	0.258120
18	9	0	-4.958846	0.108638	0.069847
19	16	0	-2.590532	-0.281730	-1.025062
20	8	0	-1.415764	-1.078561	-0.676142
21	8	0	-2.304424	1.265278	-0.740707
22	8	0	-3.250591	-0.402451	-2.310841
23	6	0	4.043003	-3.420356	-1.093286
24	6	0	4.455739	-3.026797	0.180007
25	6	0	2.733186	-3.166732	-1.510012

26	6	0	3.560682	-2.377705	1.032697
27	6	0	1.837870	-2.525100	-0.655849
28	6	0	2.247480	-2.123435	0.623899
29	6	0	1.278663	-1.431282	1.541180
30	8	0	1.069637	-0.074372	1.038669
31	6	0	0.084497	0.606540	1.633278
32	8	0	-0.544698	0.246597	2.604827
33	7	0	-0.217148	1.812186	0.953221
34	1	0	4.737821	-3.925792	-1.758788
35	1	0	5.472270	-3.223316	0.510080
36	1	0	2.407364	-3.475446	-2.499659
37	1	0	3.884001	-2.069627	2.024593
38	1	0	0.817633	-2.329686	-0.975723
39	1	0	0.304072	-1.923874	1.561914
40	1	0	1.657215	-1.364016	2.564633
41	1	0	-0.734087	2.391053	1.611953
42	1	0	-1.505095	1.387586	-0.116011
43	1	0	0.278172	3.571427	0.022063

13: B3LYP\6-31G(d) = -1580.543594
Sum of electronic and zero-point Energies = -1580.227002
Sum of electronic and thermal Energies = -1580.201017
Sum of electronic and thermal Enthalpies = -1580.200073
Sum of electronic and thermal Free Energies = -1580.290737

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.843091	2.605438	-0.622857
2	6	0	-0.324316	2.451234	0.311249
3	6	0	-1.530481	3.019515	0.151738
4	6	0	2.047876	3.285395	0.058779
5	6	0	3.273254	3.358304	-0.856669
6	1	0	0.545485	3.176325	-1.512526
7	1	0	1.158531	1.609663	-0.966684
8	1	0	-0.144788	1.827345	1.188473
9	1	0	-2.321217	2.896423	0.888509
10	1	0	-1.750534	3.665587	-0.696982
11	1	0	2.304416	2.727461	0.968340
12	1	0	1.756249	4.293915	0.380264
13	1	0	3.051711	3.908866	-1.779209
14	1	0	4.107253	3.865418	-0.358617
15	1	0	3.611125	2.353816	-1.137535

16	1	0	-1.814110	1.154919	-0.731948
17	9	0	-4.879445	-1.362208	0.790343
18	6	0	-4.380533	-0.457395	-0.046602
19	9	0	-5.041088	-0.492309	-1.198732
20	9	0	-4.483113	0.759993	0.493646
21	16	0	-2.575660	-0.842795	-0.337001
22	8	0	-2.494056	-2.059505	-1.118039
23	8	0	-1.928826	-0.714918	0.970134
24	8	0	-2.166369	0.388557	-1.275751
25	8	0	0.681897	-0.330235	2.181461
26	6	0	1.709591	-0.726085	1.365607
27	6	0	2.994732	-0.275235	1.671556
28	6	0	1.521822	-1.552962	0.247998
29	6	0	4.084933	-0.634228	0.873996
30	6	0	2.605994	-1.909763	-0.547501
31	6	0	3.895234	-1.453773	-0.244596
32	8	0	4.890098	-1.865027	-1.094240
33	6	0	6.213110	-1.443166	-0.819860
34	1	0	-0.161634	-0.670434	1.832258
35	1	0	3.135522	0.353574	2.545623
36	1	0	0.531031	-1.930282	0.007829
37	1	0	5.071545	-0.271929	1.140128
38	1	0	2.471135	-2.550682	-1.413252
39	1	0	6.837657	-1.881867	-1.600697
40	1	0	6.307434	-0.348653	-0.855618
41	1	0	6.558767	-1.798669	0.160793

TS14: B3LYP\6-31G(d) = -1580.5157878, imaginary frequency = -117 cm^{-1}

Sum of electronic and zero-point Energies = -1580.201535

Sum of electronic and thermal Energies = -1580.177278

Sum of electronic and thermal Enthalpies = -1580.176333

Sum of electronic and thermal Free Energies = -1580.260589

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.261307	2.746126	-0.497465
2	6	0	0.075668	2.761508	0.374040
3	6	0	-1.253882	2.907394	-0.086918
4	6	0	2.348097	3.756305	-0.039824
5	6	0	3.605537	3.656591	-0.907730
6	1	0	0.985739	2.912115	-1.544626
7	1	0	1.706168	1.737251	-0.421197

8	1	0	0.258171	2.670169	1.440514
9	1	0	-1.986370	3.210097	0.663647
10	1	0	-1.352885	3.427258	-1.045151
11	1	0	2.600126	3.558105	1.009503
12	1	0	1.942989	4.774857	-0.081271
13	1	0	3.381137	3.867122	-1.959581
14	1	0	4.360872	4.376835	-0.576039
15	1	0	4.042748	2.653436	-0.850591
16	1	0	-1.616700	1.818511	-0.416351
17	9	0	-4.712407	-1.646946	0.795318
18	6	0	-4.370022	-0.637430	-0.009548
19	9	0	-4.996367	-0.781690	-1.181257
20	9	0	-4.763656	0.515212	0.551146
21	16	0	-2.527159	-0.623002	-0.266023
22	8	0	-2.200636	-1.886606	-0.931226
23	8	0	-1.994880	-0.442765	1.115539
24	8	0	-2.303449	0.603887	-1.119966
25	8	0	0.518303	0.396009	1.458652
26	6	0	1.510604	-0.382271	0.932578
27	6	0	2.834378	-0.029522	1.218064
28	6	0	1.254871	-1.497553	0.113457
29	6	0	3.900502	-0.774119	0.704568
30	6	0	2.313983	-2.238671	-0.389407
31	6	0	3.643441	-1.886838	-0.103248
32	8	0	4.601326	-2.688701	-0.656566
33	6	0	5.960324	-2.395193	-0.382089
34	1	0	-0.377687	-0.022383	1.336987
35	1	0	3.023384	0.814725	1.875306
36	1	0	0.234393	-1.786473	-0.120495
37	1	0	4.914939	-0.483545	0.952789
38	1	0	2.131458	-3.105621	-1.016434
39	1	0	6.543471	-3.154059	-0.906903
40	1	0	6.243182	-1.400853	-0.754210
41	1	0	6.177109	-2.451254	0.693259

15: B3LYP\6-31G(d) = -1580.5729931
Sum of electronic and zero-point Energies = -1580.253259
Sum of electronic and thermal Energies = -1580.228866
Sum of electronic and thermal Enthalpies = -1580.227921
Sum of electronic and thermal Free Energies = -1580.311967

Standard orientation:

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

1	6	0	0.498926	2.645593	-0.339570
2	6	0	0.613857	2.055001	1.067794
3	6	0	-0.502868	2.460912	2.019730
4	6	0	0.708776	4.166741	-0.389931
5	6	0	0.708699	4.709066	-1.823323
6	1	0	-0.484716	2.387987	-0.752682
7	1	0	1.251499	2.162822	-0.976788
8	1	0	1.586633	2.320657	1.500721
9	1	0	-0.393217	1.948833	2.980945
10	1	0	-0.469343	3.539405	2.201779
11	1	0	-1.483762	2.217323	1.598297
12	1	0	1.661755	4.421301	0.096541
13	1	0	-0.076402	4.672760	0.186232
14	1	0	-0.240925	4.493926	-2.327245
15	1	0	0.855767	5.794801	-1.836153
16	1	0	1.510269	4.255411	-2.418601
17	9	0	-3.627524	-2.754123	0.215378
18	6	0	-3.969795	-1.481361	0.033289
19	9	0	-4.819991	-1.388649	-0.990003
20	9	0	-4.546381	-1.008292	1.135815
21	16	0	-2.463285	-0.462541	-0.389859
22	8	0	-1.822689	-1.074631	-1.549702
23	8	0	-1.663177	-0.783698	0.955406
24	8	0	-2.868560	0.940879	-0.433874
25	8	0	0.580107	0.586854	1.002117
26	6	0	1.728849	-0.069296	0.553656
27	6	0	2.876717	-0.089494	1.340872
28	6	0	1.694569	-0.759776	-0.661677
29	6	0	4.010685	-0.785348	0.913189
30	6	0	2.815869	-1.464399	-1.082744
31	6	0	3.982993	-1.477056	-0.304154
32	1	0	2.885774	0.425496	2.297050
33	1	0	0.788701	-0.755601	-1.260232
34	1	0	4.894846	-0.790260	1.539780
35	1	0	2.810216	-2.013113	-2.019010
36	1	0	-0.805849	-0.237837	0.987258
37	8	0	5.027500	-2.191419	-0.814811
38	6	0	6.230131	-2.253826	-0.064992
39	1	0	6.668466	-1.257321	0.079671
40	1	0	6.071450	-2.723609	0.914803
41	1	0	6.916573	-2.867155	-0.651262

16: B3LYP\6-31G(d) = -1670.5286064

Sum of electronic and zero-point Energies = -1670.241977
Sum of electronic and thermal Energies = -1670.216143
Sum of electronic and thermal Enthalpies = -1670.215199
Sum of electronic and thermal Free Energies = -1670.306178

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.212975	3.117116	-0.714124
2	6	0	-1.437937	2.790706	0.091822
3	6	0	-2.708374	2.968750	-0.304405
4	6	0	0.682643	4.161958	-0.018094
5	6	0	1.968163	4.444468	-0.800877
6	1	0	-0.499205	3.472420	-1.712624
7	1	0	0.376013	2.199204	-0.854491
8	1	0	-1.247676	2.386344	1.086549
9	1	0	-3.547492	2.742619	0.349608
10	1	0	-2.948629	3.392136	-1.278459
11	1	0	0.933479	3.800730	0.987953
12	1	0	0.113022	5.090641	0.116994
13	1	0	1.747749	4.819838	-1.807466
14	1	0	2.581689	5.196204	-0.292396
15	1	0	2.572469	3.535823	-0.908437
16	9	0	-4.425707	-2.164286	1.029808
17	6	0	-4.238931	-1.273091	0.062419
18	9	0	-4.820460	-1.685533	-1.057021
19	9	0	-4.748127	-0.094326	0.429008
20	16	0	-2.401417	-1.075477	-0.218996
21	8	0	-1.900116	-2.286666	-0.834369
22	8	0	-1.858872	-0.574078	1.048447
23	8	0	-2.392773	0.091353	-1.314566
24	1	0	-2.346638	0.994620	-0.879358
25	8	0	0.675285	0.537667	1.736782
26	6	0	1.766582	-0.035763	1.175666
27	6	0	2.994562	0.629734	1.332168
28	6	0	1.706590	-1.242395	0.457415
29	6	0	4.147651	0.100603	0.773255
30	6	0	2.861994	-1.771899	-0.103267
31	6	0	4.072382	-1.096990	0.056986
32	7	0	5.285707	-1.653021	-0.536262
33	8	0	6.339883	-1.032028	-0.379929
34	8	0	5.189157	-2.711525	-1.161369
35	1	0	-0.122639	-0.000182	1.564518
36	1	0	3.020004	1.554414	1.899361

37	1	0	0.759988	-1.761708	0.337841
38	1	0	5.105320	0.594691	0.881541
39	1	0	2.839288	-2.698670	-0.663283

TS17: B3LYP\6-31G(d) = -1670.4973549, imaginary frequency = -111 cm^{-1}

Sum of electronic and zero-point Energies = -1670.212327

Sum of electronic and thermal Energies = -1670.188204

Sum of electronic and thermal Enthalpies = -1670.187260

Sum of electronic and thermal Free Energies = -1670.271743

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.796546	2.916866	0.370657
2	6	0	0.175354	2.815666	-0.728157
3	6	0	1.581079	2.915365	-0.529920
4	6	0	-1.406344	4.358695	0.383193
5	6	0	-2.456613	4.496562	1.489812
6	1	0	-0.320040	2.708823	1.334462
7	1	0	-1.617085	2.206804	0.211663
8	1	0	-0.219623	2.779033	-1.738916
9	1	0	2.173339	3.126446	-1.420575
10	1	0	1.845369	3.540772	0.332699
11	1	0	1.936500	1.889918	-0.096003
12	1	0	-1.858567	4.572577	-0.592859
13	1	0	-0.603357	5.090176	0.531302
14	1	0	-2.021527	4.306423	2.476832
15	1	0	-2.870498	5.510303	1.492808
16	1	0	-3.283199	3.793237	1.342227
17	9	0	4.467218	-2.282215	-0.478911
18	6	0	4.336416	-1.069645	0.063997
19	9	0	4.984561	-1.039846	1.231937
20	9	0	4.882681	-0.164212	-0.758419
21	16	0	2.535805	-0.683116	0.330547
22	8	0	2.032855	-1.698411	1.259519
23	8	0	1.973893	-0.735193	-1.057104
24	8	0	2.542970	0.720990	0.873653
25	8	0	-0.303322	0.479696	-1.479846
26	6	0	-1.388799	-0.190492	-1.014954
27	6	0	-2.653772	0.268027	-1.424349
28	6	0	-1.280851	-1.291069	-0.145342
29	6	0	-3.804739	-0.362409	-0.970768
30	6	0	-2.433799	-1.924332	0.300796

31	6	0	-3.682531	-1.453651	-0.110285
32	7	0	-4.895376	-2.118041	0.371206
33	8	0	-5.981573	-1.663702	0.004743
34	8	0	-4.761351	-3.089579	1.115796
35	1	0	0.550822	-0.029129	-1.303269
36	1	0	-2.713869	1.098303	-2.121549
37	1	0	-0.305734	-1.641011	0.178184
38	1	0	-4.789931	-0.033290	-1.277241
39	1	0	-2.378874	-2.774682	0.969408

18: B3LYP\6-31G(d)=-1670.5517266

Sum of electronic and zero-point Energies= -1670.262036

Sum of electronic and thermal Energies= -1670.237588

Sum of electronic and thermal Enthalpies= -1670.236644

Sum of electronic and thermal Free Energies= -1670.322050

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.172441	2.796892	-0.436708
2	6	0	0.267147	2.262847	0.994024
3	6	0	-0.930539	2.580371	1.877464
4	6	0	0.221661	4.329744	-0.526753
5	6	0	0.239641	4.827193	-1.976296
6	1	0	-0.752685	2.421346	-0.892024
7	1	0	1.006723	2.378618	-1.016025
8	1	0	1.183351	2.630691	1.468955
9	1	0	-0.826156	2.102563	2.856684
10	1	0	-1.002596	3.660951	2.032755
11	1	0	-1.861491	2.240483	1.412602
12	1	0	1.114239	4.700066	-0.001902
13	1	0	-0.643366	4.761777	-0.007954
14	1	0	-0.652199	4.493373	-2.519365
15	1	0	0.267038	5.921486	-2.017819
16	1	0	1.117270	4.449583	-2.514429
17	9	0	-3.649907	-2.906495	0.346757
18	6	0	-4.041041	-1.668450	0.061048
19	9	0	-4.858010	-1.685077	-0.991254
20	9	0	-4.667693	-1.138517	1.107708
21	16	0	-2.561707	-0.620975	-0.394166
22	8	0	-1.823405	-1.314921	-1.444351
23	8	0	-1.818254	-0.764749	1.021381
24	8	0	-3.019241	0.750851	-0.599740

25	8	0	0.364720	0.791783	0.951045
26	6	0	1.570135	0.201140	0.625789
27	6	0	2.748058	0.518882	1.314776
28	6	0	1.566645	-0.782184	-0.370677
29	6	0	3.930120	-0.140175	0.996465
30	6	0	2.746253	-1.450524	-0.681475
31	6	0	3.914792	-1.116451	0.001317
32	7	0	5.163626	-1.813668	-0.330905
33	8	0	6.179780	-1.489813	0.284919
34	8	0	5.120314	-2.679073	-1.204810
35	1	0	2.738863	1.257205	2.109127
36	1	0	0.644751	-1.015807	-0.893836
37	1	0	4.855704	0.079354	1.513986
38	1	0	2.774002	-2.214873	-1.448166
39	1	0	-1.004213	-0.173058	1.030106

19: B3LYP\6-31G(d) = -1158.5467969
Sum of electronic and zero-point Energies = -1158.368922
Sum of electronic and thermal Energies = -1158.353109
Sum of electronic and thermal Enthalpies = -1158.352165
Sum of electronic and thermal Free Energies = -1158.414770

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.897685	-1.720689	1.448315
2	6	0	-2.478521	-1.674176	0.239663
3	6	0	-2.997433	-0.453355	-0.472373
4	6	0	-2.872222	0.878640	0.273630
5	6	0	-3.425617	2.052393	-0.540696
6	1	0	-1.749625	-0.831275	2.055192
7	1	0	-1.591557	-2.665615	1.891147
8	1	0	-2.610728	-2.612942	-0.301884
9	1	0	-4.053846	-0.640304	-0.722567
10	1	0	-2.481702	-0.378759	-1.440804
11	1	0	-1.817342	1.066862	0.506832
12	1	0	-3.401256	0.812904	1.234076
13	1	0	-4.485948	1.906662	-0.781333
14	1	0	-3.336231	2.993964	0.012091
15	1	0	-2.880672	2.166691	-1.484994
16	8	0	0.832399	-1.720423	0.026561
17	16	0	1.311284	-0.424433	-0.801221
18	6	0	1.775594	0.701662	0.615159

19	8	0	0.170485	0.197822	-1.462791
20	8	0	2.532403	-0.774044	-1.497713
21	9	0	0.721384	0.838641	1.432027
22	9	0	2.111741	1.892390	0.125648
23	9	0	2.795433	0.189987	1.296421
24	1	0	-0.135640	-1.650124	0.254282

TS20: B3LYP\6-31G(d) = -1158.5063747, imaginary frequency = -236 cm^{-1}

Sum of electronic and zero-point Energies = -1158.332734

Sum of electronic and thermal Energies = -1158.317950

Sum of electronic and thermal Enthalpies = -1158.317006

Sum of electronic and thermal Free Energies = -1158.378135

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.117542	-1.926052	-1.079184
2	6	0	2.714336	-1.489434	0.143045
3	6	0	2.926438	-0.137552	0.544569
4	6	0	3.188105	0.974826	-0.479699
5	6	0	3.090373	2.363166	0.159478
6	1	0	2.290007	-1.295095	-1.952222
7	1	0	2.227794	-2.992874	-1.283039
8	1	0	2.813014	-2.242584	0.928310
9	1	0	3.510841	-0.049986	1.465932
10	1	0	2.457919	0.898626	-1.291029
11	1	0	4.183988	0.825820	-0.917897
12	1	0	3.804754	2.474471	0.984185
13	1	0	3.309007	3.141751	-0.578298
14	1	0	2.082970	2.535285	0.550847
15	1	0	1.808762	0.021145	0.868975
16	8	0	-0.644147	-1.579044	-0.476597
17	16	0	-0.936594	-0.486115	0.512101
18	6	0	-2.251369	0.511892	-0.347951
19	8	0	0.195325	0.500066	0.608899
20	8	0	-1.509542	-0.922275	1.786695
21	9	0	-1.791516	0.969805	-1.519514
22	9	0	-2.606076	1.552673	0.412145
23	9	0	-3.327901	-0.246608	-0.574559
24	1	0	0.980238	-1.792602	-0.825548

21: B3LYP\6-31G(d) = -1158.5510344

Sum of electronic and zero-point Energies = -1158.373229
Sum of electronic and thermal Energies = -1158.357229
Sum of electronic and thermal Enthalpies = -1158.356285
Sum of electronic and thermal Free Energies = -1158.419559

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.598338	-1.733003	1.301753
2	6	0	-2.657858	-1.349221	-0.150032
3	6	0	-2.956743	-0.148763	-0.681695
4	6	0	-3.312810	1.126606	0.037111
5	6	0	-2.413906	2.310047	-0.361375
6	1	0	-2.785942	-0.891754	1.973933
7	1	0	-3.344280	-2.509546	1.516872
8	1	0	-1.616113	-2.154342	1.544366
9	1	0	-2.460756	-2.166299	-0.846405
10	1	0	-2.978277	-0.076191	-1.771625
11	1	0	-3.279763	0.986208	1.122483
12	1	0	-4.355472	1.376824	-0.209242
13	1	0	-2.432009	2.475698	-1.445045
14	1	0	-2.749566	3.233114	0.123480
15	1	0	-1.374157	2.133404	-0.067611
16	8	0	0.796455	-1.698988	0.632865
17	16	0	1.329854	-0.822187	-0.402585
18	6	0	1.835271	0.765052	0.441888
19	8	0	0.128658	-0.266605	-1.322426
20	8	0	2.421593	-1.206711	-1.274391
21	9	0	0.787418	1.267357	1.107108
22	9	0	2.253730	1.650566	-0.456835
23	9	0	2.814817	0.497159	1.302353
24	1	0	-0.752355	-0.433745	-0.887760

22: B3LYP\6-31G(d) = -1158.5466756
Sum of electronic and zero-point Energies = -1158.368951
Sum of electronic and thermal Energies = -1158.352953
Sum of electronic and thermal Enthalpies = -1158.352009
Sum of electronic and thermal Free Energies = -1158.416204

Standard orientation:

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

1	9	0	-3.109568	-0.182458	1.455582
2	6	0	-2.497239	0.373106	0.412343
3	9	0	-3.393844	0.702076	-0.512569
4	9	0	-1.847080	1.472879	0.812403
5	16	0	-1.264908	-0.845595	-0.283345
6	8	0	-2.015329	-1.910266	-0.917579
7	8	0	-0.281387	-1.081828	0.766668
8	8	0	-0.618166	0.061577	-1.448384
9	1	0	0.162148	0.566853	-1.089525
10	6	0	1.409510	2.000216	-0.121332
11	6	0	2.336216	1.230559	-0.711324
12	6	0	2.965520	0.003929	-0.111314
13	6	0	4.482361	0.173690	0.109413
14	6	0	5.135903	-1.087585	0.682042
15	1	0	1.030676	1.772319	0.873095
16	1	0	1.026746	2.900348	-0.596419
17	1	0	2.698749	1.516593	-1.701169
18	1	0	2.471282	-0.244810	0.834984
19	1	0	2.803002	-0.852079	-0.783119
20	1	0	4.652195	1.022029	0.785202
21	1	0	4.961681	0.438383	-0.843305
22	1	0	5.006688	-1.942501	0.007420
23	1	0	6.210890	-0.941167	0.834589
24	1	0	4.694318	-1.358267	1.648411

TS23: B3LYP\6-31G(d) = -1158.5063317, imaginary frequency = -236 cm^{-1}

Sum of electronic and zero-point Energies = -1158.332986

Sum of electronic and thermal Energies = -1158.318255

Sum of electronic and thermal Enthalpies = -1158.317311

Sum of electronic and thermal Free Energies = -1158.376953

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.641243	2.089906	-0.024553
2	9	0	2.663735	-1.624210	-0.525059
3	6	0	2.479778	-0.310267	-0.363134
4	9	0	3.507116	0.189633	0.329948
5	9	0	2.446447	0.272867	-1.567632
6	16	0	0.885827	0.001310	0.546461
7	8	0	1.026715	-0.625475	1.862188
8	8	0	-0.133237	-0.615919	-0.369159
9	8	0	0.790038	1.503490	0.555174

10	6	0	-1.672414	2.484043	-0.438428
11	6	0	-2.555875	1.514787	0.119469
12	6	0	-2.841528	0.235312	-0.445927
13	6	0	-3.918522	-0.653616	0.184234
14	6	0	-3.782471	-2.115895	-0.252199
15	1	0	-1.571430	2.470761	-1.525416
16	1	0	-1.758025	3.486210	-0.012941
17	1	0	-2.859857	1.672431	1.158281
18	1	0	-2.834235	0.234356	-1.543082
19	1	0	-4.910005	-0.271683	-0.091703
20	1	0	-3.846632	-0.584400	1.277432
21	1	0	-2.806972	-2.521964	0.035735
22	1	0	-4.560644	-2.731858	0.209573
23	1	0	-3.878810	-2.215494	-1.339745
24	1	0	-1.783010	-0.216788	-0.231990

24: B3LYP\6-31G(d) = -1158.5523324
Sum of electronic and zero-point Energies = -1158.375002
Sum of electronic and thermal Energies = -1158.358841
Sum of electronic and thermal Enthalpies = -1158.357896
Sum of electronic and thermal Free Energies = -1158.422266

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	2.544537	-0.327400	-1.571446
2	6	0	2.225880	0.294192	-0.440219
3	9	0	3.322292	0.496803	0.287104
4	9	0	1.657698	1.471504	-0.725596
5	16	0	1.034442	-0.747383	0.552081
6	8	0	1.612312	-2.072213	0.655819
7	8	0	-0.189706	-0.813215	-0.496803
8	8	0	0.646394	0.042499	1.714509
9	1	0	-0.900387	-0.159627	-0.247085
10	6	0	-1.511540	2.665584	0.112045
11	6	0	-2.227708	1.408589	0.522300
12	6	0	-3.010553	0.663598	-0.276164
13	6	0	-3.805019	-0.543687	0.150304
14	6	0	-3.604238	-1.768055	-0.758098
15	1	0	-1.639378	2.875627	-0.955275
16	1	0	-1.897052	3.525841	0.675138
17	1	0	-0.439158	2.604126	0.329631
18	1	0	-2.118225	1.115662	1.567991

19	1	0	-3.127875	0.966020	-1.320309
20	1	0	-4.871553	-0.271848	0.141373
21	1	0	-3.561666	-0.797976	1.189617
22	1	0	-2.566309	-2.116496	-0.737199
23	1	0	-4.245405	-2.596324	-0.438143
24	1	0	-3.857748	-1.532923	-1.798816

1(CH_3): B3LYP\6-31G(d) = -1324.3934969

Sum of electronic and zero-point Energies = -1323.992015

Sum of electronic and thermal Energies = -1323.967632

Sum of electronic and thermal Enthalpies = -1323.966688

Sum of electronic and thermal Free Energies = -1324.051792

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.615950	3.569764	1.279738
2	6	0	-1.129318	2.346492	0.503036
3	6	0	0.894916	3.753313	1.076884
4	6	0	-0.561679	2.279041	-0.894203
5	6	0	1.223347	3.983762	-0.407319
6	6	0	0.482015	3.021484	-1.305671
7	1	0	-1.138722	4.470763	0.928623
8	1	0	-0.851261	3.463036	2.345106
9	1	0	-2.225295	2.356920	0.441058
10	1	0	-0.875117	1.421679	1.040475
11	1	0	1.269155	4.590780	1.677993
12	1	0	1.413516	2.850562	1.427124
13	1	0	-1.046388	1.592337	-1.587116
14	1	0	2.304911	3.894248	-0.579244
15	1	0	0.965129	5.014297	-0.698677
16	1	0	0.805415	2.960544	-2.345751
17	6	0	3.293382	-1.661479	0.130292
18	16	0	1.634135	-0.851908	0.056972
19	8	0	1.342116	-0.143366	1.308230
20	8	0	0.651039	-1.842116	-0.427806
21	8	0	1.904824	0.237950	-1.117839
22	6	0	3.154889	-2.770510	1.187110
23	6	0	4.320359	-0.605284	0.559609
24	6	0	3.609038	-2.243665	-1.254582
25	1	0	1.274260	1.004044	-1.011127
26	1	0	4.118203	-3.283704	1.279438
27	1	0	2.889776	-2.358587	2.165337

28	1	0	2.398497	-3.504995	0.897117
29	1	0	4.057452	-0.164699	1.525155
30	1	0	5.297901	-1.090972	0.656938
31	1	0	4.406102	0.194137	-0.181047
32	1	0	4.570632	-2.766487	-1.198669
33	1	0	2.845048	-2.959996	-1.568053
34	1	0	3.687535	-1.459485	-2.012068
35	8	0	-1.797056	-0.865983	-1.518184
36	6	0	-2.868524	-1.059627	-0.696116
37	6	0	-2.778206	-1.765409	0.511535
38	6	0	-4.097357	-0.517987	-1.096202
39	6	0	-3.914710	-1.923391	1.305806
40	6	0	-5.223098	-0.683815	-0.292460
41	6	0	-5.141693	-1.386130	0.913347
42	1	0	-1.002642	-1.297592	-1.141635
43	1	0	-1.822972	-2.181487	0.820314
44	1	0	-4.149391	0.020710	-2.037805
45	1	0	-3.834892	-2.472306	2.240982
46	1	0	-6.172492	-0.261356	-0.612497
47	1	0	-6.022363	-1.513096	1.536443

TS2(CH_3): B3LYP\6-31G(d) = -1324.3539513, imaginary frequency = -99 cm^{-1}

Sum of electronic and zero-point Energies = -1323.953668

Sum of electronic and thermal Energies = -1323.931036

Sum of electronic and thermal Enthalpies = -1323.930092

Sum of electronic and thermal Free Energies = -1324.008414

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.438341	3.118200	1.605817
2	6	0	-1.192759	1.972699	0.870788
3	6	0	0.948737	3.332358	0.992639
4	6	0	-1.178088	2.140923	-0.583353
5	6	0	0.861688	3.642134	-0.505356
6	6	0	-0.002594	2.597803	-1.270990
7	1	0	-1.034353	4.039034	1.552019
8	1	0	-0.359861	2.847383	2.663389
9	1	0	-2.203801	1.803734	1.249317
10	1	0	-0.596178	1.049825	1.060684
11	1	0	1.458306	4.158478	1.504526
12	1	0	1.547388	2.428612	1.144729
13	1	0	-2.086835	1.960021	-1.146241

14	1	0	1.858231	3.650530	-0.956050
15	1	0	0.421964	4.635633	-0.666992
16	1	0	-0.197805	2.866295	-2.313005
17	1	0	0.671407	1.668357	-1.297418
18	6	0	3.200747	-1.526442	0.140991
19	16	0	1.638994	-0.580028	-0.167808
20	8	0	1.144163	-0.094667	1.157822
21	8	0	0.682451	-1.547673	-0.818805
22	8	0	2.014711	0.544978	-1.099838
23	6	0	2.853010	-2.692157	1.077293
24	6	0	4.201064	-0.565091	0.797267
25	6	0	3.716942	-2.032507	-1.212732
26	1	0	3.761841	-3.270377	1.283150
27	1	0	2.450988	-2.327224	2.026701
28	1	0	2.115635	-3.357285	0.619123
29	1	0	3.810406	-0.176938	1.742407
30	1	0	5.134604	-1.102716	1.002299
31	1	0	4.424647	0.278725	0.138352
32	1	0	4.638149	-2.606220	-1.053457
33	1	0	2.981825	-2.682851	-1.694918
34	1	0	3.937722	-1.199355	-1.885764
35	8	0	-1.579583	-0.260816	-1.351816
36	6	0	-2.616727	-0.794567	-0.639738
37	6	0	-2.416264	-1.721265	0.394434
38	6	0	-3.912918	-0.363769	-0.955616
39	6	0	-3.517218	-2.209060	1.097707
40	6	0	-5.001724	-0.854542	-0.236468
41	6	0	-4.811230	-1.778711	0.793839
42	1	0	-0.733839	-0.781998	-1.186350
43	1	0	-1.407746	-2.047661	0.627109
44	1	0	-4.051848	0.329848	-1.780749
45	1	0	-3.358294	-2.930739	1.894907
46	1	0	-6.004511	-0.520271	-0.490284
47	1	0	-5.661843	-2.163011	1.349410

3(CH_3): B3LYP\6-31G(d) = -1324.4156722
Sum of electronic and zero-point Energies = -1324.010307
Sum of electronic and thermal Energies = -1323.987699
Sum of electronic and thermal Enthalpies = -1323.986755
Sum of electronic and thermal Free Energies = -1324.064458

Standard orientation:

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

1	6	0	-2.212729	2.966407	1.432244
2	6	0	-1.741288	1.534472	1.120542
3	6	0	-1.465905	3.999250	0.574256
4	6	0	-1.887633	1.237799	-0.372649
5	6	0	-1.596109	3.678581	-0.922926
6	6	0	-1.129581	2.245100	-1.233656
7	8	0	-1.372584	-0.091333	-0.701936
8	6	0	-2.156012	-1.187220	-0.350483
9	6	0	-1.670236	-2.089564	0.597409
10	6	0	-3.379558	-1.407326	-0.988876
11	6	0	-2.425637	-3.222813	0.906020
12	6	0	-4.129644	-2.537286	-0.661876
13	6	0	-3.655679	-3.447763	0.285238
14	1	0	-3.293897	3.047899	1.244131
15	1	0	-2.066714	3.176606	2.498530
16	1	0	-2.312020	0.802888	1.704677
17	1	0	-0.685147	1.424954	1.396278
18	1	0	-1.845833	5.008278	0.778348
19	1	0	-0.402836	3.996753	0.852119
20	1	0	-2.950748	1.246866	-0.648797
21	1	0	-1.013605	4.390535	-1.519911
22	1	0	-2.645379	3.797930	-1.231843
23	1	0	-1.275750	2.005926	-2.293995
24	1	0	-0.057290	2.155996	-1.019446
25	1	0	-0.713178	-1.902912	1.075583
26	1	0	-3.727533	-0.708896	-1.744319
27	1	0	-2.048861	-3.928924	1.641043
28	1	0	-5.080599	-2.710958	-1.158449
29	1	0	-4.239832	-4.329537	0.533302
30	6	0	3.786812	-0.567339	-0.211316
31	16	0	2.062319	-0.172568	0.321485
32	8	0	1.627127	-1.132629	1.346838
33	8	0	1.286633	-0.482691	-1.069583
34	8	0	1.952725	1.262624	0.626084
35	6	0	3.840536	-2.043926	-0.626232
36	6	0	4.660162	-0.303327	1.027320
37	6	0	4.165770	0.368605	-1.367601
38	1	0	0.303900	-0.338061	-0.933713
39	1	0	4.869757	-2.289445	-0.913419
40	1	0	3.546555	-2.697444	0.199727
41	1	0	3.187492	-2.243008	-1.479874
42	1	0	4.366280	-0.943772	1.864204
43	1	0	5.703304	-0.522314	0.773710
44	1	0	4.593510	0.741368	1.345073

45	1	0	5.216399	0.195113	-1.628201
46	1	0	3.553930	0.177970	-2.253230
47	1	0	4.050183	1.417618	-1.080974

$CF_3SO_3^-$:B3LYP\6-31G(d) = -961.497981
Sum of electronic and zero-point Energies = -961.470714
Sum of electronic and thermal Energies = -961.463547
Sum of electronic and thermal Enthalpies = -961.462602
Sum of electronic and thermal Free Energies = -961.503225

F,0,1.4102590021,-0.9142075057,-0.9164816277
C,0,0.7974735868,0.2004888971,-0.4578582544
F,0,1.6867780033,0.8411781637,0.3337931093
F,0,0.5777929557,0.9973864752,-1.5280551472
S,0,-0.7848170457,-0.1974653464,0.450884449
O,0,-0.3085439632,-1.0591328087,1.5568918538
O,0,-1.5861493127,-0.8804708344,-0.5904876437
O,0,-1.267961529,1.1442658882,0.8498072064

Protonated Cyclohexane: B3LYP\6-31G(d) = -234.9595675
Sum of electronic and zero-point Energies = -234.804156
Sum of electronic and thermal Energies = -234.797964
Sum of electronic and thermal Enthalpies = -234.797020
Sum of electronic and thermal Free Energies = -234.833460

C,0,-1.1446680808,0.7515767457,0.5807415962
C,0,-1.3657270253,-0.2672828438,-0.5482157494
C,0,0.1538384678,0.4702118722,1.3522056938
C,0,-0.1849762558,-0.7767734737,-1.2103231675
C,0,1.3671418839,0.4175597482,0.411129626
C,0,1.1643151109,-0.6040444869,-0.7188258611
H,0,-1.1112945114,1.7541411815,0.1377139548
H,0,-2.0102344047,0.7355553258,1.2486833923
H,0,-2.1228769273,0.013095627,-1.3008682965
H,0,-1.8115466154,-1.2220824475,-0.1646009618
H,0,0.3081899704,1.2486949636,2.104869504
H,0,0.0650826502,-0.476799587,1.9024590141
H,0,-0.3278349779,-1.4006667235,-2.0971175476
H,0,2.2791736294,0.1653766333,0.959037394
H,0,1.5373544665,1.4018043445,-0.0414170095
H,0,1.8625617573,-0.5180905454,-1.5693146095
H,0,1.3918803591,-1.648514142,-0.3797176624

1 (B3LYP\6-31G(d) optimized structure in toluene)

6	0	1.75029	4.152	0.57322
6	0	0.51752	3.26068	0.34839
6	0	3.04165	3.32138	0.5906
6	0	0.74736	2.22366	-0.72444
6	0	3.23829	2.58084	-0.74263
6	0	1.96332	1.92758	-1.22154
1	0	1.81236	4.8924	-0.2363
1	0	1.64148	4.71478	1.50748
1	0	-0.35275	3.86916	0.06984
1	0	0.22634	2.75561	1.28184
1	0	3.90914	3.9591	0.79597
1	0	2.99074	2.58823	1.4082
1	0	-0.13625	1.7184	-1.11086
1	0	4.03067	1.82583	-0.65076
1	0	3.58741	3.27987	-1.51846
1	0	2.0467	1.20295	-2.03192
1	0	1.54164	0.51969	0.28497
9	0	2.00856	-3.50164	-0.86315
6	0	2.42991	-2.32535	-0.41013
9	0	3.54024	-2.48301	0.3015
9	0	2.6668	-1.50444	-1.43675
16	0	1.09308	-1.58261	0.66479
8	0	1.02413	-2.34965	1.8918
8	0	-0.06977	-1.4123	-0.21182
8	0	1.74301	-0.16031	1.00122
1	0	-1.53168	-0.17181	-0.04748
8	0	-2.09618	0.62342	-0.02125
6	0	-3.4125	0.25985	-0.06271
6	0	-3.81925	-1.07922	-0.1148
6	0	-4.36973	1.28163	-0.04871
6	0	-5.18008	-1.38722	-0.1512
6	0	-5.72487	0.95958	-0.08575
6	0	-6.14032	-0.37424	-0.1371
1	0	-3.0728	-1.87033	-0.12486
1	0	-4.03458	2.3138	-0.00785
1	0	-5.48713	-2.42935	-0.19037
1	0	-6.46206	1.75857	-0.07403
1	0	-7.19807	-0.61956	-0.16532

TS2 (B3LYP\6-31G(d) optimized structure in toluene)

C,0,-1.7571597812,3.5390535438,0.6547847466
C,0,-1.906175173,2.5456172156,-0.5129329925
C,0,-0.5099868909,3.2459248253,1.5008132462
C,0,-0.6477106082,2.1085860735,-1.1349832284
C,0,0.7565688316,3.258019175,0.6356732344

C,0,0.6272076891,2.272321145,-0.5346019105
H,0,-1.6915415014,4.5565355718,0.2484530151
H,0,-2.6620903022,3.505855971,1.2700085209
H,0,-2.5728252713,2.9153269873,-1.3064863022
H,0,-2.410522025,1.6117143535,-0.1895419904
H,0,-0.4219299146,3.9863861638,2.3032875952
H,0,-0.6057385867,2.2643223771,1.9839105733
H,0,-0.7126507554,1.606169044,-2.0963817806
H,0,1.6329869757,2.9810775127,1.2284145684
H,0,0.9378580287,4.2651382978,0.2375797025
H,0,1.4507949952,2.2660221506,-1.2574064323
H,0,0.7660159773,1.2169587325,-0.0493896143
F,0,3.8141603447,-1.8870122795,-1.1138383079
C,0,3.2858704549,-0.7933723609,-0.5585144872
F,0,4.2399262668,-0.1498138608,0.1234128897
F,0,2.8544202236,0.0189971363,-1.5464222065
S,0,1.8661463013,-1.2391544877,0.5592030104
O,0,2.4423861924,-2.0934983468,1.5982048288
O,0,0.9005354467,-1.8931389869,-0.3719419404
O,0,1.3852322389,0.101881319,1.0406426821
H,0,-0.4624882851,-1.0436048562,-0.9270430339
O,0,-1.2586811294,-0.5483547214,-1.2625413599
C,0,-2.3798314988,-0.9391358177,-0.588654317
C,0,-2.3241728067,-1.7218843013,0.575226664
C,0,-3.620992018,-0.5122743724,-1.0856155386
C,0,-3.5071202322,-2.0751357501,1.2213549179
C,0,-4.7957237339,-0.8679416204,-0.4213779662
C,0,-4.7466102805,-1.649160869,0.734240159
H,0,-1.3618356008,-2.0568310613,0.9483290254
H,0,-3.649538793,0.067999524,-2.0038622003
H,0,-3.4571028382,-2.6886498323,2.1171127848
H,0,-5.7527597784,-0.5382138111,-0.8173507202
H,0,-5.6623003631,-1.9280897156,1.2473578931

Cyclohexene: B3LYP\6-31+G(d) = -234.6562062
Sum of electronic and zero-point Energies = -234.509694
Sum of electronic and thermal Energies = -234.504193
Sum of electronic and thermal Enthalpies = -234.503249
Sum of electronic and thermal Free Energies = -234.538335

C,0,-0.6676980555,1.3071403272,-0.0570891454
C,0,-1.5003985623,0.0476239663,-0.1104292128
C,0,-0.6988144109,-1.1929831701,0.318816558
C,0,0.6988048449,-1.1929885683,-0.3188178165
C,0,1.5003990114,0.0476118106,0.1104293376

C,0,0.6677084748,1.3071346753,0.0570908287
H,0,-1.2006881616,2.2565205974,-0.1132775862
H,0,1.2007061167,2.2565108644,0.113277497
H,0,-2.3876450065,0.1639679385,0.5281976996
H,0,-1.8905769132,-0.0901604255,-1.132198549
H,0,-1.2453727934,-2.1070518068,0.0533369222
H,0,-0.5938686699,-1.1938640935,1.4136345202
H,0,1.2453558275,-2.1070619798,-0.0533393952
H,0,0.5938594193,-1.1938670881,-1.4136358385
H,0,2.3876466582,0.1639490107,-0.5281971553
H,0,1.8905757085,-0.0901772631,1.1321985871

PhOH: B3LYP\6-31+G(d) = -307.4803124
Sum of electronic and zero-point Energies = -307.375825
Sum of electronic and thermal Energies = -307.370282
Sum of electronic and thermal Enthalpies = -307.369338
Sum of electronic and thermal Free Energies = -307.404835

C,0,-1.2077810997,0.2316906565,0.
C,0,-1.1901596765,-1.1661381347,0.
C,0,0.0221977662,-1.8601368986,0.
C,0,1.2228229033,-1.1403654001,0.
C,0,1.2184495242,0.2545484239,0.
C,0,-0.0011387762,0.9404840117,0.
O,0,0.050095561,2.3120784471,0.
H,0,-2.1556705318,0.7680467962,0.
H,0,-2.1315957669,-1.7098008098,0.
H,0,0.03275486,-2.9463935801,0.
H,0,2.1730803651,-1.66848315,0.
H,0,2.1433342586,0.8237956393,0.
H,0,-0.8490115212,2.6757115755,0.

TfOH: B3LYP\6-31+G(d) = -962.0344822
Sum of electronic and zero-point Energies = -961.996367
Sum of electronic and thermal Energies = -961.988518
Sum of electronic and thermal Enthalpies = -961.987574
Sum of electronic and thermal Free Energies = -962.029433

F,0,1.4366123576,-0.1514402457,-1.2550351474
C,0,1.0121236877,0.0150361905,-0.0037924603
F,0,1.5608767485,-0.9097577641,0.7849971512
F,0,1.3616806187,1.2341389735,0.4275090658
S,0,-0.8641740373,-0.1552937299,0.0783124307
O,0,-1.2196695845,-1.3738123744,-0.6156776032
O,0,-1.2740282563,1.0891281275,-0.8913382926

O,0,-1.2609328731,0.1542820437,1.4439397536
H,0,-1.4414393403,1.8812314882,-0.3428746178

1: B3LYP\6-31+G(d) = -1504.1904206
Sum of electronic and zero-point Energies = -1503.898873
Sum of electronic and thermal Energies = -1503.876246
Sum of electronic and thermal Enthalpies = -1503.875302
Sum of electronic and thermal Free Energies = -1503.959157

C,0,1.9234547611,4.1965988159,0.6140101617
C,0,0.7017578956,3.2844879092,0.4097207655
C,0,3.2305512904,3.3902101191,0.5790938622
C,0,0.9153932391,2.2843880508,-0.7016879477
C,0,3.4025653601,2.6762422495,-0.7729290048
C,0,2.122754597,2.0218841657,-1.2400118183
H,0,1.9468660935,4.9524433584,-0.1841297516
H,0,1.8319839543,4.7412005918,1.5615485201
H,0,-0.1916918273,3.8797077677,0.1797001377
H,0,0.4573547212,2.7508330992,1.3413410476
H,0,4.0920286613,4.0418845938,0.7692305952
H,0,3.2180592356,2.6440965982,1.3868934365
H,0,0.0275040596,1.7899700675,-1.0942333733
H,0,4.2051165366,1.9279620842,-0.7129012343
H,0,3.7283328753,3.3942682174,-1.5423733097
H,0,2.1918865329,1.3359066386,-2.0856158378
H,0,1.7460061772,0.4723123729,0.1955414951
F,0,1.668468963,-3.7224363083,-0.7214570689
C,0,2.258522813,-2.5638766691,-0.4231797762
F,0,3.4128657243,-2.796138021,0.2014473506
F,0,2.4939937468,-1.8803181076,-1.5508255871
S,0,1.1095282721,-1.5681685878,0.6881899107
O,0,1.0427456069,-2.2502027158,1.9633159447
O,0,-0.0791630006,-1.2915074448,-0.1199886973
O,0,1.9763358401,-0.2356788745,0.8725720871
H,0,-1.5925877222,-0.0735648037,-0.0758190078
O,0,-2.1611981441,0.7170751655,-0.119248619
C,0,-3.4834546579,0.3593051162,-0.1029926417
C,0,-3.8983454421,-0.9768077603,-0.0369902334
C,0,-4.4324178548,1.387344632,-0.1554898482
C,0,-5.2632936914,-1.276848662,-0.0254158464
C,0,-5.7919590957,1.0741229381,-0.1427150276
C,0,-6.217631126,-0.2575081556,-0.0780433417
H,0,-3.1586946686,-1.7735006199,0.0046668285
H,0,-4.0910961876,2.4173978976,-0.2052059142
H,0,-5.5775746576,-2.3164757723,0.025994913

H,0,-6.5235276987,1.8775361615,-0.1833556951
H,0,-7.2775252935,-0.4959944563,-0.0682252182

TS2: B3LYP\6-31+G(d) = -1504.1593649, imaginary frequency = -51cm^{-1}
Sum of electronic and zero-point Energies = -1503.868633
Sum of electronic and thermal Energies = -1503.847819
Sum of electronic and thermal Enthalpies = -1503.846875
Sum of electronic and thermal Free Energies = -1503.922242

C,0,-2.6379096086,3.1626545548,0.3113095912
C,0,-2.4042126971,2.1706964257,-0.8476741477
C,0,-1.6014143191,2.9767102109,1.4264831318
C,0,-0.9927180077,1.9268435376,-1.1896739554
C,0,-0.1827534427,3.1736896555,0.8804237306
C,0,0.1085421524,2.2275816737,-0.3031344775
H,0,-2.5801994713,4.1891979593,-0.0752499839
H,0,-3.6561946051,3.0273092437,0.6918132235
H,0,-2.9614370477,2.433618431,-1.7573000559
H,0,-2.8179320215,1.178756459,-0.5683191844
H,0,-1.7917508236,3.6909119904,2.2363487032
H,0,-1.6953557553,1.972256524,1.8619413415
H,0,-0.7656236675,1.6048895613,-2.2009967963
H,0,0.5646433559,2.9933334546,1.6590865206
H,0,-0.0561926613,4.213596459,0.5489324039
H,0,1.0048223977,2.4921067426,-0.8804447213
H,0,0.429984156,1.2355032854,0.1428611744
F,0,4.3112666821,-0.9741671167,-1.0219385303
C,0,3.591049925,-0.1950785539,-0.204357012
F,0,4.3471627726,0.1316603599,0.8546373406
F,0,3.2909616382,0.9472380746,-0.868736809
S,0,2.0160886816,-1.062315548,0.3440406051
O,0,2.4685169339,-2.2477916458,1.0716754321
O,0,1.3176833575,-1.3109757478,-0.9596888329
O,0,1.3080891873,-0.0225848709,1.1555706555
H,0,-0.2306938239,-0.8458252915,-1.1577730518
O,0,-1.1564029564,-0.513845461,-1.3827367991
C,0,-2.1301270545,-1.1337121211,-0.6501877448
C,0,-1.8903109011,-1.6618501901,0.629690975
C,0,-3.4177695689,-1.1922892744,-1.2080364533
C,0,-2.937059371,-2.2675702909,1.3244721472
C,0,-4.4581205638,-1.7916694266,-0.4937782196
C,0,-4.2224191333,-2.3337347057,0.7723850829
H,0,-0.8989505252,-1.6001262286,1.0667431849
H,0,-3.5748918662,-0.8010930883,-2.2095174028
H,0,-2.7446055331,-2.6888417616,2.3076120486

H,0,-5.4496196362,-1.8455482268,-0.935907409
H,0,-5.0296978505,-2.8076257756,1.3237627769

3: B3LYP\6-31+G(d) = -1504.2117739
Sum of electronic and zero-point Energies = -1503.916468
Sum of electronic and thermal Energies = -1503.895650
Sum of electronic and thermal Enthalpies = -1503.894705
Sum of electronic and thermal Free Energies = -1503.971545

C,0,-1.5918096078,3.4775873286,1.3958836979
C,0,-1.4028060937,1.9517678994,1.3022909058
C,0,-0.5408943065,4.2236705878,0.55881903
C,0,-1.4123566251,1.4967178742,-0.157139336
C,0,-0.5453264305,3.7416064862,-0.9006586676
C,0,-0.3588667766,2.2151336144,-0.9952813736
H,0,-2.5992067409,3.7456531219,1.0423243375
H,0,-1.538849329,3.7890661425,2.4464554663
H,0,-2.1895091177,1.4305315541,1.8621173404
H,0,-0.4390728823,1.6736634117,1.7496685302
H,0,-0.7240101113,5.3051749745,0.5992000531
H,0,0.4549526416,4.054386048,0.9929184295
H,0,0.2473802984,4.2406450366,-1.4714968891
H,0,-1.4969588338,4.0256320232,-1.3756770158
H,0,-0.4257323949,1.8788771024,-2.0375285485
H,0,0.6373559222,1.9428094921,-0.6259934464
F,0,3.1623876373,-2.4064568248,-1.0734888375
C,0,3.1059419608,-1.0895430502,-0.8648090522
F,0,4.3416101759,-0.5807626144,-0.906001183
F,0,2.3656402329,-0.5231290572,-1.8294506788
S,0,2.3467516829,-0.7185216864,0.817715734
O,0,3.0728143624,-1.5161315003,1.7872289587
O,0,0.9036750695,-1.366311514,0.6184562489
O,0,2.2484532489,0.7349869395,0.9103110638
H,0,0.2106388008,-0.7091068121,0.2793837654
O,0,-1.164789349,0.0480202313,-0.2428379472
C,0,-2.2845469501,-0.7839787367,-0.2145357958
C,0,-2.5232617763,-1.5729541729,0.9120409639
C,0,-3.1215208757,-0.8586987518,-1.3315776429
C,0,-3.615851274,-2.445692782,0.9183952727
C,0,-4.2166360905,-1.7252323862,-1.3107935066
C,0,-4.4664643764,-2.520511888,-0.1875165291
H,0,-1.8542015482,-1.5091372681,1.7649425562
H,0,-2.9034826772,-0.2549936516,-2.2080989723
H,0,-3.800076882,-3.0650780424,1.7921432767
H,0,-4.8673495209,-1.7875596841,-2.1791121856

H,0,-5.3154470921,-3.1984978765,-0.1779501493
H,0,-2.4060311946,1.66367249,-0.5922563923