Supporting Information

Understanding the Chemo-Selectivities between Carbonyl and Hydroxyl Groups in the Rh(II)-Azavinyl Carbene Involved Reactions

Yuanzheng Lv, Abosede Adejoke Ogunlana, Hongli Li, Dafang Gao, Chenli Wang, Xiaoguang Bao*

College of Chemistry, Chemical Engineering and Materials Science, Soochow University, 199 Ren-Ai Road, Suzhou Industrial Park, Suzhou, Jiangsu 215123, China.

E-mail: xgbao@suda.edu.cn

List of Contents

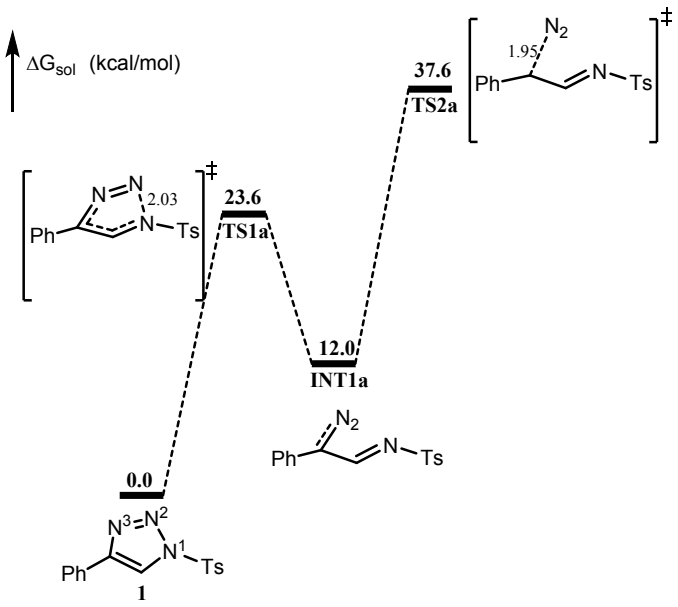

Figure S1. Energy profile for the formation of the Rh(II)-AVC intermediate in the absence of Rh-catalyst. Bond distances are shown in Å.

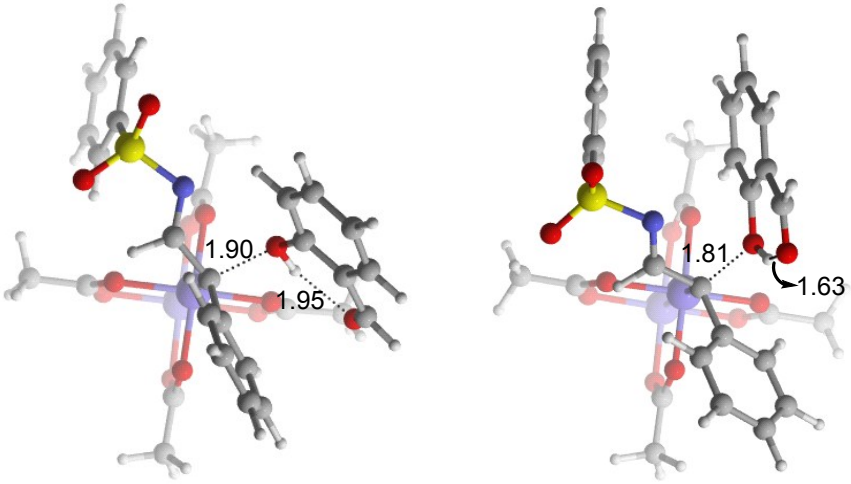

Figure S2. The nucleophilic attack of the OH group in **2** from the α-imino side is shown as **TS4'**, which is 6.8 kcal/mol higher in energy than **TS4**.

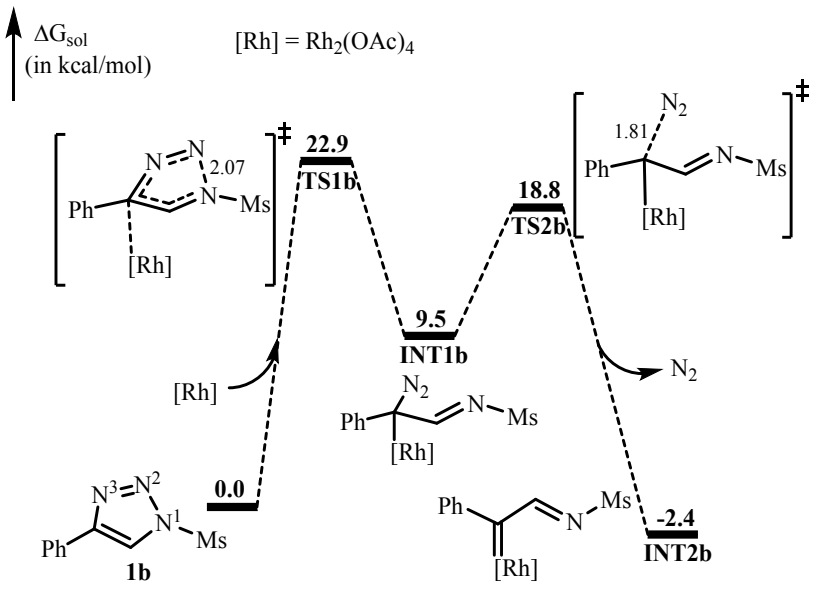

Figure S3. Energy profile for the formation of the Rh(II)-AVC intermediate (**INT2b**) from 1-methylsulfonyl-1,2,3-triazole (**1b**), in the presence of $Rh_2(OAc)_4$ catalyst. Bond distances are shown in Å.

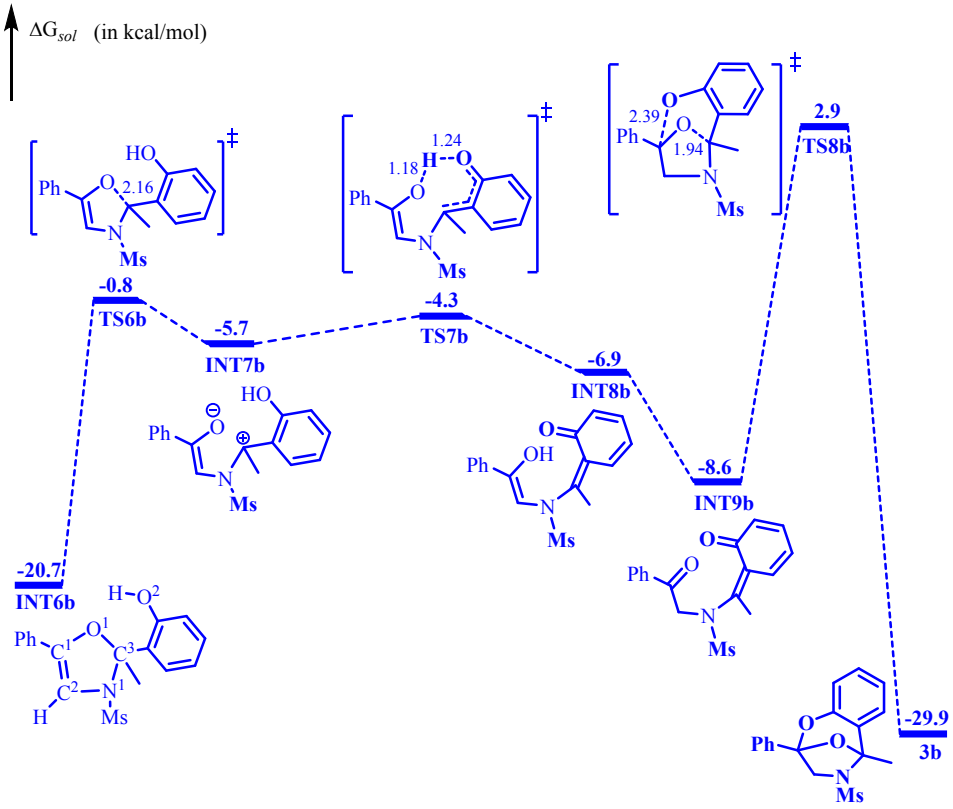

Figure S4. Energy profile for the formation of the corresponding benzoxazepine product **3b** from the oxazoline intermediate **INT6b**. Bond distances are shown in Å.

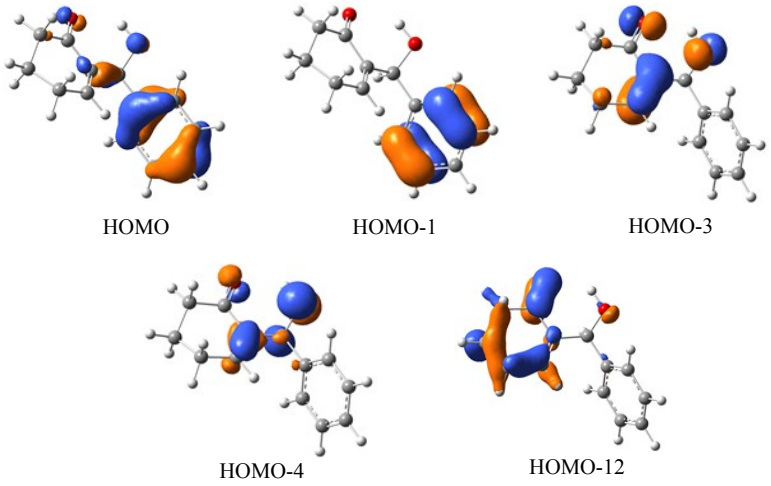

Figure S5. The high-lying occupied π orbitals of **4**.

Cartesian Coordinates and Energies

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.826636	-0.871896	0.337189
2	6	0	-1.749590	-0.125298	-0.352724
3	1	0	-0.850586	-1.447455	1.247947
4	6	0	-3.160685	0.151022	-0.052236
5	6	0	-3.905378	0.981526	-0.895001
6	6	0	-3.777536	-0.407135	1.071472
7	6	0	-5.240864	1.246368	-0.615260
8	1	0	-3.426930	1.412903	-1.767882
9	6	0	-5.112631	-0.140104	1.348497
10	1	0	-3.214995	-1.058077	1.735207
11	6	0	-5.849432	0.687822	0.505679
12	1	0	-5.809915	1.891822	-1.277576
13	1	0	-5.578742	-0.581750	2.224113
14	1	0	-6.893578	0.894462	0.720160
15	7	0	-1.131474	0.383255	-1.468508
16	7	0	0.095625	-0.005066	-1.509182
17	7	0	0.297952	-0.776555	-0.420128
18	16	0	1.864675	-1.442933	-0.093564
19	8	0	1.674489	-2.146461	1.157725
20	8	0	2.295688	-2.097745	-1.303786
21	6	0	2.824581	0.020168	0.169353
22	6	0	3.019662	0.472502	1.470983
23	6	0	3.346726	0.684608	-0.937655
24	6	0	3.764011	1.630741	1.665136
25	1	0	2.604604	-0.077821	2.308277
26	6	0	4.086091	1.841514	-0.724748
27	1	0	3.171473	0.300974	-1.936420
28	6	0	4.292287	2.311683	0.570789
29	1	0	3.932033	2.000294	2.671332
30	1	0	4.502464	2.375301	-1.572461
31	1	0	4.869600	3.217357	0.728710

Zero-point correction= 0.234521 (Hartree/Particle)
Thermal correction to Energy= 0.250426
Thermal correction to Enthalpy= 0.251370
Thermal correction to Gibbs Free Energy= 0.187718
Sum of electronic and zero-point Energies= -1252.360234
Sum of electronic and thermal Energies= -1252.344328
Sum of electronic and thermal Enthalpies= -1252.343384
Sum of electronic and thermal Free Energies= -1252.407037
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1252.84422131

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.294873	0.622753	-0.028995
2	6	0	0.745282	-0.274221	-0.047860
3	1	0	-0.365033	1.697373	0.014986
4	6	0	2.196518	-0.047934	-0.014348
5	6	0	3.069687	-1.139865	-0.015667
6	6	0	2.724070	1.246217	0.022223
7	6	0	4.443891	-0.936830	0.021142
8	1	0	2.659212	-2.143576	-0.046476
9	6	0	4.098756	1.445566	0.059277
10	1	0	2.060252	2.106679	0.020146
11	6	0	4.963629	0.354283	0.059585
12	1	0	5.112734	-1.792271	0.019885
13	1	0	4.495550	2.455896	0.087696
14	1	0	6.037700	0.510462	0.089481
15	7	0	0.211597	-1.538151	-0.096577
16	7	0	-1.073957	-1.475201	-0.117304
17	7	0	-1.402001	-0.165057	-0.073108
18	16	0	-3.062659	0.326442	-0.108791
19	8	0	-3.013362	1.740089	0.198594

20	8	0	-3.652385	-0.174260	-1.326082
21	6	0	-3.680736	-0.604016	1.275673
22	1	0	-4.754979	-0.414127	1.324772
23	1	0	-3.480575	-1.660445	1.091209
24	1	0	-3.183164	-0.256551	2.181613

Zero-point correction= 0.180598 (Hartree/Particle)
Thermal correction to Energy= 0.193400
Thermal correction to Enthalpy= 0.194344
Thermal correction to Gibbs Free Energy= 0.138811
Sum of electronic and zero-point Energies= -1060.746815
Sum of electronic and thermal Energies= -1060.734012
Sum of electronic and thermal Enthalpies= -1060.733068
Sum of electronic and thermal Free Energies= -1060.788602
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1061.13222630

[Rh] = Rh2(OAc)4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.003942	-0.000436	-1.187149
2	8	0	-1.458931	1.450200	-1.122888
3	6	0	-1.862512	1.860668	0.006633
4	8	0	-1.456715	1.446445	1.133171
5	45	0	-0.003681	-0.007380	1.187156
6	8	0	-1.456239	-1.459759	1.122996
7	6	0	-1.867875	-1.862392	-0.006459
8	8	0	-1.455400	-1.454997	-1.133071
9	8	0	1.447326	1.454728	-1.122980
10	6	0	1.860783	1.855487	0.006448
11	8	0	1.450432	1.446063	1.133055
12	8	0	1.452191	-1.451186	-1.133131
13	6	0	1.862558	-1.860809	-0.006580
14	8	0	1.449434	-1.459865	1.122915
15	6	0	-2.963404	-2.895737	-0.002033
16	1	0	-3.037833	-3.379492	-0.976373
17	1	0	-2.777604	-3.632422	0.782247
18	1	0	-3.912443	-2.397969	0.222338
19	6	0	-2.895545	2.956572	0.002372
20	1	0	-3.379147	3.031321	0.976768
21	1	0	-2.397517	3.905447	-0.222108
22	1	0	-3.632348	2.771169	-0.781921
23	6	0	2.957996	-2.894356	-0.002109
24	1	0	3.906890	-2.397168	0.224307
25	1	0	2.771098	-3.632047	0.780940
26	1	0	3.033803	-3.376773	-0.977000
27	6	0	2.955774	2.889602	0.001734
28	1	0	2.766644	3.628943	-0.779270
29	1	0	3.033739	3.369940	0.977491
30	1	0	3.904324	2.393499	-0.228338

Zero-point correction= 0.214819 (Hartree/Particle)
Thermal correction to Energy= 0.235842
Thermal correction to Enthalpy= 0.236786
Thermal correction to Gibbs Free Energy= 0.164352
Sum of electronic and zero-point Energies= -1132.577136
Sum of electronic and thermal Energies= -1132.556113
Sum of electronic and thermal Enthalpies= -1132.555169
Sum of electronic and thermal Free Energies= -1132.627603
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1133.10396399

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.305679	-1.219585	2.381265
2	8	0	0.187073	-2.319374	2.010097
3	8	0	-0.266991	-0.128193	1.728246
4	6	0	-1.047585	-1.194195	3.693354
5	1	0	-2.112785	-1.367556	3.502409
6	1	0	-0.682468	-1.983317	4.351994
7	1	0	-0.947021	-0.215834	4.166191

8	6	0	3.191482	-0.647062	1.344344
9	8	0	2.941470	-1.878768	1.186890
10	8	0	2.470380	0.314568	0.947421
11	6	0	4.449031	-0.286719	2.092367
12	1	0	5.267946	-0.937808	1.778963
13	1	0	4.698684	0.761655	1.923226
14	1	0	4.281590	-0.449811	3.161995
15	6	0	2.301655	-1.281957	-2.206258
16	8	0	2.212630	-2.373104	-1.576376
17	8	0	1.791137	-0.174824	-1.853019
18	6	0	3.105449	-1.274192	-3.480868
19	1	0	2.593908	-0.679163	-4.240713
20	1	0	4.073737	-0.803579	-3.281167
21	1	0	3.269982	-2.291682	-3.836474
22	6	0	-1.205341	-1.844362	-1.293894
23	8	0	-0.552323	-2.807080	-0.798630
24	8	0	-0.946143	-0.612507	-1.130333
25	6	0	-2.369247	-2.173084	-2.189418
26	1	0	-1.994021	-2.267055	-3.214505
27	1	0	-2.817424	-3.123467	-1.897142
28	1	0	-3.108856	-1.371608	-2.160366
29	45	0	1.204650	-2.410337	0.217253
30	45	0	0.734450	-0.078097	-0.087507
31	6	0	-0.914776	2.373547	0.165139
32	6	0	0.291828	2.349675	-0.594355
33	1	0	-0.897357	2.486691	1.244988
34	6	0	1.619504	2.897256	-0.257712
35	6	0	2.661769	2.831100	-1.186718
36	6	0	1.860922	3.453159	1.000739
37	6	0	3.922443	3.312145	-0.858410
38	1	0	2.488160	2.370596	-2.153722
39	6	0	3.127274	3.923774	1.326874
40	1	0	1.066729	3.515498	1.738240
41	6	0	4.163684	3.857462	0.400301
42	1	0	4.721810	3.256047	-1.591284
43	1	0	3.298945	4.354018	2.308912
44	1	0	5.149779	4.234664	0.653760
45	7	0	-0.111949	2.239784	-1.915010
46	7	0	-1.178074	2.102906	-2.341574
47	7	0	-2.020896	2.225167	-0.496364
48	16	0	-3.519450	2.261739	0.289121
49	8	0	-3.281072	2.559078	1.694490
50	8	0	-4.382757	3.101643	-0.516093
51	6	0	-4.069948	0.577635	0.153102
52	6	0	-3.391215	-0.404008	0.868198
53	6	0	-5.201624	0.289321	-0.600291
54	6	0	-3.859753	-1.710763	0.828247
55	1	0	-2.496958	-0.141551	1.421162
56	6	0	-5.668987	-1.023432	-0.624346
57	1	0	-5.705911	1.082283	-1.141956
58	6	0	-5.002988	-2.016795	0.089020
59	1	0	-3.327082	-2.492225	1.362236
60	1	0	-6.556370	-1.267206	-1.199774
61	1	0	-5.371511	-3.037912	0.063556

Zero-point correction= 0.448493 (Hartree/Particle)
Thermal correction to Energy= 0.486605
Thermal correction to Enthalpy= 0.487550
Thermal correction to Gibbs Free Energy= 0.377524
Sum of electronic and zero-point Energies= -2384.919860
Sum of electronic and thermal Energies= -2384.881748
Sum of electronic and thermal Enthalpies= -2384.880804
Sum of electronic and thermal Free Energies= -2384.990830

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2385.93589265

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.725899	0.583610	-0.273025
2	6	0	1.815187	-0.299063	-0.430075
3	1	0	0.828688	1.521645	0.266438
4	6	0	3.197472	-0.207330	0.039791

5	6	0	4.173951	-1.080296	-0.454026
6	6	0	3.568836	0.750593	0.989850
7	6	0	5.486367	-0.996309	-0.007239
8	1	0	3.902255	-1.826505	-1.195325
9	6	0	4.885633	0.836975	1.425869
10	1	0	2.828714	1.430218	1.402243
11	6	0	5.850684	-0.035901	0.932298
12	1	0	6.229014	-1.683972	-0.400387
13	1	0	5.155066	1.587208	2.162900
14	1	0	6.877309	0.031329	1.278249
15	7	0	1.358476	-1.347554	-1.156858
16	7	0	0.311042	-1.572175	-1.604137
17	7	0	-0.404541	0.225229	-0.815085
18	16	0	-1.759310	1.223358	-0.710493
19	8	0	-1.446986	2.364245	0.142265
20	8	0	-2.243195	1.417512	-2.062952
21	6	0	-2.885549	0.154782	0.155279
22	6	0	-3.117091	0.367001	1.509807
23	6	0	-3.506746	-0.876545	-0.544756
24	6	0	-3.991324	-0.482475	2.180839
25	1	0	-2.627488	1.190949	2.017669
26	6	0	-4.374366	-1.719843	0.138681
27	1	0	-3.315775	-1.006419	-1.604732
28	6	0	-4.614515	-1.523358	1.497726
29	1	0	-4.187168	-0.328192	3.237105
30	1	0	-4.866977	-2.529285	-0.390535
31	1	0	-5.294712	-2.184309	2.026210

Zero-point correction= 0.231454 (Hartree/Particle)
Thermal correction to Energy= 0.247522
Thermal correction to Enthalpy= 0.248466
Thermal correction to Gibbs Free Energy= 0.184335
Sum of electronic and zero-point Energies= -1252.322009
Sum of electronic and thermal Energies= -1252.305942
Sum of electronic and thermal Enthalpies= -1252.304998
Sum of electronic and thermal Free Energies= -1252.369129

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1252.80322533

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.980888	-1.610763	2.007848
2	8	0	-0.121284	-2.510721	1.797090
3	8	0	-1.065613	-0.508334	1.379635
4	6	0	-2.000055	-1.845754	3.091771
5	1	0	-2.793087	-1.098402	3.033576
6	1	0	-2.407770	-2.855789	3.002952
7	1	0	-1.504083	-1.774056	4.064960
8	6	0	2.411622	-0.053009	1.843772
9	8	0	2.533294	-1.299083	1.660456
10	8	0	1.574502	0.704302	1.267706
11	6	0	3.320688	0.591578	2.857400
12	1	0	2.875626	0.472759	3.851028
13	1	0	4.293051	0.096089	2.859062
14	1	0	3.425603	1.656683	2.644948
15	6	0	2.552484	-0.720940	-1.805813
16	8	0	2.635064	-1.818372	-1.184782
17	8	0	1.685021	0.183851	-1.606727
18	6	0	3.586782	-0.440250	-2.864900
19	1	0	3.109220	-0.006538	-3.746417
20	1	0	4.298318	0.294345	-2.473612
21	1	0	4.121901	-1.352747	-3.128785
22	6	0	-0.847538	-2.259811	-1.655069
23	8	0	-0.022594	-3.019613	-1.074992
24	8	0	-0.962981	-1.007933	-1.473038
25	6	0	-1.812867	-2.894813	-2.622901
26	1	0	-2.183436	-2.154947	-3.333883
27	1	0	-1.332230	-3.725323	-3.142940
28	1	0	-2.660867	-3.297579	-2.057928
29	45	0	1.282598	-2.221761	0.311495
30	45	0	0.286421	-0.084037	-0.120665
31	6	0	-1.808805	1.907661	0.115518

32	6	0	-0.646712	2.241232	-0.642794
33	1	0	-1.801913	1.966200	1.200279
34	6	0	0.506968	3.084380	-0.284481
35	6	0	1.550577	3.266515	-1.196661
36	6	0	0.587136	3.686955	0.973137
37	6	0	2.653408	4.037198	-0.853055
38	1	0	1.507561	2.778386	-2.164476
39	6	0	1.698634	4.448244	1.315616
40	1	0	-0.212908	3.561212	1.696170
41	6	0	2.736253	4.628150	0.405352
42	1	0	3.454787	4.171928	-1.573463
43	1	0	1.746883	4.910713	2.296794
44	1	0	3.600065	5.229386	0.672211
45	7	0	-1.001446	2.052862	-1.964986
46	7	0	-1.976086	1.637822	-2.422998
47	7	0	-2.837631	1.481110	-0.547178
48	16	0	-4.195074	0.861818	0.243871
49	8	0	-4.023022	0.994336	1.685003
50	8	0	-5.359540	1.426490	-0.407279
51	6	0	-4.046419	-0.855378	-0.205431
52	1	0	-4.898055	-1.374686	0.239448
53	1	0	-4.067351	-0.930678	-1.293247
54	1	0	-3.100233	-1.224230	0.189747

Zero-point correction= 0.394252 (Hartree/Particle)
Thermal correction to Energy= 0.429589
Thermal correction to Enthalpy= 0.430533
Thermal correction to Gibbs Free Energy= 0.326275
Sum of electronic and zero-point Energies= -2193.307216
Sum of electronic and thermal Energies= -2193.271878
Sum of electronic and thermal Enthalpies= -2193.270934
Sum of electronic and thermal Free Energies= -2193.375192
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2194.22276203

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.322908	-1.108604	-2.403759
2	8	0	-0.180741	-2.229941	-2.119431
3	8	0	0.281108	-0.066965	-1.674409
4	6	0	1.079435	-0.991830	-3.701954
5	1	0	2.141953	-1.181466	-3.511943
6	1	0	0.719557	-1.731362	-4.418451
7	1	0	0.986883	0.018354	-4.104221
8	6	0	-3.184962	-0.622762	-1.414050
9	8	0	-2.939662	-1.859131	-1.299911
10	8	0	-2.476883	0.323134	-0.956396
11	6	0	-4.421904	-0.235266	-2.183298
12	1	0	-5.252393	-0.887097	-1.903145
13	1	0	-4.670297	0.810830	-2.000143
14	1	0	-4.230891	-0.378390	-3.251708
15	6	0	-2.362791	-1.460413	2.127894
16	8	0	-2.230488	-2.512258	1.447273
17	8	0	-1.880442	-0.319262	1.835976
18	6	0	-3.179462	-1.536960	3.392012
19	1	0	-2.664251	-1.014087	4.201286
20	1	0	-4.137573	-1.034288	3.224387
21	1	0	-3.363439	-2.576495	3.663983
22	6	0	1.177109	-1.938248	1.230425
23	8	0	0.549699	-2.873079	0.655778
24	8	0	0.885372	-0.703585	1.169623
25	6	0	2.351966	-2.306312	2.096415
26	1	0	1.991286	-2.450352	3.120895
27	1	0	2.800174	-3.238471	1.750672
28	1	0	3.088700	-1.501314	2.095022
29	45	0	-1.207979	-2.439021	-0.345158
30	45	0	-0.769449	-0.121503	0.107301
31	6	0	1.009114	2.287379	0.069153
32	6	0	-0.291178	2.188001	0.717926
33	1	0	0.988260	2.439937	-1.012641
34	6	0	-1.489635	2.977493	0.303063
35	6	0	-2.737407	2.722226	0.880613

36	6	0	-1.374098	3.967638	-0.674786
37	6	0	-3.850101	3.453590	0.487389
38	1	0	-2.839636	1.923138	1.609425
39	6	0	-2.499067	4.677909	-1.082887
40	1	0	-0.411057	4.199028	-1.118593
41	6	0	-3.737804	4.428929	-0.501091
42	1	0	-4.813107	3.249293	0.945517
43	1	0	-2.398200	5.441486	-1.847936
44	1	0	-4.611103	4.993224	-0.813479
45	7	0	-0.177176	1.987699	2.056226
46	7	0	-0.096302	1.742847	3.141710
47	7	0	2.101051	2.156835	0.729193
48	16	0	3.518119	2.254499	-0.194304
49	8	0	3.192752	2.555498	-1.585712
50	8	0	4.431560	3.106881	0.544759
51	6	0	4.106177	0.576096	-0.113527
52	6	0	3.429727	-0.398727	-0.840331
53	6	0	5.247118	0.281754	0.622491
54	6	0	3.911589	-1.701468	-0.834799
55	1	0	2.528554	-0.130999	-1.379066
56	6	0	5.727067	-1.026955	0.615409
57	1	0	5.749663	1.069063	1.174164
58	6	0	5.064624	-2.012015	-0.112730
59	1	0	3.382500	-2.475784	-1.382796
60	1	0	6.622631	-1.274018	1.176837
61	1	0	5.444402	-3.029410	-0.113396

Zero-point correction= 0.449264 (Hartree/Particle)
Thermal correction to Energy= 0.488272
Thermal correction to Enthalpy= 0.489216
Thermal correction to Gibbs Free Energy= 0.377019
Sum of electronic and zero-point Energies= -2384.936478
Sum of electronic and thermal Energies= -2384.897471
Sum of electronic and thermal Enthalpies= -2384.896526
Sum of electronic and thermal Free Energies= -2385.008723
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2385.95639521

INT1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.645958	0.133083	0.531901
2	6	0	1.809521	0.695673	-0.087863
3	1	0	0.780576	-0.838553	1.016744
4	6	0	3.134597	0.055581	-0.201103
5	6	0	4.304629	0.820762	-0.259845
6	6	0	3.233505	-1.339447	-0.249332
7	6	0	5.544735	0.203464	-0.368241
8	1	0	4.249503	1.905087	-0.207739
9	6	0	4.478269	-1.951666	-0.337529
10	1	0	2.336546	-1.951552	-0.234807
11	6	0	5.638103	-1.184890	-0.401442
12	1	0	6.442763	0.811908	-0.413650
13	1	0	4.538766	-3.035121	-0.371129
14	1	0	6.607782	-1.666002	-0.479650
15	7	0	1.654435	1.910316	-0.581062
16	7	0	1.497973	2.947605	-0.994668
17	7	0	-0.490814	0.741082	0.530326
18	16	0	-1.723722	-0.043694	1.377066
19	8	0	-1.299011	-1.379382	1.791262
20	8	0	-2.220917	0.903027	2.360281
21	6	0	-2.937995	-0.220258	0.088596
22	6	0	-3.129200	-1.463505	-0.503963
23	6	0	-3.673418	0.897283	-0.298058
24	6	0	-4.078922	-1.586785	-1.513765
25	1	0	-2.550380	-2.315915	-0.165146
26	6	0	-4.616604	0.761857	-1.309779
27	1	0	-3.511714	1.849165	0.196382
28	6	0	-4.817158	-0.477019	-1.916312
29	1	0	-4.244392	-2.551538	-1.982796
30	1	0	-5.199482	1.622645	-1.621888
31	1	0	-5.558273	-0.577997	-2.703479

Zero-point correction= 0.232053 (Hartree/Particle)
Thermal correction to Energy= 0.248963
Thermal correction to Enthalpy= 0.249907
Thermal correction to Gibbs Free Energy= 0.184528
Sum of electronic and zero-point Energies= -1252.337825
Sum of electronic and thermal Energies= -1252.320915
Sum of electronic and thermal Enthalpies= -1252.319971
Sum of electronic and thermal Free Energies= -1252.385350
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1252.82185572

INT1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.455993	-1.631998	-2.131950
2	8	0	-0.634034	-2.258403	-2.013063
3	8	0	0.847139	-0.680161	-1.385172
4	6	0	1.380628	-2.024288	-3.253781
5	1	0	2.370788	-1.593532	-3.093943
6	1	0	1.431623	-3.112590	-3.333471
7	1	0	0.970913	-1.640801	-4.194024
8	6	0	-2.353450	0.794151	-1.786577
9	8	0	-2.840033	-0.370164	-1.703123
10	8	0	-1.339644	1.224542	-1.157697
11	6	0	-3.010617	1.758163	-2.739738
12	1	0	-2.545455	1.644039	-3.724616
13	1	0	-4.074255	1.533783	-2.834400
14	1	0	-2.854940	2.784237	-2.402305
15	6	0	-2.723682	-0.154192	1.814357
16	8	0	-3.093237	-1.125085	1.100129
17	8	0	-1.648250	0.510608	1.668883
18	6	0	-3.635448	0.283550	2.931349
19	1	0	-3.052858	0.469403	3.836676
20	1	0	-4.118930	1.223351	2.645351
21	1	0	-4.400591	-0.470377	3.117498
22	6	0	0.102470	-2.564861	1.445392
23	8	0	-0.880727	-3.008564	0.788673
24	8	0	0.545266	-1.374855	1.412453
25	6	0	0.842906	-3.541322	2.323047
26	1	0	1.489338	-3.012919	3.024746
27	1	0	0.133268	-4.176824	2.856814
28	1	0	1.455818	-4.188739	1.686711
29	45	0	-1.910304	-1.740184	-0.475903
30	45	0	-0.357145	-0.020902	0.147379
31	6	0	2.331202	1.134271	0.179321
32	6	0	1.196504	1.775657	0.823085
33	1	0	2.402559	1.281797	-0.901119
34	6	0	0.613025	3.073801	0.374916
35	6	0	-0.653605	3.476346	0.809109
36	6	0	1.333789	3.889537	-0.499874
37	6	0	-1.188024	4.680635	0.369728
38	1	0	-1.232066	2.824483	1.457188
39	6	0	0.781395	5.082455	-0.955895
40	1	0	2.330927	3.606182	-0.823084
41	6	0	-0.477486	5.483530	-0.520196
42	1	0	-2.172447	4.985151	0.712481
43	1	0	1.348300	5.706086	-1.640055
44	1	0	-0.903240	6.418922	-0.870259
45	7	0	1.130330	1.532492	2.152919
46	7	0	1.022085	1.277550	3.235195
47	7	0	3.143634	0.385045	0.829445
48	16	0	4.276542	-0.435840	-0.122776
49	8	0	4.150736	-0.071190	-1.532516
50	8	0	5.563261	-0.309817	0.537759
51	6	0	3.662276	-2.097405	0.085880
52	1	0	4.333529	-2.759140	-0.465632
53	1	0	3.664422	-2.336908	1.149671
54	1	0	2.650397	-2.132363	-0.318822

Zero-point correction= 0.394648 (Hartree/Particle)
Thermal correction to Energy= 0.431039
Thermal correction to Enthalpy= 0.431983
Thermal correction to Gibbs Free Energy= 0.324273

Sum of electronic and zero-point Energies= -2193.323231
Sum of electronic and thermal Energies= -2193.286840
Sum of electronic and thermal Enthalpies= -2193.285896
Sum of electronic and thermal Free Energies= -2193.393606

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2194.24211732

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.558335	-1.218273	2.084949
2	8	0	-2.473546	-2.315576	1.479194
3	8	0	-2.001748	-0.122838	1.740147
4	6	0	-3.385203	-1.165848	3.345653
5	1	0	-2.743898	-0.886651	4.186976
6	1	0	-3.849860	-2.132856	3.537741
7	1	0	-4.153614	-0.393772	3.246946
8	6	0	-3.208967	-0.601214	-1.544222
9	8	0	-3.021498	-1.832820	-1.353157
10	8	0	-2.485081	0.349249	-1.108739
11	6	0	-4.388685	-0.198364	-2.394282
12	1	0	-4.813469	0.738879	-2.029151
13	1	0	-5.140191	-0.988691	-2.401361
14	1	0	-4.040329	-0.034802	-3.419530
15	6	0	0.334170	-1.336107	-2.333953
16	8	0	-0.232859	-2.407450	-1.998013
17	8	0	0.289414	-0.231607	-1.700508
18	6	0	1.161125	-1.353216	-3.596288
19	1	0	1.629638	-0.383495	-3.768722
20	1	0	0.519488	-1.614224	-4.442781
21	1	0	1.927753	-2.129458	-3.515560
22	6	0	0.983319	-1.932332	1.364601
23	8	0	0.325834	-2.875776	0.850323
24	8	0	0.771313	-0.689390	1.189711
25	6	0	2.101631	-2.283231	2.311859
26	1	0	1.682757	-2.360999	3.321402
27	1	0	2.864770	-1.503533	2.306662
28	1	0	2.535836	-3.247447	2.044430
29	45	0	-1.369761	-2.446176	-0.269597
30	45	0	-0.826103	-0.093202	0.040237
31	6	0	-0.279410	1.961676	0.314508
32	6	0	1.062820	2.096989	-0.227489
33	1	0	1.081627	2.085452	-1.324338
34	6	0	-1.245207	3.062998	0.164984
35	6	0	-2.591897	2.861258	0.502753
36	6	0	-0.838901	4.308234	-0.340174
37	6	0	-3.511297	3.886572	0.331594
38	1	0	-2.898612	1.900849	0.901106
39	6	0	-1.768198	5.321472	-0.535003
40	1	0	0.206170	4.481149	-0.582043
41	6	0	-3.103333	5.110566	-0.196646
42	1	0	-4.551921	3.728293	0.596646
43	1	0	-1.450103	6.276517	-0.940560
44	1	0	-3.829345	5.905049	-0.342474
45	7	0	2.132602	2.100344	0.474432
46	16	0	3.577103	2.050432	-0.425845
47	8	0	3.284242	2.165676	-1.851752
48	8	0	4.490458	2.979318	0.214093
49	6	0	4.114673	0.384795	-0.100882
50	6	0	5.188351	0.163952	0.753059
51	6	0	3.461905	-0.661342	-0.746774
52	6	0	5.624456	-1.144579	0.952273
53	1	0	5.674547	1.004688	1.236115
54	6	0	3.901550	-1.962026	-0.537216
55	1	0	2.613733	-0.449074	-1.386080
56	6	0	4.986273	-2.200936	0.306904
57	1	0	6.465929	-1.336747	1.610423
58	1	0	3.392395	-2.788675	-1.023550
59	1	0	5.330883	-3.218162	0.467240
60	7	0	0.084913	1.935353	2.078156
61	7	0	-0.030545	1.686622	3.145061

Zero-point correction= 0.446277 (Hartree/Particle)

Thermal correction to Energy= 0.485316
Thermal correction to Enthalpy= 0.486260
Thermal correction to Gibbs Free Energy= 0.374076
Sum of electronic and zero-point Energies= -2384.922370
Sum of electronic and thermal Energies= -2384.883331
Sum of electronic and thermal Enthalpies= -2384.882387
Sum of electronic and thermal Free Energies= -2384.994572
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2385.94012559

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.707475	0.545720	0.425700
2	6	0	-0.636138	-0.333365	0.311711
3	1	0	-0.632519	-1.047375	1.152326
4	6	0	-3.120275	0.262425	0.310646
5	6	0	-4.043017	1.187363	0.831131
6	6	0	-3.599169	-0.925163	-0.275531
7	6	0	-5.405745	0.937803	0.762823
8	1	0	-3.663790	2.095856	1.288730
9	6	0	-4.961354	-1.183802	-0.322604
10	1	0	-2.888448	-1.634929	-0.688950
11	6	0	-5.861261	-0.249793	0.190550
12	1	0	-6.114288	1.656949	1.161038
13	1	0	-5.326488	-2.104276	-0.766618
14	1	0	-6.927825	-0.449349	0.143468
15	7	0	0.342770	-0.305511	-0.543947
16	16	0	1.585585	-1.386196	-0.234883
17	8	0	1.333813	-2.141320	0.994459
18	8	0	1.853137	-2.095081	-1.475727
19	6	0	2.941987	-0.271765	0.074444
20	6	0	3.573552	0.337620	-1.006233
21	6	0	3.333538	-0.018822	1.384504
22	6	0	4.613443	1.227665	-0.763488
23	1	0	3.257010	0.105063	-2.017469
24	6	0	4.377880	0.871647	1.615272
25	1	0	2.831515	-0.524598	2.202364
26	6	0	5.013025	1.495386	0.544637
27	1	0	5.115917	1.708982	-1.596760
28	1	0	4.697611	1.074379	2.632703
29	1	0	5.826276	2.190953	0.729384
30	7	0	-1.278649	1.774734	-1.023928
31	7	0	-1.086102	2.773802	-1.451170

Zero-point correction= 0.227611 (Hartree/Particle)
Thermal correction to Energy= 0.245203
Thermal correction to Enthalpy= 0.246147
Thermal correction to Gibbs Free Energy= 0.178523
Sum of electronic and zero-point Energies= -1252.291402
Sum of electronic and thermal Energies= -1252.273810
Sum of electronic and thermal Enthalpies= -1252.272866
Sum of electronic and thermal Free Energies= -1252.340490
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1252.77505960

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.596705	0.878319	1.794855
2	8	0	-3.280182	-0.004601	1.217813
3	8	0	-1.377013	1.164407	1.552927
4	6	0	-3.276522	1.708464	2.854979
5	1	0	-2.563295	1.996522	3.629379
6	1	0	-4.114382	1.158997	3.285778
7	1	0	-3.663744	2.621125	2.389089
8	6	0	-2.192324	1.248935	-1.911702
9	8	0	-2.978424	0.292767	-1.678108
10	8	0	-1.067386	1.454237	-1.353237
11	6	0	-2.595251	2.242718	-2.972337
12	1	0	-3.670152	2.193967	-3.149826

13	1	0	-2.071336	1.994147	-3.901244
14	1	0	-2.294975	3.250665	-2.678231
15	6	0	-0.227829	-1.934050	-1.999954
16	8	0	-1.438077	-2.195635	-1.773717
17	8	0	0.466846	-1.042401	-1.411872
18	6	0	0.483478	-2.725287	-3.068371
19	1	0	1.562806	-2.582974	-2.991473
20	1	0	0.144129	-2.375776	-4.048874
21	1	0	0.221269	-3.782408	-2.983601
22	6	0	-0.619365	-2.292597	1.665613
23	8	0	-1.735452	-2.489925	1.118264
24	8	0	0.162720	-1.310709	1.451035
25	6	0	-0.130285	-3.332104	2.643841
26	1	0	-0.975475	-3.780206	3.168865
27	1	0	0.576952	-2.894908	3.350559
28	1	0	0.379157	-4.125090	2.085011
29	45	0	-2.433159	-1.142521	-0.293282
30	45	0	-0.387198	0.122166	0.066388
31	6	0	1.435648	1.241717	0.337662
32	6	0	2.472825	0.338421	-0.120126
33	1	0	2.505374	0.253384	-1.213567
34	6	0	1.539080	2.687634	0.093513
35	6	0	0.422947	3.514787	0.290648
36	6	0	2.742848	3.248341	-0.362551
37	6	0	0.515068	4.875634	0.033239
38	1	0	-0.501208	3.076928	0.650196
39	6	0	2.822123	4.605843	-0.641937
40	1	0	3.616538	2.616611	-0.498593
41	6	0	1.708213	5.419109	-0.440264
42	1	0	-0.348154	5.514420	0.191696
43	1	0	3.751282	5.031277	-1.007038
44	1	0	1.772637	6.482724	-0.650146
45	7	0	3.169984	-0.416780	0.641966
46	16	0	4.026561	-1.638453	-0.174069
47	8	0	3.947580	-1.459692	-1.622072
48	8	0	5.321933	-1.755499	0.469535
49	7	0	1.607357	1.076303	2.128262
50	7	0	1.299425	1.045942	3.185747
51	6	0	2.999740	-3.027584	0.276035
52	1	0	3.448969	-3.917676	-0.169541
53	1	0	2.975099	-3.106206	1.363454
54	1	0	1.999765	-2.845970	-0.121801

Zero-point correction= 0.391778 (Hartree/Particle)
Thermal correction to Energy= 0.428378
Thermal correction to Enthalpy= 0.429322
Thermal correction to Gibbs Free Energy= 0.321305
Sum of electronic and zero-point Energies= -2193.307555
Sum of electronic and thermal Energies= -2193.270955
Sum of electronic and thermal Enthalpies= -2193.270011
Sum of electronic and thermal Free Energies= -2193.378028

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2194.22439380

N_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.550870
2	7	0	0.000000	0.000000	-0.550870

Zero-point correction= 0.005708 (Hartree/Particle)
Thermal correction to Energy= 0.008069
Thermal correction to Enthalpy= 0.009013
Thermal correction to Gibbs Free Energy= -0.012735
Sum of electronic and zero-point Energies= -109.479340
Sum of electronic and thermal Energies= -109.476980
Sum of electronic and thermal Enthalpies= -109.476036
Sum of electronic and thermal Free Energies= -109.497784

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -109.51208290

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.689926	-0.401515	2.094013
2	8	0	-2.736679	-1.609344	1.751275
3	8	0	-2.017967	0.521429	1.524784
4	6	0	-3.477329	0.020372	3.309795
5	1	0	-3.974061	0.975220	3.122622
6	1	0	-2.784099	0.164211	4.144854
7	1	0	-4.205573	-0.746168	3.576071
8	6	0	-3.280048	-0.566987	-1.584095
9	8	0	-3.196610	-1.737645	-1.135793
10	8	0	-2.479746	0.396294	-1.339238
11	6	0	-4.415846	-0.250909	-2.525934
12	1	0	-4.020678	-0.187286	-3.544954
13	1	0	-4.851239	0.719785	-2.277408
14	1	0	-5.173784	-1.033563	-2.483671
15	6	0	0.190603	-1.806702	-2.092354
16	8	0	-0.475146	-2.709887	-1.529104
17	8	0	0.244332	-0.579502	-1.742826
18	6	0	1.044395	-2.193175	-3.275171
19	1	0	1.135529	-1.357209	-3.970660
20	1	0	0.624403	-3.068908	-3.771935
21	1	0	2.049471	-2.447619	-2.919742
22	6	0	0.740350	-1.615276	1.649226
23	8	0	-0.022206	-2.578692	1.372956
24	8	0	0.675095	-0.440969	1.162184
25	6	0	1.814492	-1.836368	2.682462
26	1	0	1.378885	-1.655751	3.671353
27	1	0	2.640055	-1.139582	2.530987
28	1	0	2.166852	-2.868214	2.644864
29	45	0	-1.635298	-2.247879	0.122145
30	45	0	-0.852819	0.063071	-0.108831
31	6	0	-0.149760	1.946786	-0.260784
32	6	0	1.243228	1.921944	-0.664265
33	1	0	1.407125	1.716477	-1.732716
34	6	0	-0.826380	3.175832	-0.031766
35	6	0	-2.230626	3.185714	0.154430
36	6	0	-0.114568	4.402163	0.027189
37	6	0	-2.890987	4.380224	0.388112
38	1	0	-2.770955	2.250363	0.093403
39	6	0	-0.781761	5.585222	0.282079
40	1	0	0.962619	4.401011	-0.102815
41	6	0	-2.168571	5.571674	0.457832
42	1	0	-3.967771	4.389448	0.521052
43	1	0	-0.233668	6.519578	0.340178
44	1	0	-2.691213	6.504610	0.649390
45	7	0	2.210924	2.006777	0.171391
46	16	0	3.745792	1.748171	-0.531315
47	8	0	3.629851	1.723152	-1.987720
48	8	0	4.653573	2.676700	0.118103
49	6	0	4.097443	0.092964	0.020695
50	6	0	5.112943	-0.119897	0.944251
51	6	0	3.368379	-0.959390	-0.527386
52	6	0	5.413504	-1.429108	1.316467
53	1	0	5.657657	0.726179	1.349439
54	6	0	3.670543	-2.258963	-0.142126
55	1	0	2.564710	-0.755065	-1.226264
56	6	0	4.697576	-2.492471	0.773194
57	1	0	6.208723	-1.615645	2.031211
58	1	0	3.097560	-3.088805	-0.545287
59	1	0	4.933678	-3.509927	1.070025

Zero-point correction= 0.438153 (Hartree/Particle)
Thermal correction to Energy= 0.475443
Thermal correction to Enthalpy= 0.476388
Thermal correction to Gibbs Free Energy= 0.365706
Sum of electronic and zero-point Energies= -2275.463217
Sum of electronic and thermal Energies= -2275.425926
Sum of electronic and thermal Enthalpies= -2275.424982
Sum of electronic and thermal Free Energies= -2275.535664

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2276.44436137

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.267362	1.278859	0.000051
2	6	0	-0.063278	0.840398	0.000049
3	6	0	-0.332915	-0.547708	-0.000009
4	6	0	0.733581	-1.461624	-0.000047
5	6	0	2.043059	-1.024374	-0.000040
6	6	0	2.296926	0.354541	0.000006
7	1	0	1.459949	2.346188	0.000097
8	1	0	0.509048	-2.526100	-0.000091
9	1	0	2.863254	-1.733827	-0.000073
10	1	0	3.323611	0.709497	0.000010
11	8	0	-1.036116	1.754606	0.000130
12	1	0	-1.895221	1.275424	0.000149
13	6	0	-1.706323	-1.029527	-0.000054
14	8	0	-2.695830	-0.305321	-0.000099
15	1	0	-1.835546	-2.128852	-0.000070

Zero-point correction= 0.116817 (Hartree/Particle)
Thermal correction to Energy= 0.123694
Thermal correction to Enthalpy= 0.124638
Thermal correction to Gibbs Free Energy= 0.085581
Sum of electronic and zero-point Energies= -420.544923
Sum of electronic and thermal Energies= -420.538046
Sum of electronic and thermal Enthalpies= -420.537101
Sum of electronic and thermal Free Energies= -420.576159
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -420.78748388

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.176839	1.001506	-2.328771
2	8	0	2.328800	-0.150953	-2.800441
3	8	0	1.768887	1.292888	-1.155411
4	6	0	2.461681	2.170614	-3.240420
5	1	0	1.541916	2.408996	-3.786482
6	1	0	3.230291	1.904231	-3.967326
7	1	0	2.763173	3.048136	-2.664690
8	6	0	3.922490	-1.139690	0.250290
9	8	0	3.714739	-1.808875	-0.793870
10	8	0	3.082052	-0.396272	0.854283
11	6	0	5.293276	-1.217997	0.877396
12	1	0	5.208196	-1.690313	1.860746
13	1	0	5.688758	-0.210096	1.029608
14	1	0	5.968113	-1.798303	0.247956
15	6	0	0.792231	-3.057084	0.749082
16	8	0	1.262082	-3.338348	-0.381933
17	8	0	0.616704	-1.886986	1.221609
18	6	0	0.397954	-4.203890	1.647913
19	1	0	-0.235300	-4.901380	1.093116
20	1	0	-0.119853	-3.840883	2.537088
21	1	0	1.300692	-4.745843	1.946397
22	6	0	-0.922569	-0.882000	-1.817629
23	8	0	-0.110000	-1.670098	-2.370225
24	8	0	-0.700080	-0.177464	-0.779697
25	6	0	-2.275014	-0.711963	-2.456526
26	1	0	-2.199594	0.074451	-3.215879
27	1	0	-3.011926	-0.408606	-1.712165
28	1	0	-2.575708	-1.638879	-2.947130
29	45	0	1.827063	-1.803066	-1.651599
30	45	0	1.159671	-0.232448	0.107982
31	6	0	0.578916	1.022727	1.637431
32	6	0	-0.548512	0.388503	2.290936
33	1	0	-0.218631	-0.426849	2.953340
34	6	0	1.370958	2.011780	2.320302
35	6	0	2.569200	2.476416	1.744112
36	6	0	0.948801	2.545002	3.556025
37	6	0	3.321504	3.444592	2.393415
38	1	0	2.883646	2.072354	0.789806
39	6	0	1.710685	3.501787	4.204766
40	1	0	0.013594	2.207531	3.993419
41	6	0	2.896424	3.951392	3.620791

42	1	0	4.242643	3.805387	1.946876
43	1	0	1.382963	3.906340	5.156794
44	1	0	3.492037	4.705388	4.127489
45	7	0	-1.792795	0.578362	2.056958
46	16	0	-2.831548	-0.525817	2.829422
47	8	0	-2.064109	-1.502553	3.598166
48	8	0	-3.864976	0.265329	3.473766
49	6	0	-2.110412	3.687994	-3.847744
50	6	0	-1.183348	3.623649	-2.828700
51	6	0	-1.489465	3.007928	-1.601067
52	6	0	-2.770592	2.436818	-1.402017
53	6	0	-3.711045	2.519600	-2.442720
54	6	0	-3.382007	3.131129	-3.637526
55	1	0	-1.867930	4.163584	-4.791704
56	1	0	-4.688346	2.077347	-2.281645
57	1	0	-4.124531	3.176813	-4.429018
58	6	0	-0.487006	2.965020	-0.560131
59	8	0	-0.710450	2.493771	0.554009
60	1	0	-0.193839	4.057652	-2.956106
61	8	0	-3.147151	1.811098	-0.293224
62	1	0	-2.405264	1.720759	0.348509
63	1	0	0.506175	3.378556	-0.793465
64	6	0	-3.526027	-1.341417	1.410243
65	6	0	-2.846453	-2.419450	0.850154
66	6	0	-4.736015	-0.889068	0.897254
67	6	0	-3.405969	-3.072818	-0.241210
68	1	0	-1.898356	-2.731536	1.270611
69	6	0	-5.288405	-1.553290	-0.194317
70	1	0	-5.231691	-0.040166	1.354335
71	6	0	-4.628675	-2.643432	-0.756554
72	1	0	-2.887376	-3.914102	-0.690322
73	1	0	-6.236322	-1.218896	-0.603936
74	1	0	-5.064905	-3.157483	-1.607848

Zero-point correction= 0.557352 (Hartree/Particle)
Thermal correction to Energy= 0.601626
Thermal correction to Enthalpy= 0.602570
Thermal correction to Gibbs Free Energy= 0.479171
Sum of electronic and zero-point Energies= -2696.021965
Sum of electronic and thermal Energies= -2695.977692
Sum of electronic and thermal Enthalpies= -2695.976748
Sum of electronic and thermal Free Energies= -2696.100147

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.24663485

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.479624	1.653647	0.945610
2	6	0	1.219169	0.529203	0.398661
3	45	0	-0.286374	-1.007992	0.089188
4	8	0	0.366484	-2.007819	1.762103
5	6	0	-0.223979	-3.076704	2.118126
6	8	0	-1.206543	-3.616509	1.542010
7	45	0	-2.036904	-2.705240	-0.111532
8	8	0	-3.217084	-1.554106	1.126264
9	6	0	-2.774771	-0.446693	1.526806
10	8	0	-1.627071	0.037050	1.255010
11	8	0	0.886002	-2.254228	-1.090437
12	6	0	0.403263	-3.349960	-1.526863
13	8	0	-0.760692	-3.778561	-1.330628
14	8	0	-1.067617	-0.119663	-1.602751
15	6	0	-2.109475	-0.617820	-2.143375
16	8	0	-2.730487	-1.640017	-1.755900
17	8	0	5.656082	0.355784	-1.715427
18	1	0	6.156014	1.092265	-1.280974
19	6	0	2.507670	0.200702	1.000322
20	6	0	3.178901	1.117763	1.836564
21	6	0	3.127929	-1.029803	0.726491
22	6	0	4.411841	0.811235	2.387472
23	1	0	2.724432	2.083333	2.045661
24	6	0	4.375359	-1.327713	1.266101
25	1	0	2.618454	-1.741990	0.088738
26	6	0	5.017686	-0.412761	2.092840

27	1	0	4.910632	1.525935	3.034361
28	1	0	4.846282	-2.278685	1.037720
29	1	0	5.991634	-0.648052	2.511593
30	7	0	0.112713	2.713120	0.318639
31	1	0	0.142260	1.467280	1.973807
32	16	0	-0.888932	3.768272	1.177354
33	6	0	-2.301347	3.814392	0.092948
34	6	0	-2.891098	2.621964	-0.319342
35	6	0	-2.815309	5.051566	-0.276799
36	6	0	-4.031875	2.676832	-1.111746
37	1	0	-2.452207	1.672712	-0.033175
38	6	0	-3.958856	5.092823	-1.071237
39	1	0	-2.320027	5.959725	0.049800
40	6	0	-4.566323	3.910239	-1.484499
41	1	0	-4.504396	1.754193	-1.436332
42	1	0	-4.372963	6.051364	-1.367730
43	1	0	-5.458498	3.948108	-2.102353
44	8	0	-0.243998	5.073332	1.153195
45	8	0	-1.285588	3.190985	2.460140
46	6	0	4.380844	0.688873	-1.729952
47	6	0	3.929278	1.934185	-1.207934
48	6	0	3.455549	-0.208338	-2.306187
49	6	0	2.569543	2.209909	-1.192928
50	6	0	2.117827	0.079935	-2.259979
51	1	0	3.833658	-1.121717	-2.751305
52	6	0	1.631720	1.244640	-1.599265
53	1	0	2.208735	3.151708	-0.789268
54	1	0	1.396295	-0.614143	-2.669744
55	1	0	0.589578	1.520749	-1.718104
56	6	0	4.882910	2.872626	-0.630298
57	8	0	6.088817	2.662427	-0.558332
58	6	0	-3.673965	0.415701	2.374217
59	1	0	-3.130557	1.284871	2.747405
60	1	0	-4.517944	0.750443	1.762160
61	1	0	-4.078193	-0.176008	3.199483
62	6	0	0.298257	-3.734717	3.371081
63	1	0	0.033165	-4.792769	3.382868
64	1	0	1.379477	-3.602964	3.444825
65	1	0	-0.162602	-3.248696	4.237558
66	6	0	-2.612713	0.098108	-3.372942
67	1	0	-1.926199	-0.097178	-4.203325
68	1	0	-3.608177	-0.256759	-3.642046
69	1	0	-2.622919	1.176516	-3.195387
70	6	0	1.343387	-4.213413	-2.332512
71	1	0	2.008152	-3.592976	-2.937781
72	1	0	1.960941	-4.797117	-1.641403
73	1	0	0.780654	-4.902546	-2.963289
74	1	0	4.463044	3.815694	-0.236653

Zero-point correction= 0.555983 (Hartree/Particle)
Thermal correction to Energy= 0.601163
Thermal correction to Enthalpy= 0.602107
Thermal correction to Gibbs Free Energy= 0.474523
Sum of electronic and zero-point Energies= -2696.017463
Sum of electronic and thermal Energies= -2695.972283
Sum of electronic and thermal Enthalpies= -2695.971339
Sum of electronic and thermal Free Energies= -2696.098923

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.23890019

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.831918	1.511988	0.967399
2	6	0	1.308915	0.197205	0.605567
3	45	0	-0.468268	-0.894108	0.170541
4	8	0	-0.000140	-2.470259	1.424708
5	6	0	-0.778626	-3.474206	1.483274
6	8	0	-1.846167	-3.632029	0.834339
7	45	0	-2.487068	-2.129346	-0.430340
8	8	0	-3.422333	-1.218591	1.170210
9	6	0	-2.773307	-0.420048	1.893440
10	8	0	-1.559613	-0.066776	1.726137
11	8	0	0.469635	-1.802609	-1.408606

12	6	0	-0.184153	-2.616712	-2.148001
13	8	0	-1.380492	-2.955335	-1.979969
14	8	0	-1.080594	0.559736	-1.141534
15	6	0	-2.168358	0.414051	-1.782133
16	8	0	-2.982455	-0.541416	-1.660508
17	8	0	2.024183	0.426544	-1.134769
18	1	0	1.953888	-0.499562	-1.492617
19	6	0	2.486124	-0.344005	1.295592
20	6	0	3.342440	0.498301	2.024686
21	6	0	2.821376	-1.699253	1.155154
22	6	0	4.494481	-0.004306	2.615140
23	1	0	3.105165	1.554358	2.120626
24	6	0	3.982530	-2.195292	1.733547
25	1	0	2.171180	-2.345520	0.579011
26	6	0	4.816045	-1.351649	2.466209
27	1	0	5.144873	0.654956	3.181071
28	1	0	4.235572	-3.244844	1.617902
29	1	0	5.719738	-1.745516	2.922416
30	7	0	0.701626	2.538761	0.210515
31	1	0	0.471515	1.522862	2.007220
32	16	0	-0.017341	3.880824	0.947229
33	6	0	-1.631441	3.877455	0.198200
34	6	0	-2.514599	2.857771	0.541402
35	6	0	-1.990192	4.895561	-0.675977
36	6	0	-3.791567	2.859758	-0.004746
37	1	0	-2.188166	2.064504	1.204445
38	6	0	-3.277785	4.893801	-1.210160
39	1	0	-1.273981	5.672727	-0.920410
40	6	0	-4.173545	3.881904	-0.874472
41	1	0	-4.481550	2.056074	0.234981
42	1	0	-3.578755	5.684661	-1.890028
43	1	0	-5.172932	3.882873	-1.299142
44	8	0	0.726941	5.037278	0.472031
45	8	0	-0.181325	3.654737	2.381718
46	6	0	3.313141	0.917105	-1.200655
47	6	0	4.426327	0.080353	-1.394114
48	6	0	3.484219	2.282278	-1.006243
49	6	0	5.709086	0.636266	-1.335540
50	6	0	4.770321	2.810022	-0.964884
51	1	0	2.608147	2.905609	-0.873290
52	6	0	5.889889	1.992489	-1.114576
53	1	0	6.566844	-0.016220	-1.479630
54	1	0	4.893094	3.877211	-0.809081
55	1	0	6.888710	2.413303	-1.070936
56	6	0	4.290906	-1.338340	-1.732611
57	8	0	3.234877	-1.871707	-2.020240
58	6	0	-3.494997	0.222971	3.052615
59	1	0	-2.814043	0.354417	3.895606
60	1	0	-3.843971	1.216468	2.748679
61	1	0	-4.358988	-0.377035	3.340880
62	6	0	-0.387552	-4.561254	2.454797
63	1	0	-0.803876	-5.519022	2.139186
64	1	0	0.698886	-4.619599	2.543917
65	1	0	-0.797153	-4.311759	3.439419
66	6	0	-2.473978	1.475331	-2.807988
67	1	0	-2.021554	1.173889	-3.759253
68	1	0	-3.551708	1.566246	-2.949687
69	1	0	-2.042204	2.430607	-2.504835
70	6	0	0.561729	-3.182799	-3.327797
71	1	0	1.584875	-3.430087	-3.040128
72	1	0	0.038011	-4.054300	-3.721587
73	1	0	0.614247	-2.415440	-4.107617
74	1	0	5.234091	-1.917993	-1.746300

Zero-point correction= 0.556017 (Hartree/Particle)
Thermal correction to Energy= 0.600933
Thermal correction to Enthalpy= 0.601877
Thermal correction to Gibbs Free Energy= 0.476015
Sum of electronic and zero-point Energies= -2696.016367
Sum of electronic and thermal Energies= -2695.971452
Sum of electronic and thermal Enthalpies= -2695.970507
Sum of electronic and thermal Free Energies= -2696.096370

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.23707237

TS4'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.244166	1.025486	-1.189145
2	6	0	0.298996	1.540736	-0.217017
3	45	0	-1.228867	-0.022788	0.067556
4	8	0	-2.475502	1.162445	-1.066165
5	6	0	-3.650821	0.765320	-1.341684
6	8	0	-4.175395	-0.322720	-0.982519
7	45	0	-3.069308	-1.637917	0.160040
8	8	0	-2.301931	-2.499775	-1.563697
9	6	0	-1.270491	-2.005977	-2.086566
10	8	0	-0.624173	-0.995770	-1.654574
11	8	0	-1.981782	0.781019	1.822309
12	6	0	-3.048075	0.297912	2.322394
13	8	0	-3.708493	-0.675367	1.875331
14	8	0	-0.157377	-1.396086	1.197339
15	6	0	-0.704921	-2.473414	1.595822
16	8	0	-1.864963	-2.865234	1.314518
17	8	0	1.292498	1.905157	1.247550
18	1	0	1.545691	2.872939	1.115390
19	6	0	-0.228312	2.906583	-0.440828
20	6	0	0.239336	3.695910	-1.501164
21	6	0	-1.201604	3.431354	0.422216
22	6	0	-0.283009	4.965898	-1.718020
23	1	0	1.014288	3.318322	-2.162138
24	6	0	-1.695603	4.712216	0.222251
25	1	0	-1.565532	2.814229	1.236104
26	6	0	-1.247293	5.476679	-0.854121
27	1	0	0.076241	5.561361	-2.551432
28	1	0	-2.444191	5.112180	0.899613
29	1	0	-1.647367	6.473347	-1.016283
30	7	0	2.496041	0.843282	-0.978030
31	1	0	0.763603	0.702717	-2.120402
32	16	0	3.319311	-0.072040	-2.131062
33	6	0	3.500252	-1.576588	-1.190648
34	6	0	2.362513	-2.329193	-0.911048
35	6	0	4.758711	-1.952341	-0.738439
36	6	0	2.498328	-3.497285	-0.171071
37	1	0	1.386936	-1.994427	-1.250502
38	6	0	4.881227	-3.124424	0.004618
39	1	0	5.618379	-1.332731	-0.969974
40	6	0	3.755179	-3.894913	0.285700
41	1	0	1.621249	-4.099846	0.044580
42	1	0	5.858075	-3.437292	0.360652
43	1	0	3.856807	-4.812532	0.857972
44	8	0	4.627872	0.535907	-2.304338
45	8	0	2.475898	-0.342431	-3.292146
46	6	0	2.443044	1.258381	1.678784
47	6	0	3.632298	1.999483	1.778716
48	6	0	2.397885	-0.079884	2.020168
49	6	0	4.799780	1.348944	2.196355
50	6	0	3.574192	-0.701002	2.421704
51	1	0	1.469661	-0.628289	1.909289
52	6	0	4.778480	0.000638	2.511089
53	1	0	5.725045	1.916330	2.257749
54	1	0	3.552599	-1.762351	2.649933
55	1	0	5.686865	-0.505967	2.818405
56	6	0	3.669721	3.404467	1.398638
57	8	0	2.681220	4.042267	1.046395
58	6	0	-0.725296	-2.656923	-3.332955
59	1	0	-1.477694	-2.599777	-4.124951
60	1	0	0.193333	-2.164207	-3.654732
61	1	0	-0.538455	-3.716337	-3.135370
62	6	0	-4.473634	1.687690	-2.206079
63	1	0	-5.537524	1.508252	-2.044736
64	1	0	-4.217548	2.728071	-1.996380
65	1	0	-4.240748	1.484337	-3.256719
66	6	0	0.117458	-3.337571	2.522185
67	1	0	-0.123120	-3.066415	3.555796
68	1	0	-0.135191	-4.390043	2.380344
69	1	0	1.184099	-3.173551	2.357435
70	6	0	-3.549679	0.974520	3.574946

71	1	0	-2.768950	0.947819	4.340246
72	1	0	-3.761441	2.025940	3.358257
73	1	0	-4.450864	0.483651	3.942485
74	1	0	4.652415	3.904154	1.439957

Zero-point correction= 0.557174 (Hartree/Particle)
Thermal correction to Energy= 0.601592
Thermal correction to Enthalpy= 0.602537
Thermal correction to Gibbs Free Energy= 0.478317
Sum of electronic and zero-point Energies= -2696.005411
Sum of electronic and thermal Energies= -2695.960993
Sum of electronic and thermal Enthalpies= -2695.960048
Sum of electronic and thermal Free Energies= -2696.084268

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.22864709

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.479624	1.653647	0.945610
2	6	0	1.219169	0.529203	0.398661
3	45	0	-0.286374	-1.007992	0.089188
4	8	0	0.366484	-2.007819	1.762103
5	6	0	-0.223979	-3.076704	2.118126
6	8	0	-1.206543	-3.616509	1.542010
7	45	0	-2.036904	-2.705240	-0.111532
8	8	0	-3.217084	-1.554106	1.126264
9	6	0	-2.774771	-0.446693	1.526806
10	8	0	-1.627071	0.037050	1.255010
11	8	0	0.886002	-2.254228	-1.090437
12	6	0	0.403263	-3.349960	-1.526863
13	8	0	-0.760692	-3.778561	-1.330628
14	8	0	-1.067617	-0.119663	-1.602751
15	6	0	-2.109475	-0.617820	-2.143375
16	8	0	-2.730487	-1.640017	-1.755900
17	8	0	5.656082	0.355784	-1.715427
18	1	0	6.156014	1.092265	-1.280974
19	6	0	2.507670	0.200702	1.000322
20	6	0	3.178901	1.117763	1.836564
21	6	0	3.127929	-1.029803	0.726491
22	6	0	4.411841	0.811235	2.387472
23	1	0	2.724432	2.083333	2.045661
24	6	0	4.375359	-1.327713	1.266101
25	1	0	2.618454	-1.741990	0.088738
26	6	0	5.017686	-0.412761	2.092840
27	1	0	4.910632	1.525935	3.034361
28	1	0	4.846282	-2.278685	1.037720
29	1	0	5.991634	-0.648052	2.511593
30	7	0	0.112713	2.713120	0.318639
31	1	0	0.142260	1.467280	1.973807
32	16	0	-0.888932	3.768272	1.177354
33	6	0	-2.301347	3.814392	0.092948
34	6	0	-2.891098	2.621964	-0.319342
35	6	0	-2.815309	5.051566	-0.276799
36	6	0	-4.031875	2.676832	-1.111746
37	1	0	-2.452207	1.672712	-0.033175
38	6	0	-3.958856	5.092823	-1.071237
39	1	0	-2.320027	5.959725	0.049800
40	6	0	-4.566323	3.910239	-1.484499
41	1	0	-4.504396	1.754193	-1.436332
42	1	0	-4.372963	6.051364	-1.367730
43	1	0	-5.458498	3.948108	-2.102353
44	8	0	-0.243998	5.073332	1.153195
45	8	0	-1.285588	3.190985	2.460140
46	6	0	4.380844	0.688873	-1.729952
47	6	0	3.929278	1.934185	-1.207934
48	6	0	3.455549	-0.208338	-2.306187
49	6	0	2.569543	2.209909	-1.192928
50	6	0	2.117827	0.079935	-2.259979
51	1	0	3.833658	-1.121717	-2.751305
52	6	0	1.631720	1.244640	-1.599265
53	1	0	2.208735	3.151708	-0.789268
54	1	0	1.396295	-0.614143	-2.669744

55	1	0	0.589578	1.520749	-1.718104
56	6	0	4.882910	2.872626	-0.630298
57	8	0	6.088817	2.662427	-0.558332
58	6	0	-3.673965	0.415701	2.374217
59	1	0	-3.130557	1.284871	2.747405
60	1	0	-4.517944	0.750443	1.762160
61	1	0	-4.078193	-0.176008	3.199483
62	6	0	0.298257	-3.734717	3.371081
63	1	0	0.033165	-4.792769	3.382868
64	1	0	1.379477	-3.602964	3.444825
65	1	0	-0.162602	-3.248696	4.237558
66	6	0	-2.612713	0.098108	-3.372942
67	1	0	-1.926199	-0.097178	-4.203325
68	1	0	-3.608177	-0.256759	-3.642046
69	1	0	-2.622919	1.176516	-3.195387
70	6	0	1.343387	-4.213413	-2.332512
71	1	0	2.008152	-3.592976	-2.937781
72	1	0	1.960941	-4.797117	-1.641403
73	1	0	0.780654	-4.902546	-2.963289
74	1	0	4.463044	3.815694	-0.236653

Zero-point correction= 0.555983 (Hartree/Particle)
Thermal correction to Energy= 0.601163
Thermal correction to Enthalpy= 0.602107
Thermal correction to Gibbs Free Energy= 0.474523
Sum of electronic and zero-point Energies= -2696.017463
Sum of electronic and thermal Energies= -2695.972283
Sum of electronic and thermal Enthalpies= -2695.971339
Sum of electronic and thermal Free Energies= -2696.098923

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.23890019

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.158606	0.770766	-2.251455
2	8	0	2.116416	-0.342446	-2.824410
3	8	0	1.790279	1.011787	-1.050737
4	6	0	2.660036	1.959179	-3.034558
5	1	0	1.805003	2.590099	-3.302424
6	1	0	3.163296	1.632803	-3.944837
7	1	0	3.338087	2.556585	-2.419089
8	6	0	3.460038	-1.877561	0.138173
9	8	0	3.169073	-2.389427	-0.977022
10	8	0	2.738383	-1.081344	0.816439
11	6	0	4.791481	-2.236218	0.751872
12	1	0	4.618370	-2.792439	1.678029
13	1	0	5.328724	-1.321328	1.016350
14	1	0	5.384310	-2.840239	0.064651
15	6	0	0.073215	-3.249971	0.472232
16	8	0	0.498469	-3.505354	-0.685980
17	8	0	0.071179	-2.111803	1.040865
18	6	0	-0.491864	-4.398359	1.271751
19	1	0	-1.170088	-4.985065	0.647131
20	1	0	-1.007007	-4.034028	2.161752
21	1	0	0.330030	-5.055307	1.573856
22	6	0	-1.201391	-0.551027	-1.944682
23	8	0	-0.555017	-1.454623	-2.539969
24	8	0	-0.874739	0.002672	-0.846841
25	6	0	-2.455305	-0.025030	-2.594286
26	1	0	-2.191830	0.871922	-3.167257
27	1	0	-3.184027	0.259781	-1.834003
28	1	0	-2.872307	-0.767688	-3.275339
29	45	0	1.322547	-1.988846	-1.823588
30	45	0	0.906748	-0.500811	0.062300
31	6	0	0.484728	1.026220	1.639842
32	6	0	-0.682952	0.421009	2.240291
33	1	0	-0.508457	-0.394282	2.945738
34	6	0	1.635058	1.444271	2.494229
35	6	0	2.908531	1.650943	1.946421
36	6	0	1.447418	1.669707	3.863609
37	6	0	3.959406	2.082790	2.747922
38	1	0	3.077274	1.439043	0.896294

39	6	0	2.506788	2.075609	4.668769
40	1	0	0.463496	1.532085	4.303714
41	6	0	3.764071	2.289350	4.110990
42	1	0	4.940466	2.237865	2.308397
43	1	0	2.344785	2.236337	5.730172
44	1	0	4.589717	2.613219	4.737741
45	7	0	-1.876179	0.767359	1.880059
46	16	0	-3.147564	-0.117493	2.538068
47	8	0	-2.642298	-1.192657	3.386364
48	8	0	-4.097940	0.845482	3.070650
49	6	0	-0.183651	5.269020	-2.678659
50	6	0	0.461110	4.596914	-1.671499
51	6	0	-0.214929	3.640423	-0.872202
52	6	0	-1.599896	3.373912	-1.103239
53	6	0	-2.235623	4.077869	-2.146647
54	6	0	-1.546313	4.995370	-2.908827
55	1	0	0.342499	5.995242	-3.287696
56	1	0	-3.285870	3.871352	-2.320099
57	1	0	-2.068328	5.517497	-3.705349
58	6	0	0.545148	2.941455	0.095513
59	8	0	-0.048831	2.089076	0.812680
60	1	0	1.514732	4.777774	-1.474967
61	8	0	-2.367953	2.541920	-0.427732
62	1	0	-1.930872	1.976434	0.252308
63	1	0	1.604006	3.136588	0.253589
64	6	0	-3.849518	-0.840974	1.068890
65	6	0	-3.207258	-1.928638	0.485517
66	6	0	-5.030765	-0.325323	0.549004
67	6	0	-3.762729	-2.516917	-0.643965
68	1	0	-2.279551	-2.287148	0.912604
69	6	0	-5.584869	-0.927172	-0.579114
70	1	0	-5.505846	0.521311	1.032535
71	6	0	-4.954711	-2.019299	-1.170842
72	1	0	-3.262457	-3.357462	-1.114989
73	1	0	-6.511094	-0.541713	-0.993909
74	1	0	-5.390369	-2.482456	-2.051180

Zero-point correction= 0.559772 (Hartree/Particle)
Thermal correction to Energy= 0.604145
Thermal correction to Enthalpy= 0.605089
Thermal correction to Gibbs Free Energy= 0.481751
Sum of electronic and zero-point Energies= -2696.042553
Sum of electronic and thermal Energies= -2695.998180
Sum of electronic and thermal Enthalpies= -2695.997236
Sum of electronic and thermal Free Energies= -2696.120575

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.26792979

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.751088	1.589034	0.901162
2	6	0	1.405044	0.378608	0.475464
3	45	0	-0.373072	-0.884956	0.138418
4	8	0	0.288736	-2.419448	1.356719
5	6	0	-0.361880	-3.509088	1.404448
6	8	0	-1.413215	-3.782885	0.764394
7	45	0	-2.243981	-2.331196	-0.454796
8	8	0	-3.242996	-1.566324	1.185320
9	6	0	-2.670817	-0.715606	1.916251
10	8	0	-1.510429	-0.222057	1.735241
11	8	0	0.637019	-1.623533	-1.495784
12	6	0	0.066106	-2.488976	-2.252089
13	8	0	-1.067628	-2.980395	-2.053386
14	8	0	-1.164357	0.513507	-1.146522
15	6	0	-2.244387	0.257231	-1.764967
16	8	0	-2.943410	-0.786309	-1.644025
17	8	0	1.969854	0.552039	-0.996631
18	1	0	1.875892	-0.342283	-1.455196
19	6	0	2.519719	-0.153557	1.310132
20	6	0	3.168726	0.660280	2.246194
21	6	0	2.985133	-1.460179	1.115756
22	6	0	4.241671	0.174776	2.987583

23	1	0	2.838759	1.685229	2.393047
24	6	0	4.073583	-1.934934	1.836418
25	1	0	2.484733	-2.099290	0.398340
26	6	0	4.700400	-1.122076	2.779478
27	1	0	4.726932	0.817205	3.715951
28	1	0	4.423759	-2.950162	1.673242
29	1	0	5.543542	-1.500135	3.350205
30	7	0	0.467893	2.608474	0.165669
31	1	0	0.431938	1.542110	1.949284
32	16	0	-0.364332	3.847896	0.941228
33	6	0	-1.999897	3.693958	0.254073
34	6	0	-2.776668	2.603656	0.634773
35	6	0	-2.479295	4.666823	-0.613897
36	6	0	-4.065075	2.483960	0.129416
37	1	0	-2.360060	1.853049	1.297019
38	6	0	-3.777756	4.543731	-1.106099
39	1	0	-1.844826	5.503569	-0.886032
40	6	0	-4.566171	3.457359	-0.735656
41	1	0	-4.672322	1.624579	0.398443
42	1	0	-4.170196	5.297293	-1.781828
43	1	0	-5.573570	3.361663	-1.129722
44	8	0	0.231528	5.085589	0.459403
45	8	0	-0.454062	3.593888	2.377438
46	6	0	3.221294	1.188677	-1.163877
47	6	0	4.388041	0.458843	-1.429212
48	6	0	3.248559	2.562215	-1.003237
49	6	0	5.603347	1.147115	-1.474423
50	6	0	4.474011	3.222939	-1.065872
51	1	0	2.321242	3.093151	-0.821840
52	6	0	5.655081	2.521726	-1.287492
53	1	0	6.513001	0.586570	-1.674134
54	1	0	4.493967	4.299937	-0.934849
55	1	0	6.605772	3.042513	-1.325593
56	6	0	4.385721	-0.971829	-1.764416
57	8	0	3.384913	-1.592232	-2.061778
58	6	0	-3.435857	-0.188023	3.105360
59	1	0	-2.751060	0.035215	3.925389
60	1	0	-3.933763	0.746321	2.822094
61	1	0	-4.195433	-0.906255	3.416469
62	6	0	0.169802	-4.561491	2.346750
63	1	0	-0.024259	-5.557922	1.945608
64	1	0	1.236515	-4.412194	2.521438
65	1	0	-0.354935	-4.469977	3.303548
66	6	0	-2.694518	1.291873	-2.764062
67	1	0	-2.230866	1.062661	-3.730028
68	1	0	-3.778211	1.257932	-2.882867
69	1	0	-2.370821	2.285863	-2.451275
70	6	0	0.833580	-2.911458	-3.476110
71	1	0	1.873564	-3.113123	-3.213693
72	1	0	0.365112	-3.784635	-3.930455
73	1	0	0.829343	-2.085750	-4.195592
74	1	0	5.378543	-1.460164	-1.773455

Zero-point correction= 0.557564 (Hartree/Particle)
Thermal correction to Energy= 0.602462
Thermal correction to Enthalpy= 0.603407
Thermal correction to Gibbs Free Energy= 0.478193
Sum of electronic and zero-point Energies= -2696.015999
Sum of electronic and thermal Energies= -2695.971101
Sum of electronic and thermal Enthalpies= -2695.970156
Sum of electronic and thermal Free Energies= -2696.095370

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.23931234

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.998515	1.150000	-0.532477
2	6	0	-2.669033	0.011475	0.116459
3	45	0	1.065802	-1.326685	-0.004907
4	8	0	2.065369	-2.784568	-1.059874
5	6	0	3.282207	-2.596724	-1.361659
6	8	0	3.981971	-1.595054	-1.031902

7	45	0	3.129242	-0.124714	0.114272
8	8	0	2.584555	0.845774	-1.613546
9	6	0	1.541037	0.467269	-2.227946
10	8	0	0.690531	-0.365439	-1.783883
11	8	0	1.582410	-2.252206	1.760489
12	6	0	2.717278	-2.003582	2.271444
13	8	0	3.571681	-1.189636	1.817440
14	8	0	0.224347	0.207490	1.089485
15	6	0	0.964773	1.133212	1.545746
16	8	0	2.194294	1.277462	1.292122
17	8	0	-5.924351	-2.909063	1.114932
18	1	0	-6.511229	-2.763905	0.322699
19	6	0	-2.207169	-1.327898	-0.364765
20	6	0	-2.499205	-1.711196	-1.668514
21	6	0	-1.399324	-2.166044	0.421226
22	6	0	-1.979441	-2.892397	-2.202123
23	1	0	-3.128526	-1.072777	-2.283573
24	6	0	-0.878009	-3.347396	-0.110881
25	1	0	-1.210647	-1.913897	1.458323
26	6	0	-1.164040	-3.706727	-1.431685
27	1	0	-2.212471	-3.165872	-3.226506
28	1	0	-0.259660	-3.986645	0.510904
29	1	0	-0.745699	-4.617797	-1.845995
30	7	0	-2.180104	2.356772	-0.134483
31	1	0	-1.387417	0.915373	-1.409557
32	16	0	-1.563922	3.564375	-1.150091
33	6	0	-0.257162	4.267846	-0.172540
34	6	0	1.050540	3.833720	-0.365501
35	6	0	-0.574772	5.251046	0.761999
36	6	0	2.064942	4.399460	0.400683
37	1	0	1.280187	3.067009	-1.096830
38	6	0	0.448257	5.808261	1.520704
39	1	0	-1.602823	5.578982	0.872656
40	6	0	1.764673	5.383929	1.338461
41	1	0	3.085227	4.056755	0.268221
42	1	0	0.219756	6.579694	2.249320
43	1	0	2.560227	5.824152	1.932105
44	8	0	-2.629873	4.541488	-1.282362
45	8	0	-0.962862	2.974073	-2.344758
46	6	0	-5.109072	-1.871595	1.177782
47	6	0	-5.146400	-0.830007	0.268897
48	6	0	-4.208096	-1.847883	2.315786
49	6	0	-4.176755	0.275100	0.364309
50	6	0	-3.354559	-0.825876	2.495545
51	1	0	-4.298719	-2.656104	3.033355
52	6	0	-3.209933	0.268734	1.523235
53	1	0	-4.504620	1.249139	0.007519
54	1	0	-2.750396	-0.777108	3.397275
55	1	0	-2.899784	1.229669	1.922906
56	6	0	-6.142070	-0.837880	-0.767329
57	8	0	-6.956277	-1.751474	-0.945393
58	6	0	1.273091	1.063264	-3.581207
59	1	0	0.524286	1.853454	-3.471500
60	1	0	2.189003	1.485139	-3.996691
61	1	0	0.865231	0.297956	-4.245144
62	6	0	3.940143	-3.649664	-2.215304
63	1	0	5.025543	-3.587877	-2.129379
64	1	0	3.585061	-4.641467	-1.928488
65	1	0	3.657500	-3.478315	-3.259319
66	6	0	0.307387	2.108131	2.484388
67	1	0	0.112832	1.598788	3.434323
68	1	0	0.948343	2.972204	2.657841
69	1	0	-0.650604	2.427234	2.066278
70	6	0	3.091031	-2.772614	3.512332
71	1	0	2.196663	-3.058698	4.068033
72	1	0	3.617201	-3.684561	3.210578
73	1	0	3.762596	-2.180407	4.135878
74	1	0	-6.165786	0.040847	-1.438207

Zero-point correction= 0.559193 (Hartree/Particle)
Thermal correction to Energy= 0.603866
Thermal correction to Enthalpy= 0.604810
Thermal correction to Gibbs Free Energy= 0.478738
Sum of electronic and zero-point Energies= -2696.059169
Sum of electronic and thermal Energies= -2696.014496

Sum of electronic and thermal Enthalpies= -2696.013552
Sum of electronic and thermal Free Energies= -2696.139624
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.28075503

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.978051	0.070264	-2.455346
2	8	0	1.754844	-1.084036	-2.896431
3	8	0	1.650049	0.513542	-1.304048
4	6	0	2.718731	1.041349	-3.341872
5	1	0	3.748089	1.134849	-2.980582
6	1	0	2.254249	2.029396	-3.283205
7	1	0	2.733256	0.685054	-4.372241
8	6	0	2.941559	-2.455416	0.167801
9	8	0	2.533540	-3.052752	-0.867163
10	8	0	2.372558	-1.480175	0.746073
11	6	0	4.215220	-2.954667	0.802663
12	1	0	4.625470	-2.198465	1.473652
13	1	0	4.937295	-3.224581	0.029099
14	1	0	3.988069	-3.856740	1.380326
15	6	0	-0.616760	-3.246457	0.727261
16	8	0	-0.267657	-3.692779	-0.396806
17	8	0	-0.409734	-2.069007	1.168737
18	6	0	-1.370663	-4.170773	1.651460
19	1	0	-2.383967	-3.785251	1.806306
20	1	0	-0.879226	-4.192474	2.627626
21	1	0	-1.421123	-5.175356	1.231111
22	6	0	-1.541354	-0.711077	-1.984516
23	8	0	-1.046114	-1.758555	-2.470450
24	8	0	-1.112694	-0.089332	-0.957264
25	6	0	-2.720820	-0.091876	-2.689959
26	1	0	-3.322545	0.492358	-1.991595
27	1	0	-3.328636	-0.866037	-3.159922
28	1	0	-2.341895	0.568553	-3.479036
29	45	0	0.750290	-2.468955	-1.713199
30	45	0	0.622843	-0.726699	-0.010876
31	6	0	0.610653	0.964907	1.467044
32	6	0	-0.730490	0.847182	1.978719
33	1	0	-0.885512	0.067332	2.727122
34	6	0	1.789062	0.824775	2.365822
35	6	0	3.053223	1.189411	1.883979
36	6	0	1.694068	0.289688	3.653916
37	6	0	4.185719	1.043173	2.674360
38	1	0	3.152098	1.545251	0.862537
39	6	0	2.833495	0.124425	4.434613
40	1	0	0.733663	-0.001987	4.065241
41	6	0	4.082887	0.505032	3.954522
42	1	0	5.154896	1.335555	2.280566
43	1	0	2.737334	-0.292888	5.432565
44	1	0	4.967637	0.383852	4.572123
45	7	0	-1.716445	1.557248	1.537012
46	16	0	-3.211197	1.220964	2.232896
47	8	0	-3.037690	0.389878	3.421987
48	8	0	-3.921624	2.485704	2.318370
49	6	0	-4.006174	0.211546	0.994458
50	6	0	-5.142309	0.688044	0.351831
51	6	0	-3.511487	-1.067143	0.751331
52	6	0	-5.802917	-0.144011	-0.551144
53	1	0	-5.502832	1.687020	0.573307
54	6	0	-4.170282	-1.884368	-0.158769
55	1	0	-2.608947	-1.404884	1.249736
56	6	0	-5.319799	-1.425188	-0.803106
57	1	0	-6.697366	0.210311	-1.054091
58	1	0	-3.782660	-2.876320	-0.371936
59	1	0	-5.836372	-2.069004	-1.508798
60	6	0	-0.356562	5.166685	-2.804708
61	6	0	-0.509760	4.007478	-2.082979
62	6	0	0.301111	3.741079	-0.952366
63	6	0	1.290367	4.684412	-0.561273
64	6	0	1.433395	5.861455	-1.307581
65	6	0	0.624053	6.091296	-2.403734

66	1	0	-0.981082	5.369084	-3.667113
67	1	0	2.189753	6.574337	-0.999315
68	6	0	0.090783	2.510051	-0.286421
69	8	0	0.789884	2.217643	0.741427
70	1	0	-1.260026	3.272925	-2.362030
71	1	0	0.751879	7.010767	-2.967141
72	1	0	-0.639788	1.787474	-0.645547
73	1	0	1.922822	3.686067	0.939118
74	8	0	2.109730	4.520420	0.474821

Zero-point correction= 0.558453 (Hartree/Particle)
Thermal correction to Energy= 0.603659
Thermal correction to Enthalpy= 0.604603
Thermal correction to Gibbs Free Energy= 0.476266
Sum of electronic and zero-point Energies= -2696.040568
Sum of electronic and thermal Energies= -2695.995362
Sum of electronic and thermal Enthalpies= -2695.994418
Sum of electronic and thermal Free Energies= -2696.122755

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.26545824

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.693684	0.822596	2.830977
2	8	0	-2.494775	-0.149238	2.860008
3	8	0	-0.959988	1.168571	1.850222
4	6	0	-1.613460	1.689184	4.063694
5	1	0	-2.356951	2.488227	3.972143
6	1	0	-0.626838	2.148058	4.148889
7	1	0	-1.847506	1.103937	4.954369
8	6	0	-3.888589	0.944273	-0.166412
9	8	0	-4.218564	-0.071999	0.506998
10	8	0	-2.709649	1.277428	-0.492312
11	6	0	-4.993308	1.865700	-0.618952
12	1	0	-4.602406	2.620899	-1.302130
13	1	0	-5.429209	2.353695	0.258304
14	1	0	-5.783584	1.283466	-1.099702
15	6	0	-2.164998	-2.029539	-1.590517
16	8	0	-2.845854	-2.400147	-0.600347
17	8	0	-1.366660	-1.036107	-1.628534
18	6	0	-2.269134	-2.835710	-2.862490
19	1	0	-1.308284	-3.320656	-3.065497
20	1	0	-2.481828	-2.169789	-3.702795
21	1	0	-3.048390	-3.592947	-2.774274
22	6	0	0.025813	-2.136863	1.566941
23	8	0	-1.146732	-2.511866	1.816464
24	8	0	0.354253	-1.157014	0.820791
25	6	0	1.160155	-2.870529	2.235461
26	1	0	2.071961	-2.792489	1.640661
27	1	0	0.897359	-3.917630	2.391484
28	1	0	1.331726	-2.411471	3.216147
29	45	0	-2.735862	-1.336178	1.176644
30	45	0	-1.114506	0.117451	0.081392
31	6	0	0.332905	1.588761	-0.867797
32	6	0	1.072726	0.655981	-1.660129
33	1	0	0.678795	0.318616	-2.616465
34	6	0	-0.463389	2.676400	-1.484467
35	6	0	-0.632351	3.893225	-0.819608
36	6	0	-1.112784	2.479875	-2.709022
37	6	0	-1.417024	4.898724	-1.377435
38	1	0	-0.169039	4.046951	0.149479
39	6	0	-1.894881	3.484460	-3.259964
40	1	0	-1.041763	1.524305	-3.219058
41	6	0	-2.049761	4.702504	-2.599943
42	1	0	-1.535535	5.839325	-0.847487
43	1	0	-2.389608	3.313681	-4.211593
44	1	0	-2.660638	5.487975	-3.034391
45	7	0	2.195413	0.209854	-1.182271
46	16	0	3.097191	-0.882393	-2.081164
47	8	0	2.596850	-0.885218	-3.449392
48	8	0	4.489190	-0.590817	-1.793010
49	6	0	2.688126	-2.455052	-1.350975

50	6	0	3.701226	-3.215342	-0.778598
51	6	0	1.380350	-2.925495	-1.441485
52	6	0	3.394878	-4.485824	-0.293998
53	1	0	4.708610	-2.815734	-0.729574
54	6	0	1.084220	-4.188465	-0.944634
55	1	0	0.601917	-2.299478	-1.865569
56	6	0	2.092512	-4.970423	-0.379711
57	1	0	4.176219	-5.095976	0.148121
58	1	0	0.064722	-4.559823	-0.989626
59	1	0	1.857864	-5.959140	0.002912
60	6	0	5.172343	1.082431	2.629458
61	6	0	3.948063	0.777758	2.079662
62	6	0	3.274702	1.698060	1.248081
63	6	0	3.874399	2.948451	0.960248
64	6	0	5.119195	3.248322	1.527065
65	6	0	5.750585	2.329248	2.344745
66	1	0	5.686457	0.371320	3.265992
67	1	0	5.567171	4.209486	1.301313
68	6	0	2.028941	1.273979	0.693463
69	8	0	1.270564	2.144818	0.084353
70	1	0	3.479480	-0.184643	2.267475
71	1	0	6.716927	2.580391	2.771675
72	1	0	1.573979	0.344294	1.022732
73	1	0	2.463962	3.562308	-0.160271
74	8	0	3.319044	3.878427	0.178222

Zero-point correction= 0.559574 (Hartree/Particle)
Thermal correction to Energy= 0.603449
Thermal correction to Enthalpy= 0.604393
Thermal correction to Gibbs Free Energy= 0.480352
Sum of electronic and zero-point Energies= -2696.036067
Sum of electronic and thermal Energies= -2695.992193
Sum of electronic and thermal Enthalpies= -2695.991249
Sum of electronic and thermal Free Energies= -2696.115290

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2697.26164738

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.337840	-0.198690	-0.177601
2	6	0	1.547545	-1.275250	-0.124392
3	1	0	1.767452	-2.307398	0.096144
4	6	0	3.761675	-0.000232	0.063018
5	6	0	4.340114	1.255450	-0.147635
6	6	0	4.566469	-1.057653	0.507387
7	6	0	5.698436	1.447513	0.081668
8	1	0	3.720422	2.075747	-0.493095
9	6	0	5.921962	-0.861212	0.727403
10	1	0	4.129129	-2.035980	0.684605
11	6	0	6.493947	0.392733	0.517184
12	1	0	6.136449	2.427160	-0.083756
13	1	0	6.535346	-1.689144	1.069842
14	1	0	7.554240	0.544778	0.693873
15	7	0	0.216523	-0.847862	-0.343593
16	16	0	-1.003935	-1.909351	-0.783323
17	8	0	-0.562110	-3.209632	-0.309482
18	8	0	-1.354070	-1.697661	-2.179761
19	6	0	-2.343638	-1.317242	0.224120
20	6	0	-3.518475	-0.898777	-0.386930
21	6	0	-2.176191	-1.274657	1.606267
22	6	0	-4.553604	-0.421873	0.411605
23	1	0	-3.605413	-0.929745	-1.466976
24	6	0	-3.215313	-0.794167	2.390443
25	1	0	-1.240929	-1.591569	2.054572
26	6	0	-4.401021	-0.368150	1.793090
27	1	0	-5.473838	-0.080151	-0.050792
28	1	0	-3.096086	-0.741293	3.467607
29	1	0	-5.208012	0.013651	2.411123
30	6	0	-2.229794	2.586708	0.807212
31	6	0	-1.069108	1.854887	0.558606
32	6	0	-0.804066	1.392764	-0.740867
33	6	0	-1.688054	1.704572	-1.773092

34	6	0	-2.836763	2.445802	-1.530062
35	6	0	-3.104807	2.874486	-0.231086
36	1	0	-2.420925	2.921753	1.820970
37	1	0	-1.481548	1.326562	-2.770705
38	1	0	-3.520042	2.678555	-2.339949
39	1	0	-4.005599	3.444804	-0.023495
40	8	0	-0.248104	1.601207	1.602097
41	6	0	0.341834	0.468007	-1.008506
42	8	0	1.571030	0.939998	-0.450168
43	1	0	0.607434	1.307576	1.250691
44	1	0	0.481312	0.317928	-2.090820

Zero-point correction= 0.344264 (Hartree/Particle)
Thermal correction to Energy= 0.366092
Thermal correction to Enthalpy= 0.367037
Thermal correction to Gibbs Free Energy= 0.292076
Sum of electronic and zero-point Energies= -1563.479641
Sum of electronic and thermal Energies= -1563.457813
Sum of electronic and thermal Enthalpies= -1563.456868
Sum of electronic and thermal Free Energies= -1563.531829
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.16639125

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.822662	-0.985985	0.427362
2	6	0	1.292947	-0.539660	1.627365
3	1	0	1.802351	-0.024101	2.423201
4	6	0	3.235919	-0.708667	0.059130
5	6	0	3.840842	-1.490678	-0.928776
6	6	0	3.967269	0.324037	0.656143
7	6	0	5.159055	-1.255160	-1.301634
8	1	0	3.262934	-2.282317	-1.393506
9	6	0	5.286184	0.556088	0.284353
10	1	0	3.500600	0.963037	1.399897
11	6	0	5.885427	-0.234472	-0.693306
12	1	0	5.621585	-1.871042	-2.067094
13	1	0	5.843602	1.362140	0.751881
14	1	0	6.916042	-0.051907	-0.982945
15	7	0	-0.113968	-0.533727	1.602439
16	16	0	-0.912084	1.050576	1.791838
17	8	0	0.058208	1.798401	2.563309
18	8	0	-2.241553	0.771466	2.289860
19	6	0	-0.994165	1.700777	0.151021
20	6	0	-2.237479	1.820816	-0.460168
21	6	0	0.191392	2.053482	-0.492981
22	6	0	-2.291357	2.311787	-1.759008
23	1	0	-3.133807	1.515138	0.068386
24	6	0	0.118959	2.525920	-1.796720
25	1	0	1.145189	1.957026	0.014347
26	6	0	-1.118225	2.654994	-2.424773
27	1	0	-3.251325	2.411341	-2.254480
28	1	0	1.029920	2.793826	-2.321524
29	1	0	-1.167018	3.025797	-3.443941
30	6	0	-3.242830	-1.230336	-1.793788
31	6	0	-1.990722	-1.211059	-1.162533
32	6	0	-1.923451	-1.538319	0.207303
33	6	0	-3.090784	-1.907626	0.889529
34	6	0	-4.321381	-1.911596	0.256762
35	6	0	-4.388183	-1.567008	-1.095252
36	1	0	-3.276665	-0.970900	-2.846599
37	1	0	-3.021288	-2.154119	1.944721
38	1	0	-5.217500	-2.176596	0.807176
39	1	0	-5.345069	-1.569578	-1.609179
40	8	0	-0.944277	-0.854714	-1.915047
41	6	0	-0.646672	-1.561574	0.952162
42	8	0	1.084043	-1.625713	-0.406873
43	1	0	-0.095805	-1.031632	-1.445474
44	1	0	-0.206436	-2.519320	1.205491

Zero-point correction= 0.341850 (Hartree/Particle)
Thermal correction to Energy= 0.363356

Thermal correction to Enthalpy= 0.364301
Thermal correction to Gibbs Free Energy= 0.289505
Sum of electronic and zero-point Energies= -1563.443588
Sum of electronic and thermal Energies= -1563.422081
Sum of electronic and thermal Enthalpies= -1563.421137
Sum of electronic and thermal Free Energies= -1563.495932
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.13020378

INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.984248	-0.661926	-0.654967
2	6	0	-1.390007	0.370161	-1.407097
3	1	0	-1.905319	1.254811	-1.740028
4	6	0	-3.435174	-0.519684	-0.304892
5	6	0	-4.158065	-1.681496	-0.020771
6	6	0	-4.075622	0.720099	-0.214754
7	6	0	-5.502963	-1.608489	0.320652
8	1	0	-3.645867	-2.636333	-0.072049
9	6	0	-5.420446	0.792640	0.133995
10	1	0	-3.521695	1.637558	-0.390247
11	6	0	-6.137992	-0.370999	0.396791
12	1	0	-6.056556	-2.518935	0.530635
13	1	0	-5.905760	1.761147	0.208930
14	1	0	-7.188695	-0.312535	0.665630
15	7	0	-0.004875	0.399089	-1.451915
16	16	0	0.758651	1.937883	-0.816650
17	8	0	-0.341726	2.875915	-0.828562
18	8	0	1.967137	2.163278	-1.579677
19	6	0	1.126462	1.447066	0.838763
20	6	0	2.448807	1.204082	1.197110
21	6	0	0.062222	1.244960	1.717785
22	6	0	2.709441	0.745444	2.482618
23	1	0	3.246383	1.346703	0.476656
24	6	0	0.342774	0.775458	2.993961
25	1	0	-0.957374	1.442567	1.404834
26	6	0	1.661217	0.526089	3.372152
27	1	0	3.732744	0.540970	2.778397
28	1	0	-0.468672	0.599074	3.691778
29	1	0	1.870825	0.150795	4.368895
30	6	0	3.410315	-2.240786	0.437238
31	6	0	2.137349	-1.901058	-0.039452
32	6	0	2.036860	-1.003559	-1.125650
33	6	0	3.198124	-0.501606	-1.725205
34	6	0	4.450642	-0.849911	-1.245115
35	6	0	4.547124	-1.720529	-0.156842
36	1	0	3.469401	-2.920163	1.280859
37	1	0	3.103143	0.175437	-2.565844
38	1	0	5.342747	-0.454010	-1.718278
39	1	0	5.523678	-2.000410	0.227979
40	8	0	1.086928	-2.434667	0.590447
41	6	0	0.680103	-0.706945	-1.609135
42	8	0	-1.375215	-1.680818	-0.239414
43	1	0	0.217982	-2.096059	0.261138
44	1	0	0.100222	-1.514084	-2.044943

Zero-point correction= 0.342079 (Hartree/Particle)
Thermal correction to Energy= 0.364520
Thermal correction to Enthalpy= 0.365465
Thermal correction to Gibbs Free Energy= 0.288111
Sum of electronic and zero-point Energies= -1563.446080
Sum of electronic and thermal Energies= -1563.423638
Sum of electronic and thermal Enthalpies= -1563.422694
Sum of electronic and thermal Free Energies= -1563.500048
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.13428010

TS8

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

1	6	0	1.484151	-1.020209	-0.023144
2	6	0	0.950484	-0.778463	1.230796
3	1	0	1.528096	-0.505758	2.101756
4	6	0	2.962525	-1.130682	-0.169869
5	6	0	3.537561	-0.807726	-1.401961
6	6	0	3.786508	-1.542676	0.881714
7	6	0	4.915098	-0.873255	-1.572067
8	1	0	2.886078	-0.509045	-2.215936
9	6	0	5.164304	-1.611544	0.708631
10	1	0	3.348262	-1.837826	1.830333
11	6	0	5.732092	-1.272841	-0.516892
12	1	0	5.353510	-0.617185	-2.532048
13	1	0	5.795151	-1.940429	1.529071
14	1	0	6.808066	-1.331013	-0.652552
15	7	0	-0.445729	-0.611049	1.282691
16	16	0	-1.061449	0.999136	1.700316
17	8	0	-0.332609	1.269103	2.924377
18	8	0	-2.505579	0.921362	1.667056
19	6	0	-0.459563	2.093744	0.448481
20	6	0	-1.350330	2.587163	-0.498861
21	6	0	0.886428	2.456522	0.459828
22	6	0	-0.875388	3.468257	-1.462358
23	1	0	-2.390343	2.285218	-0.474365
24	6	0	1.349995	3.321352	-0.523453
25	1	0	1.552214	2.076580	1.225431
26	6	0	0.470355	3.824529	-1.479882
27	1	0	-1.556699	3.866569	-2.206813
28	1	0	2.396761	3.606399	-0.537526
29	1	0	0.836891	4.505102	-2.242408
30	6	0	-3.550394	-0.810591	-1.842085
31	6	0	-2.370626	-0.790911	-1.053059
32	6	0	-2.344559	-1.637816	0.105413
33	6	0	-3.393297	-2.566350	0.332233
34	6	0	-4.514732	-2.561790	-0.454228
35	6	0	-4.590226	-1.654062	-1.535975
36	1	0	-3.585367	-0.151874	-2.703218
37	1	0	-3.315624	-3.245029	1.177737
38	1	0	-5.334663	-3.242364	-0.253332
39	1	0	-5.481170	-1.645594	-2.158173
40	8	0	-1.355545	-0.077884	-1.427498
41	6	0	-1.200199	-1.653515	0.933347
42	8	0	0.796678	-1.123269	-1.110017
43	1	0	-0.301978	-0.569015	-1.192948
44	1	0	-0.800597	-2.602901	1.290097

Zero-point correction= 0.336829 (Hartree/Particle)
Thermal correction to Energy= 0.358686
Thermal correction to Enthalpy= 0.359630
Thermal correction to Gibbs Free Energy= 0.284283
Sum of electronic and zero-point Energies= -1563.440957
Sum of electronic and thermal Energies= -1563.419100
Sum of electronic and thermal Enthalpies= -1563.418156
Sum of electronic and thermal Free Energies= -1563.493503

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.12561759

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.370490	-1.007012	-0.111276
2	6	0	0.741495	-0.946848	1.086609
3	1	0	1.249039	-1.064246	2.035665
4	6	0	2.804593	-1.342928	-0.236432
5	6	0	3.550860	-0.761153	-1.265711
6	6	0	3.434784	-2.204380	0.665939
7	6	0	4.910832	-1.024271	-1.377188
8	1	0	3.053844	-0.100152	-1.967252
9	6	0	4.795302	-2.465860	0.550893
10	1	0	2.854180	-2.689080	1.445089
11	6	0	5.536568	-1.874499	-0.468787
12	1	0	5.483809	-0.565299	-2.177299
13	1	0	5.274920	-3.141593	1.252494
14	1	0	6.598545	-2.081877	-0.560568

15	7	0	-0.620837	-0.539775	1.072610
16	16	0	-0.937326	1.072830	1.611271
17	8	0	-0.294493	1.153204	2.911528
18	8	0	-2.356381	1.313509	1.457142
19	6	0	0.003688	2.083788	0.494100
20	6	0	-0.637084	2.711221	-0.568768
21	6	0	1.371130	2.233968	0.722050
22	6	0	0.121057	3.488566	-1.437917
23	1	0	-1.700007	2.574611	-0.718055
24	6	0	2.117189	3.001604	-0.163127
25	1	0	1.836191	1.759273	1.577890
26	6	0	1.492336	3.625023	-1.241534
27	1	0	-0.362560	3.982742	-2.274188
28	1	0	3.184361	3.118723	-0.005431
29	1	0	2.078910	4.227493	-1.928668
30	6	0	-4.066476	-0.417237	-1.727692
31	6	0	-2.802100	-0.439595	-1.010305
32	6	0	-2.706904	-1.405395	0.106348
33	6	0	-3.759068	-2.381033	0.285476
34	6	0	-4.892176	-2.332858	-0.450027
35	6	0	-5.046974	-1.311377	-1.454411
36	1	0	-4.169669	0.332201	-2.505061
37	1	0	-3.633485	-3.132537	1.061185
38	1	0	-5.689774	-3.050442	-0.291233
39	1	0	-5.975423	-1.277019	-2.018646
40	8	0	-1.841954	0.254042	-1.383252
41	6	0	-1.599201	-1.489453	0.901561
42	8	0	0.787602	-0.715586	-1.274230
43	1	0	-0.125747	-0.352428	-1.160930
44	1	0	-1.414291	-2.410195	1.458102

Zero-point correction= 0.342394 (Hartree/Particle)
Thermal correction to Energy= 0.364814
Thermal correction to Enthalpy= 0.365758
Thermal correction to Gibbs Free Energy= 0.289334
Sum of electronic and zero-point Energies= -1563.447372
Sum of electronic and thermal Energies= -1563.424953
Sum of electronic and thermal Enthalpies= -1563.424008
Sum of electronic and thermal Free Energies= -1563.500432
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.13642038

INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.510611	-0.750754	-0.689398
2	6	0	0.281420	-0.463555	0.172884
3	1	0	-0.247834	-1.393362	0.397481
4	6	0	2.486726	-1.750697	-0.165157
5	6	0	3.536526	-2.143097	-1.001055
6	6	0	2.386054	-2.296286	1.118244
7	6	0	4.467380	-3.075026	-0.563521
8	1	0	3.601244	-1.703084	-1.990693
9	6	0	3.322491	-3.226266	1.556699
10	1	0	1.591506	-1.990359	1.791690
11	6	0	4.360033	-3.618642	0.715651
12	1	0	5.277725	-3.379625	-1.218685
13	1	0	3.242227	-3.643714	2.555554
14	1	0	5.088992	-4.347072	1.058288
15	7	0	-0.624208	0.452474	-0.493351
16	16	0	-1.863411	-0.297765	-1.426752
17	8	0	-1.316173	-1.503505	-2.014845
18	8	0	-2.456383	0.751969	-2.232665
19	6	0	-2.993399	-0.772360	-0.138825
20	6	0	-3.667142	0.220995	0.568965
21	6	0	-3.181698	-2.123820	0.128070
22	6	0	-4.547070	-0.157513	1.573769
23	1	0	-3.502704	1.268396	0.338047
24	6	0	-4.069438	-2.488527	1.136700
25	1	0	-2.644926	-2.867605	-0.451011
26	6	0	-4.747044	-1.508841	1.855742
27	1	0	-5.078552	0.601896	2.137748

28	1	0	-4.231247	-3.538788	1.356220
29	1	0	-5.437798	-1.797731	2.641762
30	6	0	1.965549	3.556186	1.671879
31	6	0	1.049595	2.504067	1.253040
32	6	0	0.467556	2.658836	-0.097349
33	6	0	0.705881	3.893656	-0.816668
34	6	0	1.532504	4.854780	-0.343543
35	6	0	2.184561	4.662862	0.921303
36	1	0	2.436917	3.415282	2.638937
37	1	0	0.220864	4.020479	-1.781745
38	1	0	1.711094	5.762368	-0.909914
39	1	0	2.860496	5.433449	1.283785
40	8	0	0.755180	1.582299	2.030947
41	6	0	-0.341427	1.756256	-0.753709
42	8	0	1.682338	-0.175497	-1.742440
43	1	0	0.577905	0.005050	1.122260
44	1	0	-0.859579	2.115683	-1.638534

Zero-point correction= 0.343055 (Hartree/Particle)
Thermal correction to Energy= 0.365684
Thermal correction to Enthalpy= 0.366628
Thermal correction to Gibbs Free Energy= 0.287073
Sum of electronic and zero-point Energies= -1563.466067
Sum of electronic and thermal Energies= -1563.443439
Sum of electronic and thermal Enthalpies= -1563.442494
Sum of electronic and thermal Free Energies= -1563.522050
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.15385998

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.901936	-0.381304	-0.803182
2	6	0	0.917043	-1.490685	-0.559561
3	1	0	1.294782	-2.430097	-0.982176
4	6	0	3.191057	-0.273274	-0.111341
5	6	0	4.061171	0.764815	-0.460679
6	6	0	3.565643	-1.198890	0.866800
7	6	0	5.293524	0.875375	0.166059
8	1	0	3.754110	1.477413	-1.218238
9	6	0	4.803083	-1.087399	1.487787
10	1	0	2.892866	-2.001865	1.150846
11	6	0	5.666021	-0.051496	1.138271
12	1	0	5.966868	1.683014	-0.102689
13	1	0	5.093333	-1.806582	2.246797
14	1	0	6.631743	0.035620	1.626899
15	7	0	-0.244870	-1.046405	-1.309510
16	16	0	-1.713268	-1.801708	-1.079999
17	8	0	-1.389720	-3.198984	-0.856186
18	8	0	-2.556286	-1.359120	-2.175244
19	6	0	-2.370150	-1.136844	0.433276
20	6	0	-3.159184	0.009457	0.385734
21	6	0	-2.021251	-1.733265	1.642276
22	6	0	-3.593829	0.575096	1.578587
23	1	0	-3.419180	0.452184	-0.568755
24	6	0	-2.464399	-1.158687	2.827552
25	1	0	-1.429658	-2.642497	1.646885
26	6	0	-3.242881	-0.004117	2.794985
27	1	0	-4.198335	1.475798	1.554762
28	1	0	-2.203125	-1.614236	3.777258
29	1	0	-3.581664	0.444518	3.723855
30	6	0	-0.656526	2.688501	1.096995
31	6	0	-0.204842	1.521223	0.375984
32	6	0	-0.615368	1.431495	-1.015599
33	6	0	-1.314563	2.510198	-1.635388
34	6	0	-1.717583	3.590952	-0.908245
35	6	0	-1.385078	3.660825	0.478345
36	1	0	-0.388690	2.753970	2.146514
37	1	0	-1.564173	2.429230	-2.691205
38	1	0	-2.283676	4.392832	-1.370041
39	1	0	-1.713238	4.526022	1.049902
40	8	0	0.534438	0.652735	0.901161
41	6	0	-0.263447	0.314154	-1.787005

42	8	0	1.622266	0.363004	-1.763413
43	1	0	0.722507	-1.611271	0.507357
44	1	0	-0.475938	0.370239	-2.851847

Zero-point correction= 0.342482 (Hartree/Particle)
Thermal correction to Energy= 0.363973
Thermal correction to Enthalpy= 0.364917
Thermal correction to Gibbs Free Energy= 0.290557
Sum of electronic and zero-point Energies= -1563.439498
Sum of electronic and thermal Energies= -1563.418008
Sum of electronic and thermal Enthalpies= -1563.417063
Sum of electronic and thermal Free Energies= -1563.491423
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.12308860

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.091231	-0.323697	-0.477910
2	6	0	1.094495	-1.206381	0.067576
3	1	0	1.371958	-2.201402	0.404103
4	6	0	3.443086	-0.088671	-0.024166
5	6	0	4.159177	1.019539	-0.500045
6	6	0	4.034700	-0.965740	0.895703
7	6	0	5.453988	1.242316	-0.057559
8	1	0	3.687601	1.698973	-1.201283
9	6	0	5.329989	-0.735029	1.333038
10	1	0	3.484787	-1.824846	1.265620
11	6	0	6.038505	0.366910	0.856735
12	1	0	6.007741	2.101804	-0.420381
13	1	0	5.788589	-1.412767	2.045226
14	1	0	7.052273	0.545358	1.201804
15	7	0	0.090272	-1.180873	-0.981472
16	16	0	-1.341829	-2.028977	-0.847796
17	8	0	-0.945709	-3.304393	-0.276964
18	8	0	-1.961749	-1.911060	-2.154888
19	6	0	-2.372237	-1.189576	0.330964
20	6	0	-3.377383	-0.344828	-0.131014
21	6	0	-2.114285	-1.346813	1.689655
22	6	0	-4.136207	0.361064	0.792788
23	1	0	-3.545501	-0.237360	-1.195866
24	6	0	-2.877903	-0.630824	2.603389
25	1	0	-1.334273	-2.022211	2.023567
26	6	0	-3.882175	0.222630	2.154879
27	1	0	-4.911871	1.035513	0.446083
28	1	0	-2.684408	-0.736934	3.665703
29	1	0	-4.469661	0.787456	2.872332
30	6	0	-1.374610	2.608611	0.953210
31	6	0	-0.545962	1.548954	0.481274
32	6	0	-0.633124	1.267077	-0.923775
33	6	0	-1.485466	2.012166	-1.752999
34	6	0	-2.278564	3.027142	-1.254907
35	6	0	-2.205326	3.319753	0.116627
36	1	0	-1.319962	2.828666	2.014730
37	1	0	-1.532620	1.764214	-2.812219
38	1	0	-2.938449	3.587050	-1.909206
39	1	0	-2.818751	4.118396	0.527483
40	8	0	0.227817	0.926177	1.304839
41	6	0	0.132737	0.164116	-1.561080
42	8	0	1.601244	0.421227	-1.413682
43	1	0	0.708121	-0.442830	0.912423
44	1	0	-0.049030	0.112742	-2.633818

Zero-point correction= 0.340203 (Hartree/Particle)
Thermal correction to Energy= 0.361297
Thermal correction to Enthalpy= 0.362241
Thermal correction to Gibbs Free Energy= 0.288927
Sum of electronic and zero-point Energies= -1563.433885
Sum of electronic and thermal Energies= -1563.412791
Sum of electronic and thermal Enthalpies= -1563.411847
Sum of electronic and thermal Free Energies= -1563.485161
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.11889551

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.672171	0.110670	-0.199377
2	6	0	0.881431	-1.171297	0.147400
3	1	0	1.523435	-2.055020	0.142772
4	6	0	3.129637	0.071443	0.182639
5	6	0	4.006190	-0.684542	-0.596685
6	6	0	3.598394	0.727747	1.317565
7	6	0	5.347108	-0.775700	-0.244830
8	1	0	3.635078	-1.187228	-1.484167
9	6	0	4.942511	0.630881	1.668572
10	1	0	2.916163	1.320644	1.915783
11	6	0	5.817743	-0.119109	0.890077
12	1	0	6.025676	-1.359818	-0.858813
13	1	0	5.305216	1.147045	2.552244
14	1	0	6.865830	-0.192148	1.164541
15	7	0	-0.073030	-1.218978	-0.961895
16	16	0	-1.553122	-1.943796	-0.794030
17	8	0	-1.288843	-3.305259	-0.366741
18	8	0	-2.270996	-1.632361	-2.019284
19	6	0	-2.369897	-1.129040	0.568372
20	6	0	-3.206408	-0.045723	0.319928
21	6	0	-2.122744	-1.569703	1.867775
22	6	0	-3.774250	0.630964	1.393018
23	1	0	-3.408580	0.256989	-0.699509
24	6	0	-2.699952	-0.887888	2.933881
25	1	0	-1.507240	-2.447778	2.033091
26	6	0	-3.516044	0.215554	2.696799
27	1	0	-4.419866	1.482995	1.206326
28	1	0	-2.516995	-1.224164	3.949502
29	1	0	-3.962159	0.745993	3.532569
30	6	0	-0.620133	2.897632	0.404789
31	6	0	-0.042025	1.766417	-0.157204
32	6	0	-0.573274	1.198238	-1.318201
33	6	0	-1.663025	1.790121	-1.940501
34	6	0	-2.252767	2.923790	-1.386079
35	6	0	-1.732762	3.463584	-0.211555
36	1	0	-0.192427	3.321909	1.306758
37	1	0	-2.062554	1.341510	-2.846052
38	1	0	-3.111058	3.382093	-1.866498
39	1	0	-2.189066	4.345860	0.227173
40	8	0	1.062062	1.233870	0.444385
41	6	0	0.148217	-0.028453	-1.806024
42	8	0	1.530423	0.201678	-1.594716
43	1	0	0.404744	-1.065730	1.126758
44	1	0	-0.026951	-0.256527	-2.856036

Zero-point correction= 0.347227 (Hartree/Particle)
Thermal correction to Energy= 0.367702
Thermal correction to Enthalpy= 0.368647
Thermal correction to Gibbs Free Energy= 0.296407
Sum of electronic and zero-point Energies= -1563.501137
Sum of electronic and thermal Energies= -1563.480661
Sum of electronic and thermal Enthalpies= -1563.479717
Sum of electronic and thermal Free Energies= -1563.551957
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1564.18133580

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.006594	1.171552	-0.000023
2	6	0	1.390781	1.239690	-0.000009
3	6	0	2.138994	0.060704	-0.000001
4	6	0	1.493013	-1.179079	-0.000019
5	6	0	0.108825	-1.231832	-0.000066
6	6	0	-0.656245	-0.061579	-0.000030
7	1	0	-0.557879	2.099087	0.000022
8	1	0	1.910456	2.191638	0.000036

9	1	0	2.075161	-2.098250	-0.000006
10	1	0	-0.409378	-2.185185	-0.000074
11	8	0	3.488373	0.180700	0.000041
12	1	0	3.888146	-0.697653	0.000080
13	6	0	-2.143508	-0.188255	-0.000008
14	8	0	-2.675952	-1.282746	0.000065
15	6	0	-2.979273	1.077275	-0.000012
16	1	0	-2.763517	1.687195	0.884309
17	1	0	-2.763109	1.687643	-0.883906
18	1	0	-4.034333	0.801037	-0.000300

Zero-point correction= 0.144318 (Hartree/Particle)
Thermal correction to Energy= 0.153171
Thermal correction to Enthalpy= 0.154115
Thermal correction to Gibbs Free Energy= 0.110390
Sum of electronic and zero-point Energies= -459.818808
Sum of electronic and thermal Energies= -459.809955
Sum of electronic and thermal Enthalpies= -459.809011
Sum of electronic and thermal Free Energies= -459.852736
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -460.10335421

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.137306	0.472219	-1.083803
2	6	0	-0.128845	0.823982	-0.276988
3	8	0	0.423879	-0.171035	0.515904
4	1	0	-1.030655	-1.542948	-0.719086
5	6	0	0.382840	2.194100	-0.098153
6	6	0	0.290033	3.142999	-1.122722
7	6	0	0.971426	2.564942	1.116202
8	6	0	0.746577	4.440682	-0.924953
9	1	0	-0.119692	2.858771	-2.087799
10	6	0	1.439218	3.859444	1.305331
11	1	0	1.056829	1.833262	1.913137
12	6	0	1.323843	4.803875	0.288913
13	1	0	0.668401	5.165853	-1.729282
14	1	0	1.895039	4.131470	2.252551
15	1	0	1.693140	5.813943	0.437428
16	7	0	-1.524233	-0.855757	-1.280768
17	1	0	-1.694465	1.204817	-1.654559
18	16	0	-3.149068	-1.225074	-1.481630
19	6	0	-3.899159	-0.905925	0.103290
20	6	0	-4.299182	0.391492	0.413561
21	6	0	-4.023110	-1.946502	1.019450
22	6	0	-4.829678	0.648141	1.672841
23	1	0	-4.214620	1.177961	-0.328619
24	6	0	-4.558934	-1.677255	2.274392
25	1	0	-3.721390	-2.950774	0.740729
26	6	0	-4.956768	-0.382791	2.600822
27	1	0	-5.149563	1.653783	1.926384
28	1	0	-4.669699	-2.479926	2.996484
29	1	0	-5.375987	-0.178357	3.581188
30	8	0	-3.184098	-2.653497	-1.722592
31	8	0	-3.664753	-0.250781	-2.424625
32	6	0	1.747315	-0.487943	0.338485
33	6	0	2.357288	-1.174844	1.386079
34	6	0	2.454729	-0.181497	-0.823262
35	6	0	3.686295	-1.553702	1.270501
36	6	0	3.783782	-0.563335	-0.921128
37	1	0	1.968748	0.345929	-1.636718
38	6	0	4.418701	-1.249695	0.118006
39	1	0	4.151076	-2.085570	2.094907
40	1	0	4.357768	-0.335956	-1.813344
41	1	0	1.780066	-1.398610	2.277047
42	6	0	5.855926	-1.624732	-0.054813
43	8	0	6.453373	-1.340049	-1.075181
44	6	0	6.551512	-2.367093	1.069211
45	1	0	6.524222	-1.787540	1.998614
46	1	0	6.060235	-3.327177	1.263103
47	1	0	7.589039	-2.543913	0.783664

Zero-point correction= 0.370866 (Hartree/Particle)
Thermal correction to Energy= 0.395271
Thermal correction to Enthalpy= 0.396215
Thermal correction to Gibbs Free Energy= 0.312377
Sum of electronic and zero-point Energies= -1602.760157
Sum of electronic and thermal Energies= -1602.735751
Sum of electronic and thermal Enthalpies= -1602.734807
Sum of electronic and thermal Free Energies= -1602.818645
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1603.48682027

INT3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.225820	-1.680133	-2.301057
2	8	0	0.278816	-2.451791	-2.594639
3	8	0	1.279250	-0.898898	-1.294986
4	6	0	2.440034	-1.685064	-3.198967
5	1	0	2.996815	-0.750735	-3.099143
6	1	0	2.142910	-1.850746	-4.236052
7	1	0	3.093733	-2.510339	-2.897401
8	6	0	0.215277	-3.679280	0.703622
9	8	0	-0.545433	-4.015836	-0.245811
10	8	0	0.524381	-2.495864	1.035011
11	6	0	0.813936	-4.788421	1.533499
12	1	0	0.007973	-5.321622	2.046734
13	1	0	1.511567	-4.383123	2.267516
14	1	0	1.318089	-5.504176	0.878607
15	6	0	-2.920974	-1.693419	0.971710
16	8	0	-2.993581	-2.440237	-0.039619
17	8	0	-1.940149	-0.947064	1.292453
18	6	0	-4.107829	-1.654318	1.903599
19	1	0	-4.549383	-0.652281	1.890528
20	1	0	-3.776175	-1.849418	2.926768
21	1	0	-4.855519	-2.388064	1.602261
22	6	0	-1.928586	0.221852	-2.122570
23	8	0	-2.218983	-0.954740	-2.459468
24	8	0	-1.252257	0.559209	-1.098511
25	6	0	-2.369598	1.341412	-3.029092
26	1	0	-1.646160	1.418057	-3.849145
27	1	0	-2.396127	2.288377	-2.489138
28	1	0	-3.347010	1.119143	-3.459947
29	45	0	-1.414407	-2.526907	-1.377637
30	45	0	-0.297070	-0.884454	0.042414
31	6	0	0.848245	0.595559	1.313650
32	6	0	-0.165856	1.591573	1.529272
33	1	0	-0.925368	1.275733	2.246915
34	6	0	1.359263	-0.137476	2.520102
35	6	0	2.457102	-0.997413	2.377076
36	6	0	0.780569	-0.012443	3.786977
37	6	0	2.969003	-1.694215	3.462679
38	1	0	2.886242	-1.147939	1.391736
39	6	0	1.279803	-0.731512	4.870030
40	1	0	-0.053893	0.659100	3.956478
41	6	0	2.377683	-1.570487	4.718112
42	1	0	3.820609	-2.354452	3.322549
43	1	0	0.812519	-0.614402	5.843288
44	1	0	2.770773	-2.119961	5.568217
45	7	0	-0.244925	2.737689	0.938218
46	16	0	-1.557350	3.672574	1.438465
47	8	0	-1.988534	3.251576	2.769973
48	8	0	-1.184408	5.054104	1.187412
49	6	0	5.591229	2.288063	-2.196539
50	6	0	4.234501	2.213669	-1.951990
51	6	0	3.741795	1.645603	-0.762446
52	6	0	4.665051	1.163978	0.183770
53	6	0	6.023538	1.232009	-0.054805
54	6	0	6.494742	1.793354	-1.248645
55	1	0	5.977499	2.725983	-3.109897
56	1	0	6.724571	0.856624	0.686424
57	6	0	2.310708	1.553968	-0.500968
58	8	0	2.042962	1.048929	0.631929
59	1	0	3.552234	2.610407	-2.695071

60	6	0	-2.880583	3.238935	0.317626
61	6	0	-3.472192	1.981236	0.416821
62	6	0	-3.360723	4.198979	-0.565523
63	6	0	-4.564230	1.683358	-0.388483
64	1	0	-3.075662	1.237960	1.100571
65	6	0	-4.464562	3.894080	-1.360695
66	1	0	-2.882373	5.171740	-0.607378
67	6	0	-5.065132	2.641654	-1.270079
68	1	0	-5.024575	0.701406	-0.330968
69	1	0	-4.854336	4.638171	-2.048434
70	1	0	-5.924173	2.406403	-1.891452
71	1	0	4.302944	0.739041	1.113212
72	6	0	1.312638	2.076122	-1.464180
73	1	0	1.306269	3.169668	-1.384957
74	1	0	1.596229	1.789879	-2.479499
75	1	0	0.310209	1.717440	-1.251682
76	8	0	7.804336	1.889852	-1.539684
77	1	0	8.332890	1.527109	-0.817080

Zero-point correction= 0.587170 (Hartree/Particle)
Thermal correction to Energy= 0.633595
Thermal correction to Enthalpy= 0.634539
Thermal correction to Gibbs Free Energy= 0.502454
Sum of electronic and zero-point Energies= -2735.307409
Sum of electronic and thermal Energies= -2735.260984
Sum of electronic and thermal Enthalpies= -2735.260040
Sum of electronic and thermal Free Energies= -2735.392126
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2736.57492042

INT4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.430837	1.381299	1.413040
2	6	0	0.991039	0.167424	0.879824
3	45	0	-0.791737	-0.875333	0.158220
4	8	0	-0.606127	-2.479613	1.438002
5	6	0	-1.400462	-3.463675	1.315108
6	8	0	-2.331831	-3.574748	0.471806
7	45	0	-2.706504	-2.017272	-0.830492
8	8	0	-3.880811	-1.125122	0.616608
9	6	0	-3.347691	-0.365697	1.465121
10	8	0	-2.115886	-0.039088	1.514591
11	8	0	0.389593	-1.840824	-1.246667
12	6	0	-0.166697	-2.597628	-2.107863
13	8	0	-1.394734	-2.847198	-2.197524
14	8	0	-1.096363	0.640237	-1.201210
15	6	0	-2.065236	0.557823	-2.021940
16	8	0	-2.921948	-0.364432	-2.069017
17	8	0	1.605422	0.670363	-0.493367
18	1	0	1.197860	1.621884	-0.498672
19	6	0	1.991645	-0.596440	1.665177
20	6	0	2.662672	0.011694	2.733625
21	6	0	2.301583	-1.922274	1.337168
22	6	0	3.603328	-0.694447	3.476017
23	1	0	2.453885	1.048599	2.984412
24	6	0	3.258784	-2.617808	2.063925
25	1	0	1.782640	-2.395432	0.512112
26	6	0	3.905513	-2.009989	3.138371
27	1	0	4.107955	-0.211826	4.307170
28	1	0	3.493014	-3.644697	1.799173
29	1	0	4.645856	-2.561215	3.710704
30	7	0	0.448492	2.444515	0.668227
31	1	0	-0.056957	1.350250	2.387853
32	16	0	-0.310314	3.843720	1.222441
33	6	0	-1.756534	3.917768	0.191004
34	6	0	-2.718451	2.921418	0.327866
35	6	0	-1.918411	4.979995	-0.690322
36	6	0	-3.874405	2.991460	-0.438863
37	1	0	-2.542305	2.091853	1.003122
38	6	0	-3.087314	5.045722	-1.446868
39	1	0	-1.146652	5.738031	-0.770247
40	6	0	-4.060225	4.057510	-1.319748

41	1	0	-4.620994	2.206801	-0.360427
42	1	0	-3.235186	5.870991	-2.136143
43	1	0	-4.965570	4.111687	-1.916734
44	8	0	0.573053	4.943024	0.875282
45	8	0	-0.728886	3.631336	2.601917
46	6	0	2.999748	0.691020	-0.673303
47	6	0	3.551369	-0.413047	-1.298174
48	6	0	3.748851	1.775102	-0.239316
49	6	0	4.926839	-0.433564	-1.493534
50	6	0	5.119817	1.740441	-0.453538
51	1	0	3.271177	2.618416	0.249904
52	6	0	5.719051	0.639587	-1.073923
53	1	0	5.375063	-1.295186	-1.977137
54	1	0	5.751453	2.563105	-0.136613
55	6	0	-4.239706	0.259306	2.509902
56	1	0	-4.461551	1.292931	2.220914
57	1	0	-5.176838	-0.292750	2.588472
58	1	0	-3.726294	0.289423	3.473115
59	6	0	-1.218425	-4.590729	2.302008
60	1	0	-1.582787	-5.528033	1.878804
61	1	0	-0.169322	-4.674512	2.591656
62	1	0	-1.803273	-4.365231	3.200124
63	6	0	-2.154211	1.656777	-3.050420
64	1	0	-1.531224	1.378131	-3.907601
65	1	0	-3.183198	1.773244	-3.392739
66	1	0	-1.779391	2.595358	-2.637855
67	6	0	0.760422	-3.237570	-3.113615
68	1	0	1.547882	-3.786110	-2.588356
69	1	0	0.209581	-3.913223	-3.768080
70	1	0	1.239434	-2.455428	-3.710974
71	1	0	2.897831	-1.222849	-1.604233
72	6	0	7.210501	0.663762	-1.258448
73	8	0	7.858191	1.620337	-0.883363
74	6	0	7.879087	-0.525152	-1.915681
75	1	0	7.691888	-1.442213	-1.345779
76	1	0	7.492186	-0.679444	-2.929312
77	1	0	8.952980	-0.341147	-1.963076

Zero-point correction= 0.584331 (Hartree/Particle)
Thermal correction to Energy= 0.631398
Thermal correction to Enthalpy= 0.632342
Thermal correction to Gibbs Free Energy= 0.499230
Sum of electronic and zero-point Energies= -2735.300357
Sum of electronic and thermal Energies= -2735.253290
Sum of electronic and thermal Enthalpies= -2735.252346
Sum of electronic and thermal Free Energies= -2735.385459

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2736.56310295

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.170760	1.403937	-1.514811
2	8	0	-1.500424	2.347079	-2.005410
3	8	0	-1.811977	0.639185	-0.558974
4	6	0	-3.528929	1.115178	-2.105735
5	1	0	-3.504797	0.141719	-2.606274
6	1	0	-3.807217	1.889941	-2.820327
7	1	0	-4.272010	1.045580	-1.307189
8	6	0	-0.841594	3.473383	1.314110
9	8	0	-0.499462	3.982132	0.214553
10	8	0	-0.742096	2.249326	1.646131
11	6	0	-1.399723	4.399594	2.367132
12	1	0	-0.577720	4.731858	3.010088
13	1	0	-2.124868	3.872317	2.989972
14	1	0	-1.850925	5.276223	1.900143
15	6	0	2.590650	2.296864	0.593191
16	8	0	2.220552	3.068671	-0.326918
17	8	0	1.933204	1.309747	1.061924
18	6	0	3.959874	2.525350	1.186620
19	1	0	4.715304	2.144803	0.490241
20	1	0	4.063648	2.002366	2.137995
21	1	0	4.134829	3.595763	1.313250

22	6	0	1.256457	0.210807	-2.253603
23	8	0	1.216896	1.430767	-2.560128
24	8	0	0.884357	-0.302660	-1.150721
25	6	0	1.752723	-0.756443	-3.299959
26	1	0	0.917465	-1.008857	-3.963475
27	1	0	2.127274	-1.669594	-2.834830
28	1	0	2.531642	-0.288450	-3.903727
29	45	0	0.373842	2.777303	-1.225410
30	45	0	0.048215	0.889829	0.304839
31	6	0	-0.180740	-0.698190	1.630322
32	6	0	1.079254	-1.399477	1.724349
33	1	0	1.786112	-0.848028	2.364495
34	6	0	-1.072667	-0.662146	2.775863
35	6	0	-2.286740	0.042462	2.687240
36	6	0	-0.758349	-1.338469	3.967153
37	6	0	-3.159319	0.064918	3.764615
38	1	0	-2.531006	0.543849	1.758255
39	6	0	-1.619827	-1.285281	5.054211
40	1	0	0.167125	-1.902306	4.042541
41	6	0	-2.822229	-0.588555	4.950253
42	1	0	-4.101043	0.599881	3.687758
43	1	0	-1.362726	-1.797284	5.975909
44	1	0	-3.502687	-0.557665	5.796428
45	7	0	1.448212	-2.444508	1.083077
46	16	0	3.079529	-2.859995	1.325740
47	8	0	3.645043	-2.080775	2.424850
48	8	0	3.133845	-4.310465	1.350052
49	6	0	-4.785184	-2.648516	-2.680173
50	6	0	-3.465161	-2.736860	-2.268711
51	6	0	-3.084553	-2.350653	-0.976513
52	6	0	-4.067959	-1.880727	-0.098431
53	6	0	-5.391298	-1.794270	-0.494694
54	6	0	-5.754417	-2.174649	-1.791617
55	1	0	-5.087186	-2.940677	-3.679924
56	1	0	-6.146022	-1.428607	0.198141
57	6	0	-1.673506	-2.368205	-0.524818
58	8	0	-1.437385	-2.022943	0.634257
59	1	0	-2.724144	-3.104582	-2.971271
60	6	0	3.816182	-2.279352	-0.189793
61	6	0	3.967816	-0.907776	-0.376854
62	6	0	4.273358	-3.200835	-1.123858
63	6	0	4.600651	-0.451763	-1.526066
64	1	0	3.577072	-0.214491	0.359602
65	6	0	4.912072	-2.732042	-2.270692
66	1	0	4.140615	-4.261753	-0.940536
67	6	0	5.079226	-1.363957	-2.467257
68	1	0	4.712582	0.615393	-1.693507
69	1	0	5.282338	-3.438659	-3.006809
70	1	0	5.576788	-1.003210	-3.362523
71	1	0	-3.771739	-1.577415	0.899872
72	6	0	-0.601424	-2.838552	-1.462787
73	1	0	-0.808747	-3.877726	-1.745734
74	1	0	-0.598712	-2.233075	-2.373355
75	1	0	0.366075	-2.769092	-0.970306
76	8	0	-7.026434	-2.106280	-2.242344
77	1	0	-7.602067	-1.772614	-1.542884

Zero-point correction= 0.585404 (Hartree/Particle)
Thermal correction to Energy= 0.631536
Thermal correction to Enthalpy= 0.632480
Thermal correction to Gibbs Free Energy= 0.504745
Sum of electronic and zero-point Energies= -2735.290376
Sum of electronic and thermal Energies= -2735.244244
Sum of electronic and thermal Enthalpies= -2735.243300
Sum of electronic and thermal Free Energies= -2735.371035

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2736.55671689

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.567976	1.303386	1.340636
2	6	0	0.911403	-0.024515	0.873788

3	45	0	-0.898371	-0.890034	0.179477
4	8	0	-0.849399	-2.493663	1.475056
5	6	0	-1.748587	-3.389447	1.383858
6	8	0	-2.706679	-3.408056	0.566567
7	45	0	-2.954914	-1.829637	-0.744053
8	8	0	-3.985085	-0.806711	0.727909
9	6	0	-3.351920	-0.093057	1.546092
10	8	0	-2.091752	0.106606	1.554211
11	8	0	0.132702	-2.005003	-1.219690
12	6	0	-0.522615	-2.692078	-2.068888
13	8	0	-1.773521	-2.798243	-2.137778
14	8	0	-1.094535	0.640959	-1.183702
15	6	0	-2.093094	0.657491	-1.972531
16	8	0	-3.038984	-0.173256	-1.989166
17	8	0	1.628396	0.471920	-0.798775
18	1	0	1.250444	1.392090	-0.790024
19	6	0	2.003571	-0.758793	1.506138
20	6	0	2.979029	-0.079891	2.258071
21	6	0	2.142805	-2.140167	1.297962
22	6	0	4.057736	-0.764131	2.799680
23	1	0	2.894986	0.993692	2.404197
24	6	0	3.225070	-2.821025	1.839109
25	1	0	1.402673	-2.658212	0.701796
26	6	0	4.180012	-2.136241	2.588044
27	1	0	4.805149	-0.229647	3.376953
28	1	0	3.326640	-3.889553	1.675770
29	1	0	5.025315	-2.673323	3.008697
30	7	0	0.658403	2.349756	0.594339
31	1	0	0.125681	1.343987	2.342291
32	16	0	0.063094	3.807074	1.219699
33	6	0	-1.395039	4.031898	0.227696
34	6	0	-2.441402	3.126225	0.376837
35	6	0	-1.474053	5.111466	-0.643554
36	6	0	-3.600467	3.309509	-0.366003
37	1	0	-2.329289	2.277331	1.041835
38	6	0	-2.646017	5.290718	-1.376442
39	1	0	-0.636294	5.794581	-0.734468
40	6	0	-3.703431	4.395371	-1.236173
41	1	0	-4.414764	2.596351	-0.278518
42	1	0	-2.730176	6.131380	-2.057749
43	1	0	-4.611011	4.537749	-1.814956
44	8	0	1.042000	4.820499	0.865218
45	8	0	-0.334723	3.610134	2.608317
46	6	0	3.004317	0.495932	-0.896595
47	6	0	3.615320	-0.701283	-1.246267
48	6	0	3.737270	1.645071	-0.609433
49	6	0	5.001246	-0.754264	-1.293143
50	6	0	5.121027	1.577369	-0.677736
51	1	0	3.232109	2.563825	-0.325957
52	6	0	5.766695	0.381093	-1.007369
53	1	0	5.480669	-1.692123	-1.554278
54	1	0	5.728776	2.449320	-0.460790
55	6	0	-4.143983	0.637065	2.603409
56	1	0	-4.315518	1.668321	2.274231
57	1	0	-5.110250	0.154018	2.753296
58	1	0	-3.580774	0.676820	3.537734
59	6	0	-1.662245	-4.518916	2.381108
60	1	0	-2.155975	-5.409084	1.988737
61	1	0	-0.620091	-4.729045	2.629023
62	1	0	-2.174929	-4.212807	3.299214
63	6	0	-2.103028	1.761610	-2.999323
64	1	0	-1.549186	1.417819	-3.879967
65	1	0	-3.126152	1.989642	-3.300750
66	1	0	-1.611950	2.653383	-2.605257
67	6	0	0.307943	-3.435401	-3.087292
68	1	0	1.031410	-4.074533	-2.572858
69	1	0	-0.328402	-4.038776	-3.734805
70	1	0	0.870307	-2.714111	-3.688061
71	1	0	2.991285	-1.562266	-1.458777
72	6	0	7.265718	0.372669	-1.031166
73	8	0	7.892711	1.381174	-0.771652
74	6	0	7.977866	-0.918471	-1.380089
75	1	0	7.714113	-1.712895	-0.672791
76	1	0	7.696786	-1.260835	-2.382396
77	1	0	9.054137	-0.745380	-1.345665

Zero-point correction= 0.584167 (Hartree/Particle)
Thermal correction to Energy= 0.630869
Thermal correction to Enthalpy= 0.631813
Thermal correction to Gibbs Free Energy= 0.499453
Sum of electronic and zero-point Energies= -2735.298927
Sum of electronic and thermal Energies= -2735.252225
Sum of electronic and thermal Enthalpies= -2735.251281
Sum of electronic and thermal Free Energies= -2735.383641
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2736.56111684

TS5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.404791	1.370396	1.443112
2	6	0	1.006228	0.190386	0.894538
3	45	0	-0.780369	-0.867526	0.156400
4	8	0	-0.565637	-2.479605	1.421234
5	6	0	-1.341997	-3.476550	1.290903
6	8	0	-2.272537	-3.596757	0.447441
7	45	0	-2.669374	-2.037349	-0.845548
8	8	0	-3.866095	-1.175351	0.600247
9	6	0	-3.350517	-0.414748	1.458568
10	8	0	-2.124489	-0.069233	1.518393
11	8	0	0.418878	-1.794486	-1.259274
12	6	0	-0.119653	-2.559816	-2.123938
13	8	0	-1.341696	-2.837635	-2.214000
14	8	0	-1.111113	0.652697	-1.190032
15	6	0	-2.070844	0.554241	-2.018967
16	8	0	-2.909213	-0.384852	-2.076837
17	8	0	1.603520	0.731622	-0.440937
18	1	0	1.179628	1.715809	-0.381407
19	6	0	1.990807	-0.593400	1.681206
20	6	0	2.610812	-0.023842	2.799975
21	6	0	2.333306	-1.899086	1.308663
22	6	0	3.532556	-0.749552	3.547735
23	1	0	2.378026	0.998570	3.086450
24	6	0	3.272877	-2.612540	2.040789
25	1	0	1.850521	-2.343691	0.446488
26	6	0	3.868308	-2.044362	3.165475
27	1	0	3.997375	-0.296741	4.417983
28	1	0	3.532725	-3.623465	1.740733
29	1	0	4.594832	-2.609924	3.741494
30	7	0	0.420143	2.437655	0.696149
31	1	0	-0.095538	1.328500	2.409431
32	16	0	-0.352152	3.839892	1.218105
33	6	0	-1.801631	3.891836	0.190663
34	6	0	-2.755763	2.889656	0.339144
35	6	0	-1.976584	4.948560	-0.694910
36	6	0	-3.916504	2.947480	-0.421300
37	1	0	-2.570221	2.064698	1.017634
38	6	0	-3.150576	5.002300	-1.444392
39	1	0	-1.210945	5.711813	-0.783313
40	6	0	-4.115428	4.007753	-1.306317
41	1	0	-4.657137	2.158149	-0.334292
42	1	0	-3.308553	5.823038	-2.136791
43	1	0	-5.024842	4.052370	-1.897860
44	8	0	0.523140	4.938794	0.852072
45	8	0	-0.765957	3.641229	2.600419
46	6	0	2.994609	0.742159	-0.632175
47	6	0	3.528314	-0.327729	-1.328676
48	6	0	3.762292	1.790183	-0.144737
49	6	0	4.900973	-0.350448	-1.542655
50	6	0	5.130233	1.754770	-0.376806
51	1	0	3.300039	2.608685	0.398350
52	6	0	5.710133	0.687332	-1.069726
53	1	0	5.333966	-1.186191	-2.082432
54	1	0	5.774517	2.550562	-0.019305
55	6	0	-4.257894	0.185233	2.504734
56	1	0	-4.461250	1.231105	2.248323
57	1	0	-5.201834	-0.358989	2.546706
58	1	0	-3.763616	0.176053	3.478554

59	6	0	-1.138126	-4.608844	2.267316
60	1	0	-1.483510	-5.549270	1.835195
61	1	0	-0.087552	-4.673967	2.556426
62	1	0	-1.727682	-4.403569	3.167205
63	6	0	-2.173572	1.653908	-3.045135
64	1	0	-1.546717	1.384572	-3.902451
65	1	0	-3.203785	1.757562	-3.387980
66	1	0	-1.810815	2.596331	-2.630835
67	6	0	0.820870	-3.171162	-3.134868
68	1	0	1.635985	-3.683233	-2.615182
69	1	0	0.289790	-3.872802	-3.778255
70	1	0	1.260469	-2.375162	-3.744315
71	1	0	2.862681	-1.112361	-1.672078
72	6	0	7.199080	0.707618	-1.271641
73	8	0	7.862062	1.633274	-0.848497
74	6	0	7.846846	-0.446401	-2.007478
75	1	0	7.657575	-1.393928	-1.490552
76	1	0	7.445295	-0.536459	-3.023141
77	1	0	8.921888	-0.270137	-2.058300

Zero-point correction= 0.582750 (Hartree/Particle)
Thermal correction to Energy= 0.629142
Thermal correction to Enthalpy= 0.630086
Thermal correction to Gibbs Free Energy= 0.498746
Sum of electronic and zero-point Energies= -2735.301875
Sum of electronic and thermal Energies= -2735.255483
Sum of electronic and thermal Enthalpies= -2735.254539
Sum of electronic and thermal Free Energies= -2735.385879

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2736.56303522

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.985477	0.861375	-0.000079
2	6	0	-0.586982	0.969891	-0.000042
3	6	0	0.206036	-0.204249	0.000009
4	6	0	-0.441440	-1.453610	0.000110
5	6	0	-1.818479	-1.553588	0.000098
6	6	0	-2.586935	-0.382019	-0.000019
7	1	0	-2.567324	1.776855	-0.000156
8	1	0	0.154561	-2.361069	0.000252
9	1	0	-2.298848	-2.526007	0.000176
10	1	0	-3.671141	-0.448975	-0.000066
11	8	0	-0.063346	2.197235	-0.000104
12	1	0	0.916904	2.092331	-0.000108
13	6	0	1.675044	-0.092708	0.000022
14	8	0	2.232398	1.006402	0.000309
15	6	0	2.523047	-1.344704	-0.000277
16	1	0	3.573664	-1.052588	-0.001815
17	1	0	2.316577	-1.955165	0.885068
18	1	0	2.314306	-1.956816	-0.883915

Zero-point correction= 0.145070 (Hartree/Particle)
Thermal correction to Energy= 0.153511
Thermal correction to Enthalpy= 0.154455
Thermal correction to Gibbs Free Energy= 0.111668
Sum of electronic and zero-point Energies= -459.829554
Sum of electronic and thermal Energies= -459.821114
Sum of electronic and thermal Enthalpies= -459.820170
Sum of electronic and thermal Free Energies= -459.862957

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -460.11144562

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.157744	0.078082	0.016294
2	6	0	-0.495509	-1.130221	-0.674421
3	1	0	-1.123283	-2.021197	-0.604000
4	6	0	-2.664485	0.062178	-0.016087

5	6	0	-3.349194	-0.786051	0.854618
6	6	0	-3.372547	0.831337	-0.936129
7	6	0	-4.736206	-0.858954	0.807349
8	1	0	-2.791240	-1.377308	1.573754
9	6	0	-4.761639	0.752740	-0.982550
10	1	0	-2.837452	1.495292	-1.605321
11	6	0	-5.445544	-0.090852	-0.113016
12	1	0	-5.264755	-1.515696	1.491502
13	1	0	-5.310188	1.356604	-1.699053
14	1	0	-6.529092	-0.150587	-0.151300
15	7	0	0.721100	-1.294864	0.129734
16	16	0	2.100688	-1.848718	-0.607712
17	8	0	1.696650	-3.017836	-1.367839
18	8	0	3.127895	-1.917176	0.418472
19	6	0	0.987829	2.929812	-0.764183
20	6	0	0.529331	1.742914	-0.205013
21	6	0	1.315768	1.032208	0.709448
22	6	0	2.569131	1.521880	1.055170
23	6	0	3.045311	2.702251	0.488775
24	6	0	2.251170	3.399720	-0.418117
25	1	0	0.353752	3.465328	-1.462761
26	1	0	3.186862	0.964064	1.751616
27	1	0	4.028851	3.074741	0.755215
28	1	0	2.615591	4.320743	-0.862737
29	6	0	0.710150	-0.262835	1.209284
30	8	0	-0.688323	-0.019962	1.330022
31	1	0	-0.301610	-0.917812	-1.729423
32	6	0	1.218339	-0.779096	2.533530
33	1	0	0.637462	-1.661836	2.808338
34	1	0	2.268249	-1.062793	2.458407
35	1	0	1.093827	-0.006122	3.296435
36	6	0	2.625636	-0.618259	-1.802945
37	1	0	1.813131	-0.408797	-2.500614
38	1	0	2.940096	0.288236	-1.286170
39	1	0	3.464481	-1.064406	-2.340892
40	8	0	-0.701494	1.292971	-0.586879

Zero-point correction= 0.320820 (Hartree/Particle)
Thermal correction to Energy= 0.339773
Thermal correction to Enthalpy= 0.340718
Thermal correction to Gibbs Free Energy= 0.273382
Sum of electronic and zero-point Energies= -1411.170075
Sum of electronic and thermal Energies= -1411.151122
Sum of electronic and thermal Enthalpies= -1411.150177
Sum of electronic and thermal Free Energies= -1411.217513

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.78936604

INT2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.980061	0.833139	2.295780
2	8	0	-2.879656	0.080984	1.844613
3	8	0	-0.849603	1.072790	1.753976
4	6	0	-2.227413	1.500678	3.626125
5	1	0	-1.699090	2.454001	3.682282
6	1	0	-1.842935	0.849058	4.417876
7	1	0	-3.297829	1.640485	3.783683
8	6	0	-2.537010	1.650251	-1.303524
9	8	0	-3.321543	0.724415	-0.979491
10	8	0	-1.288912	1.710896	-1.046968
11	6	0	-3.097901	2.799715	-2.103904
12	1	0	-2.929025	2.598069	-3.167001
13	1	0	-2.583241	3.728539	-1.850528
14	1	0	-4.171163	2.892037	-1.932994
15	6	0	-0.976380	-1.616146	-2.268624
16	8	0	-2.096610	-1.834581	-1.743979
17	8	0	-0.075264	-0.829892	-1.821434
18	6	0	-0.635004	-2.327778	-3.553317
19	1	0	-0.527833	-1.590324	-4.354564
20	1	0	-1.415278	-3.043296	-3.812687
21	1	0	0.326471	-2.836411	-3.442400
22	6	0	-0.438512	-2.435774	1.292301

23	8	0	-1.673060	-2.473091	1.065074
24	8	0	0.363749	-1.495648	0.975779
25	6	0	0.180460	-3.619211	1.996177
26	1	0	-0.595968	-4.283822	2.375703
27	1	0	0.816339	-3.274763	2.816144
28	1	0	0.807599	-4.168937	1.286458
29	45	0	-2.579905	-0.913894	0.049269
30	45	0	-0.378555	0.159016	-0.035222
31	6	0	1.433438	1.026732	-0.209060
32	6	0	2.418122	0.004802	-0.518967
33	1	0	2.213064	-0.636005	-1.385363
34	6	0	1.782207	2.400504	-0.117277
35	6	0	0.828026	3.338708	0.349496
36	6	0	3.078591	2.857396	-0.473022
37	6	0	1.164066	4.677304	0.457127
38	1	0	-0.154426	2.985629	0.633838
39	6	0	3.399178	4.197810	-0.371213
40	1	0	3.820808	2.146399	-0.818331
41	6	0	2.441942	5.103970	0.093668
42	1	0	0.435528	5.393772	0.821878
43	1	0	4.389835	4.544503	-0.645704
44	1	0	2.698171	6.156480	0.176143
45	7	0	3.372518	-0.223295	0.307730
46	16	0	4.284236	-1.623962	-0.042774
47	8	0	3.751211	-2.321170	-1.208873
48	8	0	5.681265	-1.225798	-0.012725
49	6	0	3.890128	-2.568936	1.415306
50	1	0	4.260024	-2.031998	2.289416
51	1	0	2.805460	-2.679280	1.457552
52	1	0	4.382934	-3.538408	1.316558

Zero-point correction= 0.385121 (Hartree/Particle)
Thermal correction to Energy= 0.419091
Thermal correction to Enthalpy= 0.420035
Thermal correction to Gibbs Free Energy= 0.317969
Sum of electronic and zero-point Energies= -2083.847484
Sum of electronic and thermal Energies= -2083.813514
Sum of electronic and thermal Enthalpies= -2083.812570
Sum of electronic and thermal Free Energies= -2083.914636

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2084.72993670

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.837537	-2.625368	1.263970
2	8	0	-1.623739	-3.001315	0.361117
3	8	0	-0.396129	-1.441032	1.440505
4	6	0	-0.329878	-3.665169	2.234069
5	1	0	0.734492	-3.834693	2.037103
6	1	0	-0.872732	-4.602261	2.109508
7	1	0	-0.432233	-3.304785	3.261534
8	6	0	-3.662828	-0.123076	0.910440
9	8	0	-3.826494	-1.064043	0.092357
10	8	0	-2.579349	0.510436	1.126978
11	6	0	-4.863803	0.335171	1.700841
12	1	0	-5.327924	1.174926	1.172787
13	1	0	-4.558772	0.684345	2.689242
14	1	0	-5.594087	-0.471144	1.781541
15	6	0	-2.215202	0.946112	-2.359173
16	8	0	-2.716936	-0.200991	-2.478000
17	8	0	-1.442469	1.331820	-1.421583
18	6	0	-2.557665	1.988944	-3.392376
19	1	0	-2.693654	1.519519	-4.368462
20	1	0	-1.781007	2.755481	-3.426316
21	1	0	-3.503048	2.463859	-3.108934
22	6	0	0.508652	-1.511856	-1.987496
23	8	0	-0.567243	-2.131691	-2.195353
24	8	0	0.691438	-0.585270	-1.132821
25	6	0	1.703752	-1.919493	-2.811404
26	1	0	2.170977	-2.789232	-2.337291
27	1	0	2.439230	-1.115540	-2.846639
28	1	0	1.382065	-2.208244	-3.813748
29	45	0	-2.238547	-1.657809	-1.089511

30	45	0	-0.880791	0.023227	0.061267
31	6	0	0.227101	1.523066	1.010474
32	6	0	0.681996	2.393396	-0.052256
33	1	0	-0.130741	3.052055	-0.394722
34	6	0	0.031981	2.038709	2.349611
35	6	0	-0.714528	1.302646	3.287143
36	6	0	0.598965	3.268372	2.736210
37	6	0	-0.891200	1.790772	4.574105
38	1	0	-1.135086	0.350144	2.990818
39	6	0	0.415502	3.754511	4.021292
40	1	0	1.193797	3.830808	2.021869
41	6	0	-0.330511	3.014074	4.939277
42	1	0	-1.466964	1.219889	5.295793
43	1	0	0.853295	4.703917	4.312044
44	1	0	-0.473970	3.394062	5.946696
45	7	0	1.792167	2.338265	-0.687058
46	16	0	1.840200	3.271875	-2.107116
47	8	0	0.591069	4.006909	-2.300199
48	8	0	3.103341	3.988449	-2.111221
49	6	0	4.268731	-3.668478	0.994448
50	6	0	3.505241	-2.726707	1.651442
51	6	0	3.231429	-1.464521	1.085154
52	6	0	3.769821	-1.158888	-0.191808
53	6	0	4.573769	-2.116203	-0.836228
54	6	0	4.811648	-3.346317	-0.257750
55	1	0	4.454882	-4.637937	1.443524
56	1	0	4.988909	-1.855501	-1.803984
57	1	0	5.427542	-4.071064	-0.782288
58	6	0	2.419656	-0.485838	1.807402
59	8	0	2.079120	0.554175	1.226296
60	1	0	3.093142	-2.965867	2.626909
61	8	0	3.596878	-0.009257	-0.836411
62	1	0	2.922292	0.555108	-0.393681
63	6	0	2.052887	-0.710927	3.251569
64	1	0	1.265316	-1.466375	3.314082
65	1	0	2.918820	-1.049847	3.826952
66	1	0	1.677182	0.218336	3.677911
67	6	0	1.903494	1.930919	-3.280525
68	1	0	2.784747	1.327117	-3.059097
69	1	0	0.992666	1.340636	-3.165501
70	1	0	1.967965	2.372014	-4.277321

Zero-point correction= 0.530041 (Hartree/Particle)
Thermal correction to Energy= 0.573637
Thermal correction to Enthalpy= 0.574581
Thermal correction to Gibbs Free Energy= 0.451058
Sum of electronic and zero-point Energies= -2543.692969
Sum of electronic and thermal Energies= -2543.649373
Sum of electronic and thermal Enthalpies= -2543.648429
Sum of electronic and thermal Free Energies= -2543.771953
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2544.85230976

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.304576	-2.832864	-0.482714
2	8	0	-1.487978	-2.955854	-0.878536
3	8	0	0.239095	-1.750472	-0.078146
4	6	0	0.582828	-4.053490	-0.460843
5	1	0	1.533109	-3.828258	-0.953113
6	1	0	0.090098	-4.894097	-0.949590
7	1	0	0.808049	-4.319800	0.577415
8	6	0	-2.771054	-1.184147	1.857063
9	8	0	-3.441407	-1.565797	0.864531
10	8	0	-1.655058	-0.571007	1.820013
11	6	0	-3.314708	-1.464966	3.236234
12	1	0	-2.625303	-2.126298	3.769984
13	1	0	-4.297805	-1.931675	3.173634
14	1	0	-3.372157	-0.529131	3.798987
15	6	0	-3.194919	1.583449	-0.621545
16	8	0	-3.695708	0.549169	-1.135419
17	8	0	-2.063719	1.664913	-0.040161
18	6	0	-3.986877	2.864691	-0.693490

19	1	0	-4.958941	2.689776	-1.154675
20	1	0	-3.424231	3.600273	-1.275955
21	1	0	-4.115327	3.272899	0.312904
22	6	0	-0.757150	-0.163109	-2.910248
23	8	0	-1.791297	-0.880154	-2.857586
24	8	0	-0.181543	0.410418	-1.930895
25	6	0	-0.147272	0.046823	-4.276181
26	1	0	-0.516030	-0.709206	-4.970212
27	1	0	0.942372	0.006758	-4.211899
28	1	0	-0.435028	1.034105	-4.653337
29	45	0	-2.678828	-1.250279	-1.036682
30	45	0	-0.852156	-0.000294	-0.000971
31	6	0	0.819703	1.029655	1.065151
32	6	0	1.093684	2.128784	0.157379
33	1	0	0.401665	2.973076	0.204236
34	6	0	0.589048	1.489892	2.480134
35	6	0	-0.650224	2.019951	2.851012
36	6	0	1.627939	1.484664	3.417676
37	6	0	-0.847960	2.506752	4.138630
38	1	0	-1.455008	2.047484	2.125193
39	6	0	1.420097	1.953675	4.710811
40	1	0	2.615431	1.129563	3.134540
41	6	0	0.178317	2.463383	5.078397
42	1	0	-1.816153	2.917921	4.409400
43	1	0	2.237152	1.936914	5.426159
44	1	0	0.016382	2.836894	6.084984
45	7	0	2.075097	2.093940	-0.676451
46	16	0	2.256353	3.450840	-1.665863
47	8	0	1.154376	4.386812	-1.469183
48	8	0	3.627598	3.907003	-1.514355
49	6	0	4.611964	-3.764278	0.764853
50	6	0	3.662876	-2.967187	1.354755
51	6	0	3.206022	-1.767046	0.752349
52	6	0	3.770517	-1.370229	-0.499365
53	6	0	4.720767	-2.224267	-1.097918
54	6	0	5.132293	-3.385297	-0.484884
55	1	0	4.951189	-4.671174	1.252446
56	1	0	5.124195	-1.915993	-2.056016
57	1	0	5.873929	-4.010292	-0.973390
58	6	0	2.129543	-1.044080	1.372123
59	8	0	1.958035	0.140237	0.921024
60	6	0	1.328956	-1.564192	2.517235
61	1	0	1.837830	-1.307908	3.454846
62	1	0	0.336487	-1.110669	2.534877
63	1	0	1.222135	-2.646185	2.451498
64	1	0	3.256782	-3.254926	2.318266
65	8	0	3.482672	-0.292751	-1.208915
66	1	0	2.925601	0.404991	-0.785073
67	6	0	2.072721	2.686210	-3.262062
68	1	0	2.825616	1.902577	-3.360451
69	1	0	1.069251	2.266724	-3.314061
70	1	0	2.219923	3.463639	-4.014549

Zero-point correction= 0.534087 (Hartree/Particle)
Thermal correction to Energy= 0.576685
Thermal correction to Enthalpy= 0.577630
Thermal correction to Gibbs Free Energy= 0.457314
Sum of electronic and zero-point Energies= -2543.710915
Sum of electronic and thermal Energies= -2543.668317
Sum of electronic and thermal Enthalpies= -2543.667372
Sum of electronic and thermal Free Energies= -2543.787688

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2544.87452410

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.902777	1.784851	0.756218
2	6	0	1.044681	0.359411	0.594307
3	45	0	-0.931464	-0.253406	0.127480
4	8	0	-1.041052	-1.460330	1.797428
5	6	0	-2.108126	-2.115585	2.024035
6	8	0	-3.142928	-2.130187	1.307780

7	45	0	-3.200148	-0.980706	-0.408499
8	8	0	-3.891381	0.629119	0.693771
9	6	0	-3.060710	1.405202	1.233403
10	8	0	-1.792365	1.297541	1.186017
11	8	0	-0.238445	-1.823531	-0.993684
12	6	0	-1.074798	-2.610943	-1.550781
13	8	0	-2.326572	-2.528648	-1.476918
14	8	0	-1.001726	0.912463	-1.569943
15	6	0	-2.049738	0.901540	-2.289196
16	8	0	-3.093876	0.227783	-2.083089
17	8	0	1.932189	0.188237	-1.137391
18	1	0	1.697495	-0.745728	-1.389578
19	6	0	1.990236	-0.390309	1.419251
20	6	0	3.031619	0.267206	2.096340
21	6	0	1.916365	-1.791433	1.474386
22	6	0	3.969346	-0.454941	2.822291
23	1	0	3.107782	1.349632	2.040373
24	6	0	2.861698	-2.511034	2.193614
25	1	0	1.126302	-2.297048	0.932464
26	6	0	3.884656	-1.845118	2.868564
27	1	0	4.767708	0.062957	3.343932
28	1	0	2.798633	-3.594358	2.233242
29	1	0	4.617962	-2.412223	3.435026
30	7	0	1.070864	2.696837	-0.128365
31	1	0	0.461171	2.021864	1.736017
32	16	0	0.484360	4.219933	0.311330
33	6	0	-0.958897	4.272093	-0.736430
34	8	0	1.464104	5.190580	-0.151309
35	8	0	0.041275	4.250625	1.704536
36	6	0	3.301453	0.318941	-1.102542
37	6	0	4.160098	-0.797038	-1.073081
38	6	0	3.808185	1.612438	-1.027157
39	6	0	5.534752	-0.569394	-0.924083
40	6	0	5.176803	1.804086	-0.893698
41	1	0	3.113022	2.443169	-1.058142
42	6	0	6.045702	0.715450	-0.830025
43	1	0	6.213687	-1.415182	-0.893450
44	1	0	5.564924	2.816205	-0.836329
45	1	0	7.113747	0.869832	-0.718698
46	6	0	3.624129	-2.165474	-1.256588
47	8	0	2.476195	-2.327445	-1.656100
48	6	0	-3.592513	2.571183	2.029311
49	1	0	-2.816916	3.328204	2.159378
50	1	0	-4.472554	2.989593	1.536214
51	1	0	-3.901370	2.209856	3.015860
52	6	0	-2.127804	-2.925707	3.297409
53	1	0	-2.859018	-3.731749	3.223205
54	1	0	-1.132785	-3.321520	3.510370
55	1	0	-2.414246	-2.267708	4.124690
56	6	0	-2.044482	1.818222	-3.489014
57	1	0	-2.547055	1.335297	-4.329475
58	1	0	-2.607516	2.724399	-3.239825
59	1	0	-1.023974	2.095333	-3.757102
60	6	0	-0.495450	-3.731064	-2.377449
61	1	0	0.586595	-3.778291	-2.255894
62	1	0	-0.963940	-4.674950	-2.086834
63	1	0	-0.740052	-3.553487	-3.429431
64	6	0	4.500905	-3.357406	-0.963656
65	1	0	5.332123	-3.413822	-1.675139
66	1	0	4.920946	-3.284488	0.044621
67	1	0	3.898328	-4.262445	-1.050094
68	1	0	-0.639942	4.158387	-1.772886
69	1	0	-1.610523	3.447497	-0.442858
70	1	0	-1.442463	5.238292	-0.577917

Zero-point correction= 0.530383 (Hartree/Particle)
Thermal correction to Energy= 0.573122
Thermal correction to Enthalpy= 0.574066
Thermal correction to Gibbs Free Energy= 0.453337
Sum of electronic and zero-point Energies= -2543.687563
Sum of electronic and thermal Energies= -2543.644824
Sum of electronic and thermal Enthalpies= -2543.643880
Sum of electronic and thermal Free Energies= -2543.764610

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2544.84729521

INT4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.942708	1.735846	0.724565
2	6	0	1.200251	0.349389	0.449369
3	45	0	-0.894386	-0.240670	0.090550
4	8	0	-0.926040	-1.525951	1.699682
5	6	0	-1.953943	-2.242779	1.909898
6	8	0	-3.002210	-2.270479	1.211065
7	45	0	-3.141966	-1.024134	-0.429502
8	8	0	-3.862137	0.485528	0.781784
9	6	0	-3.045243	1.261875	1.345761
10	8	0	-1.777101	1.212508	1.254451
11	8	0	-0.156920	-1.698329	-1.151217
12	6	0	-0.975057	-2.484721	-1.742892
13	8	0	-2.222604	-2.470480	-1.614254
14	8	0	-1.039796	0.998145	-1.554050
15	6	0	-2.110257	0.993891	-2.238106
16	8	0	-3.128545	0.280179	-2.032340
17	8	0	1.856632	0.179054	-0.975594
18	1	0	1.606368	-0.732335	-1.323706
19	6	0	2.017724	-0.442236	1.413296
20	6	0	2.914353	0.194913	2.278993
21	6	0	1.955377	-1.841650	1.416380
22	6	0	3.721390	-0.544536	3.138358
23	1	0	2.989602	1.279145	2.272621
24	6	0	2.776686	-2.580384	2.259832
25	1	0	1.259589	-2.342032	0.753010
26	6	0	3.658543	-1.934668	3.125560
27	1	0	4.406134	-0.033485	3.808169
28	1	0	2.716167	-3.665037	2.253021
29	1	0	4.290601	-2.514477	3.792025
30	7	0	1.000456	2.705945	-0.122453
31	1	0	0.568064	1.896944	1.741905
32	16	0	0.384298	4.170440	0.421436
33	6	0	-1.135615	4.228463	-0.511456
34	8	0	1.286781	5.204296	-0.065425
35	8	0	0.044615	4.128377	1.843460
36	6	0	3.253698	0.397675	-1.076215
37	6	0	4.149476	-0.679937	-1.106391
38	6	0	3.678454	1.713345	-1.083568
39	6	0	5.516029	-0.384901	-1.096674
40	6	0	5.046493	1.972909	-1.089452
41	1	0	2.939960	2.506978	-1.067519
42	6	0	5.966105	0.929157	-1.083929
43	1	0	6.235897	-1.196357	-1.114285
44	1	0	5.386301	3.003333	-1.095538
45	1	0	7.030968	1.136357	-1.080687
46	6	0	3.658538	-2.074991	-1.246689
47	8	0	2.531282	-2.269567	-1.681662
48	6	0	-3.600883	2.352513	2.227180
49	1	0	-2.848843	3.126290	2.391741
50	1	0	-4.505042	2.770741	1.779496
51	1	0	-3.876298	1.916137	3.193040
52	6	0	-1.911247	-3.119864	3.137314
53	1	0	-2.547758	-3.995357	2.999624
54	1	0	-0.883412	-3.414575	3.357012
55	1	0	-2.291578	-2.545727	3.988885
56	6	0	-2.174080	1.966414	-3.391397
57	1	0	-2.656768	1.495152	-4.250200
58	1	0	-2.788984	2.822626	-3.093534
59	1	0	-1.175724	2.318029	-3.655453
60	6	0	-0.370172	-3.486716	-2.691953
61	1	0	0.647382	-3.733774	-2.387675
62	1	0	-0.998877	-4.376923	-2.744813
63	1	0	-0.329422	-3.036090	-3.689691
64	6	0	4.555830	-3.222594	-0.868422
65	1	0	5.405793	-3.296385	-1.555927
66	1	0	4.946144	-3.077311	0.143962
67	1	0	3.980569	-4.147877	-0.917471
68	1	0	-0.893446	4.172831	-1.573093
69	1	0	-1.742491	3.373654	-0.210065

70	1	0	-1.629650	5.172316	-0.271226

Zero-point correction= 0.531397 (Hartree/Particle)
Thermal correction to Energy= 0.575254
Thermal correction to Enthalpy= 0.576198
Thermal correction to Gibbs Free Energy= 0.451889
Sum of electronic and zero-point Energies= -2543.689520
Sum of electronic and thermal Energies= -2543.645663
Sum of electronic and thermal Enthalpies= -2543.644719
Sum of electronic and thermal Free Energies= -2543.769028
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2544.85073432

INT5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.586094	-1.919776	-2.305206
2	8	0	-1.833813	-1.878062	-2.451444
3	8	0	0.092927	-1.306710	-1.419046
4	6	0	0.193269	-2.789546	-3.263762
5	1	0	-0.107463	-2.568320	-4.290893
6	1	0	-0.049285	-3.838675	-3.068763
7	1	0	1.267753	-2.642000	-3.140187
8	6	0	-2.223268	-2.564497	0.944286
9	8	0	-3.153462	-2.365033	0.117496
10	8	0	-1.181990	-1.854462	1.088973
11	6	0	-2.322009	-3.777946	1.835751
12	1	0	-3.368830	-4.022426	2.023442
13	1	0	-1.789583	-3.599651	2.771856
14	1	0	-1.855876	-4.628226	1.326319
15	6	0	-3.279820	1.001861	1.170028
16	8	0	-3.951433	0.437047	0.265425
17	8	0	-2.017053	0.945707	1.319016
18	6	0	-4.023988	1.815284	2.199245
19	1	0	-3.543096	2.789723	2.316671
20	1	0	-3.968253	1.300323	3.163462
21	1	0	-5.068407	1.937252	1.911455
22	6	0	-1.771044	1.707536	-2.128006
23	8	0	-2.735441	0.931977	-2.335727
24	8	0	-0.853006	1.553595	-1.255777
25	6	0	-1.687621	2.953211	-2.978106
26	1	0	-2.444751	2.928409	-3.761809
27	1	0	-0.691905	3.039654	-3.422996
28	1	0	-1.851900	3.831247	-2.345041
29	45	0	-2.994491	-0.741969	-1.143741
30	45	0	-0.907318	-0.145557	-0.024329
31	6	0	0.982492	0.340670	1.061882
32	6	0	1.024367	1.788614	1.056880
33	1	0	0.191832	2.272674	1.573869
34	6	0	0.886185	-0.315830	2.408171
35	6	0	1.170737	-1.681398	2.539610
36	6	0	0.482201	0.387299	3.549361
37	6	0	1.088468	-2.315007	3.773287
38	1	0	1.413548	-2.266765	1.658791
39	6	0	0.372105	-0.256138	4.777262
40	1	0	0.248742	1.444268	3.495569
41	6	0	0.683357	-1.606757	4.900423
42	1	0	1.322519	-3.373062	3.846588
43	1	0	0.057214	0.312421	5.647221
44	1	0	0.609854	-2.101283	5.864126
45	7	0	1.924660	2.476214	0.445966
46	16	0	1.705559	4.149377	0.513618
47	8	0	0.534606	4.501107	1.311941
48	8	0	2.996846	4.737345	0.825325
49	6	0	5.587694	-1.604282	-2.566394
50	6	0	4.437720	-0.912002	-2.276128
51	6	0	3.864249	-0.911403	-0.977028
52	6	0	4.532552	-1.649289	0.043794
53	6	0	5.710316	-2.348806	-0.269986
54	6	0	6.225557	-2.329543	-1.546597
55	1	0	5.999558	-1.586169	-3.569048
56	1	0	6.193040	-2.895331	0.532353
57	6	0	2.659700	-0.147139	-0.744303

58	8	0	2.178274	-0.245280	0.438054
59	1	0	3.956076	-0.348764	-3.065780
60	1	0	7.137556	-2.877990	-1.761874
61	1	0	3.337335	-1.233735	1.479115
62	6	0	1.319191	4.467787	-1.199565
63	1	0	2.172656	4.175110	-1.813045
64	1	0	0.433083	3.885470	-1.455733
65	1	0	1.128196	5.538390	-1.298417
66	8	0	4.150550	-1.739323	1.314456
67	6	0	2.077942	0.706927	-1.815486
68	1	0	2.790968	1.510078	-2.028220
69	1	0	1.932036	0.106188	-2.715518
70	1	0	1.125649	1.144101	-1.536025

Zero-point correction= 0.534054 (Hartree/Particle)
Thermal correction to Energy= 0.577061
Thermal correction to Enthalpy= 0.578005
Thermal correction to Gibbs Free Energy= 0.455022
Sum of electronic and zero-point Energies= -2543.695660
Sum of electronic and thermal Energies= -2543.652653
Sum of electronic and thermal Enthalpies= -2543.651709
Sum of electronic and thermal Free Energies= -2543.774692

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2544.86138411

TS5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.680613	-0.222214	-2.926922
2	8	0	2.851738	-0.554440	-2.603870
3	8	0	0.718762	0.028172	-2.133172
4	6	0	1.382480	-0.074493	-4.399624
5	1	0	2.110536	-0.628138	-4.993585
6	1	0	1.444664	0.986440	-4.663865
7	1	0	0.368211	-0.415722	-4.618575
8	6	0	3.045091	2.121658	-0.425731
9	8	0	3.935705	1.239896	-0.575644
10	8	0	1.805233	1.912534	-0.262578
11	6	0	3.471431	3.567367	-0.469781
12	1	0	4.465850	3.678397	-0.033251
13	1	0	2.742415	4.188803	0.053459
14	1	0	3.521677	3.887180	-1.516064
15	6	0	2.750464	-0.483459	2.224410
16	8	0	3.664459	-0.838671	1.434841
17	8	0	1.590627	-0.073857	1.895843
18	6	0	3.039624	-0.521447	3.704308
19	1	0	2.214827	-1.007730	4.231326
20	1	0	3.112886	0.505591	4.076368
21	1	0	3.977013	-1.043283	3.898119
22	6	0	1.443267	-2.899812	-0.290417
23	8	0	2.636924	-2.668944	-0.602204
24	8	0	0.561834	-2.030363	0.017961
25	6	0	1.004968	-4.345236	-0.254819
26	1	0	1.734559	-4.973805	-0.766016
27	1	0	0.020409	-4.454360	-0.717168
28	1	0	0.928131	-4.670809	0.788215
29	45	0	3.347275	-0.728888	-0.604642
30	45	0	1.078274	0.002693	-0.099344
31	6	0	-0.963861	0.865019	0.414567
32	6	0	-1.417915	-0.103804	1.366428
33	1	0	-0.912906	-0.181088	2.328221
34	6	0	-0.685693	2.262872	0.862954
35	6	0	-0.906623	3.334163	-0.008003
36	6	0	-0.151818	2.528311	2.130457
37	6	0	-0.615223	4.638150	0.381609
38	1	0	-1.279034	3.147657	-1.009599
39	6	0	0.146723	3.829620	2.509391
40	1	0	0.074583	1.714753	2.809811
41	6	0	-0.086424	4.894858	1.640966
42	1	0	-0.795889	5.453981	-0.312230
43	1	0	0.562215	4.012987	3.495997
44	1	0	0.141831	5.911715	1.945571
45	7	0	-2.391835	-0.890560	1.035388

46	16	0	-2.888776	-2.068890	2.126066
47	8	0	-2.211235	-1.880056	3.402740
48	8	0	-4.337648	-2.116232	2.057504
49	6	0	-6.187533	-0.530141	-2.297453
50	6	0	-4.838850	-0.697938	-2.089441
51	6	0	-4.090530	0.185375	-1.273990
52	6	0	-4.774674	1.276162	-0.667165
53	6	0	-6.155961	1.420905	-0.869759
54	6	0	-6.847881	0.536327	-1.668443
55	1	0	-6.733783	-1.218695	-2.932207
56	1	0	-6.649272	2.252620	-0.379538
57	6	0	-2.688923	-0.081196	-1.026780
58	8	0	-2.002539	0.954452	-0.607234
59	1	0	-4.334472	-1.524311	-2.575606
60	1	0	-7.915419	0.672175	-1.812932
61	1	0	-3.248440	2.095958	0.119829
62	6	0	-2.213939	-3.528348	1.354366
63	1	0	-2.727347	-3.694734	0.406175
64	1	0	-1.149009	-3.356434	1.192441
65	1	0	-2.386860	-4.365838	2.033506
66	8	0	-4.213918	2.199193	0.113176
67	6	0	-2.001465	-1.256993	-1.638682
68	1	0	-2.622778	-2.148124	-1.552041
69	1	0	-1.836618	-1.028795	-2.698740
70	1	0	-1.038002	-1.449149	-1.176568

Zero-point correction= 0.532179 (Hartree/Particle)
Thermal correction to Energy= 0.575086
Thermal correction to Enthalpy= 0.576030
Thermal correction to Gibbs Free Energy= 0.453259
Sum of electronic and zero-point Energies= -2543.693371
Sum of electronic and thermal Energies= -2543.650464
Sum of electronic and thermal Enthalpies= -2543.649520
Sum of electronic and thermal Free Energies= -2543.772291

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2544.85600251

INT6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.628284	0.257339	0.120716
2	6	0	0.909994	1.347117	-0.160051
3	1	0	1.211150	2.319471	-0.515302
4	6	0	3.049959	-0.045734	0.022190
5	6	0	3.554431	-1.234068	0.560366
6	6	0	3.927651	0.843030	-0.612950
7	6	0	4.911777	-1.523825	0.466448
8	1	0	2.879306	-1.924270	1.054533
9	6	0	5.281311	0.551855	-0.695778
10	1	0	3.547197	1.761525	-1.050579
11	6	0	5.779670	-0.634044	-0.157806
12	1	0	5.291910	-2.449581	0.887813
13	1	0	5.950730	1.249501	-1.189787
14	1	0	6.838769	-0.861470	-0.229661
15	7	0	-0.439410	1.071874	0.119094
16	16	0	-1.688635	2.137608	-0.140341
17	8	0	-1.057072	3.368274	-0.584085
18	8	0	-2.560132	2.109060	1.021359
19	6	0	-2.646280	-2.468704	-1.294872
20	6	0	-1.538727	-1.768199	-0.811646
21	6	0	-1.615474	-1.098091	0.426772
22	6	0	-2.809943	-1.173005	1.148752
23	6	0	-3.911613	-1.866561	0.665683
24	6	0	-3.825613	-2.510019	-0.566716
25	1	0	-2.549847	-2.971507	-2.251342
26	1	0	-2.893738	-0.648020	2.092796
27	1	0	-4.829904	-1.895330	1.242312
28	1	0	-4.679854	-3.052260	-0.961138
29	6	0	-0.491954	-0.194497	0.901276
30	8	0	0.787748	-0.774907	0.552812
31	1	0	0.311346	-1.481019	-1.052401
32	6	0	-0.472640	0.097180	2.397001

33	1	0	-1.328534	0.709772	2.684910
34	1	0	-0.471499	-0.839237	2.960667
35	1	0	0.439680	0.654310	2.626788
36	8	0	-0.443351	-1.750820	-1.602465
37	6	0	-2.588653	1.444390	-1.517366
38	1	0	-1.888151	1.263041	-2.333440
39	1	0	-3.068002	0.517455	-1.200502
40	1	0	-3.337158	2.184931	-1.806976

Zero-point correction= 0.318856 (Hartree/Particle)
Thermal correction to Energy= 0.338911
Thermal correction to Enthalpy= 0.339855
Thermal correction to Gibbs Free Energy= 0.269179
Sum of electronic and zero-point Energies= -1411.144431
Sum of electronic and thermal Energies= -1411.124375
Sum of electronic and thermal Enthalpies= -1411.123431
Sum of electronic and thermal Free Energies= -1411.194107
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.77062188

TS6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.560116	-0.223336	0.473786
2	6	0	1.012219	0.955891	0.919085
3	1	0	1.507647	1.879650	1.167683
4	6	0	3.001539	-0.366692	0.154142
5	6	0	3.552438	-1.649167	0.085403
6	6	0	3.818423	0.741456	-0.095864
7	6	0	4.898869	-1.820591	-0.214884
8	1	0	2.909864	-2.502822	0.272086
9	6	0	5.165166	0.568691	-0.390088
10	1	0	3.396842	1.742121	-0.078480
11	6	0	5.708840	-0.712702	-0.449667
12	1	0	5.318224	-2.820971	-0.265132
13	1	0	5.789539	1.435386	-0.585254
14	1	0	6.760991	-0.847059	-0.682473
15	7	0	-0.403787	0.925730	0.847486
16	16	0	-1.111993	2.161850	-0.185303
17	8	0	-0.482024	3.376516	0.290697
18	8	0	-2.548232	1.999333	-0.152275
19	6	0	-3.248616	-1.745531	-1.512205
20	6	0	-2.082961	-1.277911	-0.896910
21	6	0	-2.148225	-0.790476	0.423056
22	6	0	-3.375054	-0.830431	1.101156
23	6	0	-4.525887	-1.280446	0.479909
24	6	0	-4.456462	-1.736071	-0.837443
25	1	0	-3.167814	-2.121405	-2.526520
26	1	0	-3.433405	-0.446047	2.114566
27	1	0	-5.470730	-1.270217	1.012360
28	1	0	-5.351166	-2.096827	-1.335844
29	6	0	-0.953152	-0.274026	1.131442
30	8	0	0.788533	-1.255940	0.321439
31	1	0	-0.164708	-1.336560	-1.013473
32	6	0	-0.648830	-0.884614	2.467541
33	1	0	-1.498021	-0.686432	3.133112
34	1	0	-0.538432	-1.963570	2.359440
35	1	0	0.252367	-0.458521	2.907028
36	8	0	-0.948348	-1.318759	-1.623140
37	6	0	-0.467840	1.793096	-1.805709
38	1	0	0.619960	1.851989	-1.756880
39	1	0	-0.790709	0.796146	-2.110201
40	1	0	-0.864994	2.563403	-2.469822

Zero-point correction= 0.316413 (Hartree/Particle)
Thermal correction to Energy= 0.336219
Thermal correction to Enthalpy= 0.337163
Thermal correction to Gibbs Free Energy= 0.267331
Sum of electronic and zero-point Energies= -1411.111447
Sum of electronic and thermal Energies= -1411.091641
Sum of electronic and thermal Enthalpies= -1411.090697
Sum of electronic and thermal Free Energies= -1411.160529

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.73699310

INT7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.663100	-0.420664	0.185117
2	6	0	1.037066	0.761325	0.610108
3	1	0	1.533870	1.710886	0.733623
4	6	0	3.156791	-0.432689	0.085848
5	6	0	3.749955	-1.348904	-0.786250
6	6	0	3.970837	0.416425	0.840600
7	6	0	5.131774	-1.397328	-0.922120
8	1	0	3.107819	-2.018379	-1.348529
9	6	0	5.354703	0.361695	0.710549
10	1	0	3.527032	1.105147	1.553446
11	6	0	5.937547	-0.541086	-0.174807
12	1	0	5.582327	-2.107943	-1.608793
13	1	0	5.978850	1.018898	1.308702
14	1	0	7.018040	-0.583303	-0.276706
15	7	0	-0.357098	0.773785	0.593258
16	16	0	-1.090825	2.131856	-0.331105
17	8	0	-0.314860	3.276185	0.100468
18	8	0	-2.522584	2.084643	-0.143685
19	6	0	-3.575685	-1.685090	-1.227335
20	6	0	-2.365401	-1.208632	-0.712436
21	6	0	-2.349118	-0.652403	0.582154
22	6	0	-3.519326	-0.649807	1.351087
23	6	0	-4.712766	-1.113564	0.827806
24	6	0	-4.734685	-1.625081	-0.472225
25	1	0	-3.570879	-2.111132	-2.224958
26	1	0	-3.487585	-0.230191	2.352696
27	1	0	-5.620661	-1.075309	1.420044
28	1	0	-5.664405	-1.996015	-0.893189
29	8	0	-1.273966	-1.304042	-1.497858
30	6	0	-1.068535	-0.196920	1.145649
31	8	0	1.033685	-1.468036	-0.141622
32	1	0	-0.427452	-1.355381	-0.967363
33	6	0	-0.640884	1.711050	-2.000656
34	1	0	-1.056555	0.730749	-2.241936
35	1	0	-1.056823	2.497775	-2.633285
36	1	0	0.447787	1.698666	-2.062369
37	6	0	-0.488768	-0.972375	2.272510
38	1	0	-1.293306	-1.331893	2.919481
39	1	0	0.033919	-1.845198	1.853735
40	1	0	0.243072	-0.379282	2.828278

Zero-point correction= 0.317031 (Hartree/Particle)
Thermal correction to Energy= 0.337305
Thermal correction to Enthalpy= 0.338249
Thermal correction to Gibbs Free Energy= 0.268177
Sum of electronic and zero-point Energies= -1411.118367
Sum of electronic and thermal Energies= -1411.098093
Sum of electronic and thermal Enthalpies= -1411.097149
Sum of electronic and thermal Free Energies= -1411.167221
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.74559849

TS7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.597495	-0.330888	0.097263
2	6	0	1.003111	0.798424	0.607411
3	1	0	1.524350	1.703981	0.878199
4	6	0	3.079950	-0.439884	0.050226
5	6	0	3.654631	-1.324224	-0.867248
6	6	0	3.912186	0.307765	0.889626
7	6	0	5.036263	-1.439674	-0.960995
8	1	0	3.002131	-1.916472	-1.499038
9	6	0	5.294126	0.190524	0.794780

10	1	0	3.481719	0.966654	1.637629
11	6	0	5.859494	-0.680153	-0.133529
12	1	0	5.471455	-2.126613	-1.680674
13	1	0	5.930365	0.773964	1.453389
14	1	0	6.939032	-0.773556	-0.205733
15	7	0	-0.409166	0.829227	0.607808
16	16	0	-1.134775	2.182042	-0.292246
17	8	0	-0.452874	3.327303	0.277830
18	8	0	-2.572202	2.056250	-0.216387
19	6	0	-3.382770	-1.690724	-1.324215
20	6	0	-2.230104	-1.078366	-0.772728
21	6	0	-2.301777	-0.680967	0.603000
22	6	0	-3.449042	-0.977576	1.371310
23	6	0	-4.554877	-1.554534	0.795976
24	6	0	-4.512235	-1.901956	-0.568345
25	1	0	-3.334653	-1.984518	-2.367380
26	1	0	-3.475076	-0.679868	2.416182
27	1	0	-5.450858	-1.733605	1.380071
28	1	0	-5.383342	-2.359354	-1.029389
29	8	0	-1.155700	-0.950974	-1.500009
30	6	0	-1.112791	-0.136982	1.199712
31	8	0	0.937886	-1.355645	-0.364740
32	1	0	-0.091756	-1.125008	-0.887989
33	6	0	-0.552761	1.926341	-1.952805
34	1	0	-0.887731	0.940299	-2.282787
35	1	0	-0.990403	2.734175	-2.542996
36	1	0	0.535072	1.996412	-1.947598
37	6	0	-0.530838	-0.788979	2.409678
38	1	0	-1.339521	-1.128325	3.062743
39	1	0	0.018697	-1.681364	2.083747
40	1	0	0.153839	-0.128411	2.944634

Zero-point correction= 0.312147 (Hartree/Particle)
Thermal correction to Energy= 0.332071
Thermal correction to Enthalpy= 0.333015
Thermal correction to Gibbs Free Energy= 0.263940
Sum of electronic and zero-point Energies= -1411.115345
Sum of electronic and thermal Energies= -1411.095421
Sum of electronic and thermal Enthalpies= -1411.094477
Sum of electronic and thermal Free Energies= -1411.163552

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.73919800

INT8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.670641	-0.280664	-0.142316
2	6	0	1.023301	0.584981	0.673135
3	1	0	1.530729	1.269297	1.339045
4	6	0	3.136669	-0.471723	-0.083315
5	6	0	3.823989	-0.887551	-1.227655
6	6	0	3.851262	-0.243850	1.096863
7	6	0	5.204230	-1.048365	-1.195850
8	1	0	3.267176	-1.081592	-2.137757
9	6	0	5.231479	-0.404014	1.125243
10	1	0	3.323464	0.035302	2.003680
11	6	0	5.911917	-0.803696	-0.021856
12	1	0	5.728791	-1.367170	-2.091474
13	1	0	5.773941	-0.228688	2.049241
14	1	0	6.989672	-0.934267	0.002427
15	7	0	-0.395803	0.649310	0.576950
16	16	0	-1.019834	2.163149	-0.015306
17	8	0	-0.295630	3.162415	0.749991
18	8	0	-2.464540	2.101974	0.029468
19	6	0	-3.679296	-1.350115	-1.475801
20	6	0	-2.455070	-0.805969	-0.929940
21	6	0	-2.353503	-0.770417	0.540235
22	6	0	-3.420921	-1.338902	1.321449
23	6	0	-4.546791	-1.830871	0.746274
24	6	0	-4.670124	-1.826495	-0.678810
25	1	0	-3.760794	-1.354736	-2.557441
26	1	0	-3.355650	-1.297041	2.403820
27	1	0	-5.359880	-2.207264	1.357347

28	1	0	-5.577918	-2.220146	-1.128686
29	8	0	-1.518487	-0.483058	-1.698298
30	6	0	-1.190919	-0.310671	1.151342
31	8	0	1.066963	-1.032337	-1.064916
32	1	0	0.118777	-0.767077	-1.214396
33	6	0	-0.440376	2.234461	-1.696768
34	1	0	-0.940684	1.450581	-2.264498
35	1	0	-0.696321	3.233656	-2.054932
36	1	0	0.642415	2.101538	-1.691128
37	6	0	-0.659637	-0.886928	2.433336
38	1	0	-1.416110	-1.473963	2.953397
39	1	0	0.172288	-1.561655	2.204234
40	1	0	-0.279493	-0.099548	3.090018

Zero-point correction= 0.316421 (Hartree/Particle)
Thermal correction to Energy= 0.337396
Thermal correction to Enthalpy= 0.338340
Thermal correction to Gibbs Free Energy= 0.265158
Sum of electronic and zero-point Energies= -1411.116469
Sum of electronic and thermal Energies= -1411.095495
Sum of electronic and thermal Enthalpies= -1411.094550
Sum of electronic and thermal Free Energies= -1411.167733
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.74453270

INT9b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.411609	-0.260065	0.707773
2	6	0	-0.425439	-0.814880	-0.314365
3	1	0	-0.770090	-1.807272	-0.617682
4	6	0	-2.830064	-0.104326	0.264604
5	6	0	-3.757373	0.362553	1.201402
6	6	0	-3.255394	-0.403480	-1.033843
7	6	0	-5.089304	0.526609	0.848150
8	1	0	-3.409403	0.589043	2.203694
9	6	0	-4.589881	-0.235941	-1.387084
10	1	0	-2.554149	-0.763267	-1.780076
11	6	0	-5.506585	0.227857	-0.447822
12	1	0	-5.804417	0.886880	1.581152
13	1	0	-4.913327	-0.466702	-2.397253
14	1	0	-6.548450	0.357548	-0.725290
15	7	0	0.901609	-0.970649	0.257691
16	16	0	1.731700	-2.407425	-0.112095
17	8	0	0.721119	-3.436622	-0.276928
18	8	0	2.817314	-2.568901	0.835738
19	6	0	1.603152	2.975445	-1.626751
20	6	0	1.429137	1.600492	-1.167751
21	6	0	1.599742	1.363777	0.291037
22	6	0	1.942749	2.501187	1.124980
23	6	0	2.083507	3.749545	0.625822
24	6	0	1.910582	3.985087	-0.782069
25	1	0	1.467158	3.134257	-2.691356
26	1	0	2.048524	2.345658	2.192417
27	1	0	2.314372	4.581096	1.283341
28	1	0	2.028735	4.995413	-1.165331
29	6	0	1.549497	0.110451	0.871626
30	8	0	-1.062271	0.045636	1.829408
31	1	0	-0.393494	-0.181704	-1.209880
32	6	0	2.082127	-0.140386	2.256266
33	1	0	2.170738	-1.205855	2.451976
34	1	0	3.053242	0.332815	2.414573
35	1	0	1.357304	0.269050	2.969468
36	6	0	2.451724	-2.062411	-1.707408
37	1	0	1.660485	-1.803518	-2.409347
38	1	0	3.140150	-1.224226	-1.602039
39	1	0	2.977815	-2.969311	-2.013177
40	8	0	1.203455	0.704180	-1.993582

Zero-point correction= 0.318130 (Hartree/Particle)
Thermal correction to Energy= 0.338827
Thermal correction to Enthalpy= 0.339771

Thermal correction to Gibbs Free Energy= 0.267263
Sum of electronic and zero-point Energies= -1411.124560
Sum of electronic and thermal Energies= -1411.103863
Sum of electronic and thermal Enthalpies= -1411.102919
Sum of electronic and thermal Free Energies= -1411.175427
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.74935699

TS8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.279894	-0.451095	0.663508
2	6	0	-0.445053	-1.601956	0.180141
3	1	0	-0.719041	-2.513462	0.727310
4	6	0	-2.690640	-0.266960	0.293854
5	6	0	-3.381786	0.835447	0.806662
6	6	0	-3.351154	-1.183687	-0.528489
7	6	0	-4.720591	1.019916	0.494969
8	1	0	-2.852307	1.537730	1.441249
9	6	0	-4.694893	-1.000213	-0.830571
10	1	0	-2.824585	-2.041690	-0.934553
11	6	0	-5.378496	0.100683	-0.321009
12	1	0	-5.253917	1.879340	0.888467
13	1	0	-5.208049	-1.714214	-1.466715
14	1	0	-6.427930	0.243950	-0.560145
15	7	0	0.916478	-1.203695	0.505413
16	16	0	2.166091	-1.926921	-0.327390
17	8	0	1.709162	-3.281861	-0.584122
18	8	0	3.379096	-1.658660	0.424767
19	6	0	0.821701	2.652173	-1.585481
20	6	0	0.574152	1.432753	-0.852784
21	6	0	1.348034	1.243101	0.368884
22	6	0	2.219884	2.281298	0.819802
23	6	0	2.419152	3.412051	0.084458
24	6	0	1.708919	3.585473	-1.138063
25	1	0	0.264387	2.787552	-2.506868
26	1	0	2.777412	2.139885	1.740178
27	1	0	3.119330	4.170802	0.417009
28	1	0	1.874777	4.489522	-1.718997
29	6	0	1.145587	0.081167	1.147112
30	8	0	-0.750258	0.242304	1.547709
31	1	0	-0.582479	-1.772436	-0.888011
32	6	0	1.699205	-0.051276	2.533548
33	1	0	1.213289	-0.890386	3.032541
34	1	0	2.769013	-0.275483	2.463123
35	1	0	1.547405	0.859429	3.115004
36	6	0	2.308898	-1.098227	-1.904479
37	1	0	1.323072	-1.028590	-2.365311
38	1	0	2.720950	-0.102684	-1.740190
39	1	0	2.986450	-1.703200	-2.509954
40	8	0	-0.290340	0.604049	-1.241624

Zero-point correction= 0.316804 (Hartree/Particle)
Thermal correction to Energy= 0.336819
Thermal correction to Enthalpy= 0.337764
Thermal correction to Gibbs Free Energy= 0.267055
Sum of electronic and zero-point Energies= -1411.108172
Sum of electronic and thermal Energies= -1411.088157
Sum of electronic and thermal Enthalpies= -1411.087212
Sum of electronic and thermal Free Energies= -1411.157921
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1411.73082252

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.975559	-2.102341	-0.510785
2	6	0	0.836435	-1.158037	-0.252510
3	6	0	0.983257	0.133337	0.082458
4	6	0	2.342950	0.728551	0.151760
5	6	0	3.523288	-0.156041	-0.197989

6	6	0	3.271964	-1.623009	0.141284
7	1	0	-0.168381	-1.564621	-0.346373
8	8	0	2.506463	1.908933	0.430692
9	6	0	-0.166385	1.090898	0.401395
10	8	0	-0.097412	2.242110	-0.414528
11	1	0	3.685256	-0.046255	-1.280739
12	1	0	4.409022	0.248210	0.299089
13	1	0	4.116883	-2.240044	-0.180491
14	1	0	3.187031	-1.735269	1.229276
15	1	0	1.707541	-3.102120	-0.151277
16	1	0	2.111840	-2.200719	-1.598607
17	1	0	0.764331	2.640522	-0.215066
18	1	0	-0.053471	1.376250	1.460251
19	6	0	-1.525574	0.454625	0.225873
20	6	0	-2.119935	-0.245606	1.275351
21	6	0	-2.182242	0.525519	-1.002613
22	6	0	-3.352187	-0.869747	1.102463
23	1	0	-1.615131	-0.300831	2.237340
24	6	0	-3.416225	-0.093530	-1.175726
25	1	0	-1.721957	1.082500	-1.811637
26	6	0	-4.003834	-0.794456	-0.125290
27	1	0	-3.806945	-1.406080	1.930297
28	1	0	-3.922687	-0.025597	-2.134244
29	1	0	-4.968164	-1.275259	-0.261155

Zero-point correction= 0.245930 (Hartree/Particle)
Thermal correction to Energy= 0.258576
Thermal correction to Enthalpy= 0.259520
Thermal correction to Gibbs Free Energy= 0.205952
Sum of electronic and zero-point Energies= -653.795238
Sum of electronic and thermal Energies= -653.782591
Sum of electronic and thermal Enthalpies= -653.781647
Sum of electronic and thermal Free Energies= -653.835216
ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -654.23101760

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.031413	-2.250407	-2.333511
2	8	0	-2.182160	-1.886221	-2.684291
3	8	0	-0.434951	-1.942976	-1.252393
4	6	0	-0.243295	-3.115664	-3.288461
5	1	0	-0.907607	-3.591756	-4.010577
6	1	0	0.323578	-3.866667	-2.732811
7	1	0	0.471214	-2.483744	-3.826922
8	6	0	-3.311846	-2.850187	0.528258
9	8	0	-3.976558	-2.368032	-0.424751
10	8	0	-2.202567	-2.413936	0.978096
11	6	0	-3.880876	-4.051930	1.243217
12	1	0	-3.082966	-4.755532	1.490723
13	1	0	-4.643775	-4.533310	0.630402
14	1	0	-4.335576	-3.718308	2.181847
15	6	0	-3.677247	0.815009	1.042019
16	8	0	-4.255427	0.516462	-0.032338
17	8	0	-2.506620	0.453310	1.395258
18	6	0	-4.422131	1.705151	2.008036
19	1	0	-4.571151	2.686923	1.547045
20	1	0	-3.867945	1.821327	2.940194
21	1	0	-5.410822	1.282296	2.204078
22	6	0	-1.321509	1.412029	-1.845118
23	8	0	-2.423753	0.989744	-2.283719
24	8	0	-0.694336	0.956037	-0.835381
25	6	0	-0.641334	2.529159	-2.593499
26	1	0	-0.096588	2.087143	-3.435700
27	1	0	0.070411	3.047014	-1.949425
28	1	0	-1.385119	3.219770	-2.994487
29	45	0	-3.285294	-0.682771	-1.414353
30	45	0	-1.377013	-0.729027	0.125978
31	6	0	0.213754	-0.699821	1.413184
32	6	0	0.250523	0.589497	2.080119
33	1	0	-0.536689	0.704759	2.839690
34	6	0	0.951017	-1.799361	1.962758

35	6	0	0.844129	-3.080338	1.385240
36	6	0	1.805740	-1.613429	3.072564
37	6	0	1.573783	-4.137889	1.903879
38	1	0	0.209765	-3.207658	0.517162
39	6	0	2.517220	-2.678471	3.596156
40	1	0	1.906441	-0.625837	3.513059
41	6	0	2.403850	-3.938179	3.005335
42	1	0	1.510242	-5.117809	1.442922
43	1	0	3.167952	-2.532635	4.452233
44	1	0	2.974758	-4.771264	3.405273
45	7	0	1.026906	1.555127	1.759473
46	16	0	0.711447	3.023887	2.550211
47	8	0	-0.260372	2.823086	3.623315
48	8	0	2.006025	3.618858	2.835547
49	6	0	-0.083275	3.935393	1.245791
50	6	0	-1.403205	3.625307	0.931068
51	6	0	0.612179	4.940325	0.586465
52	6	0	-2.046925	4.352494	-0.061662
53	1	0	-1.903328	2.814362	1.447539
54	6	0	-0.045990	5.669617	-0.400931
55	1	0	1.643520	5.143007	0.852140
56	6	0	-1.369997	5.379299	-0.719836
57	1	0	-3.071562	4.112017	-0.328894
58	1	0	0.477975	6.464795	-0.921929
59	1	0	-1.876304	5.948966	-1.493485
60	6	0	5.861300	1.180353	-2.528216
61	6	0	5.016576	0.321041	-1.632014
62	6	0	3.874384	0.715632	-1.043859
63	6	0	3.328686	2.065702	-1.353279
64	6	0	4.102361	2.939478	-2.323250
65	6	0	5.602667	2.667379	-2.296809
66	1	0	5.375324	-0.690021	-1.453858
67	8	0	2.261056	2.451663	-0.901258
68	6	0	3.097658	-0.156717	-0.048382
69	6	0	3.541385	-1.603283	-0.097521
70	6	0	2.976040	-2.464789	-1.041241
71	6	0	4.541748	-2.078974	0.746716
72	6	0	3.419902	-3.777944	-1.145042
73	1	0	2.162957	-2.100645	-1.659864
74	6	0	4.987193	-3.395615	0.643177
75	1	0	4.973425	-1.416507	1.493332
76	6	0	4.430269	-4.246675	-0.306668
77	1	0	2.973124	-4.441237	-1.880878
78	1	0	5.766222	-3.755640	1.309111
79	1	0	4.777079	-5.272788	-0.389152
80	1	0	3.701600	2.724685	-3.325429
81	1	0	3.856401	3.980885	-2.098673
82	1	0	6.116084	3.272278	-3.050916
83	1	0	6.008471	2.955372	-1.319195
84	1	0	6.918015	0.937699	-2.369125
85	1	0	5.645993	0.915830	-3.575012
86	8	0	1.712137	-0.129839	-0.318379
87	1	0	1.430634	0.807270	-0.356842
88	1	0	3.280859	0.253384	0.957900

Zero-point correction= 0.684264 (Hartree/Particle)
Thermal correction to Energy= 0.735259
Thermal correction to Enthalpy= 0.736203
Thermal correction to Gibbs Free Energy= 0.595074
Sum of electronic and zero-point Energies= -2929.280318
Sum of electronic and thermal Energies= -2929.229324
Sum of electronic and thermal Enthalpies= -2929.228380
Sum of electronic and thermal Free Energies= -2929.369509

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2930.69366593

INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.042963	1.608130	-1.483242
2	8	0	3.657966	0.603598	-1.925650
3	8	0	2.098908	1.599247	-0.630427
4	6	0	3.475540	2.966970	-1.978913
5	1	0	4.232780	3.359393	-1.291702

6	1	0	2.632059	3.661186	-1.982620
7	1	0	3.918605	2.886502	-2.972624
8	6	0	4.107932	-0.537757	1.395312
9	8	0	4.480819	-1.083855	0.319915
10	8	0	2.952545	-0.072228	1.648190
11	6	0	5.117643	-0.437468	2.512042
12	1	0	5.020658	0.527425	3.014289
13	1	0	6.128143	-0.573440	2.125116
14	1	0	4.908093	-1.221499	3.247150
15	6	0	1.601585	-3.108400	0.410408
16	8	0	2.510255	-3.098428	-0.462401
17	8	0	1.013763	-2.084543	0.886785
18	6	0	1.136050	-4.444250	0.931072
19	1	0	0.755207	-5.038557	0.094811
20	1	0	0.353196	-4.309450	1.678504
21	1	0	1.986617	-4.982885	1.358261
22	6	0	0.507048	-0.857380	-2.465135
23	8	0	1.631173	-1.361513	-2.692991
24	8	0	0.141716	-0.358195	-1.340979
25	6	0	-0.514322	-0.809962	-3.568282
26	1	0	-0.692196	0.235742	-3.837200
27	1	0	-1.466463	-1.203427	-3.205551
28	1	0	-0.160168	-1.363814	-4.437948
29	45	0	3.141958	-1.286691	-1.240960
30	45	0	1.504826	-0.204168	0.199827
31	6	0	-0.112354	0.851206	1.319827
32	6	0	-0.841602	-0.271663	1.846503
33	1	0	-0.360312	-0.822669	2.657436
34	6	0	0.470831	1.889078	2.204652
35	6	0	0.903882	3.116579	1.684664
36	6	0	0.640925	1.650819	3.575528
37	6	0	1.480336	4.073217	2.511796
38	1	0	0.812585	3.311147	0.623387
39	6	0	1.238723	2.602090	4.392838
40	1	0	0.315342	0.715515	4.017848
41	6	0	1.657552	3.821865	3.868722
42	1	0	1.802917	5.018209	2.084356
43	1	0	1.366451	2.390008	5.450188
44	1	0	2.113676	4.568110	4.512070
45	7	0	-1.937074	-0.692301	1.305457
46	16	0	-2.577180	-2.119668	1.890111
47	8	0	-1.614226	-2.872381	2.687639
48	8	0	-3.880556	-1.816604	2.477809
49	6	0	-2.869798	-2.946279	0.337352
50	6	0	-1.844807	-3.026513	-0.601720
51	6	0	-4.121857	-3.501524	0.099837
52	6	0	-2.082630	-3.683932	-1.802967
53	1	0	-0.888112	-2.559503	-0.397713
54	6	0	-4.349993	-4.154912	-1.109356
55	1	0	-4.900488	-3.412083	0.850099
56	6	0	-3.333669	-4.246285	-2.056781
57	1	0	-1.290578	-3.753192	-2.542730
58	1	0	-5.322566	-4.594285	-1.308191
59	1	0	-3.515841	-4.755249	-2.998520
60	6	0	-5.590036	1.334592	1.089345
61	6	0	-4.232445	1.970962	1.139150
62	6	0	-3.268466	1.723753	0.242748
63	6	0	-3.491378	0.803325	-0.897301
64	6	0	-4.862326	0.192732	-1.052204
65	6	0	-5.586652	0.032477	0.284947
66	1	0	-4.037275	2.673093	1.949594
67	8	0	-2.590771	0.599383	-1.697980
68	6	0	-1.935417	2.419734	0.280756
69	6	0	-1.750331	3.441952	-0.830600
70	6	0	-0.637948	3.431190	-1.673298
71	6	0	-2.721523	4.431483	-0.988511
72	6	0	-0.507897	4.401577	-2.663641
73	1	0	0.132534	2.675274	-1.557599
74	6	0	-2.582978	5.403080	-1.973842
75	1	0	-3.593933	4.441975	-0.340434
76	6	0	-1.475523	5.389248	-2.817634
77	1	0	0.357098	4.379726	-3.320332
78	1	0	-3.344160	6.169645	-2.083253
79	1	0	-1.369174	6.144150	-3.590650
80	1	0	-5.427464	0.862565	-1.718165

81	1	0	-4.748202	-0.762500	-1.572847
82	1	0	-6.613778	-0.304973	0.113543
83	1	0	-5.085684	-0.734200	0.882273
84	1	0	-5.932091	1.143212	2.111862
85	1	0	-6.297872	2.061282	0.660723
86	8	0	-0.827602	1.461498	0.175219
87	1	0	-0.918639	0.821529	-0.602150
88	1	0	-1.776104	2.889265	1.254282

Zero-point correction= 0.688634 (Hartree/Particle)
Thermal correction to Energy= 0.738600
Thermal correction to Enthalpy= 0.739545
Thermal correction to Gibbs Free Energy= 0.604090
Sum of electronic and zero-point Energies= -2929.302191
Sum of electronic and thermal Energies= -2929.252225
Sum of electronic and thermal Enthalpies= -2929.251280
Sum of electronic and thermal Free Energies= -2929.386735
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2930.71731618

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.953367	1.853899	-1.805487
2	8	0	3.238734	0.920956	-2.595443
3	8	0	2.385913	1.733607	-0.670093
4	6	0	3.283733	3.259961	-2.244590
5	1	0	2.568154	3.561622	-3.016538
6	1	0	4.281217	3.284774	-2.688668
7	1	0	3.220077	3.956370	-1.407133
8	6	0	4.548135	-0.830672	0.253089
9	8	0	4.563146	-1.122470	-0.970510
10	8	0	3.543750	-0.418701	0.920181
11	6	0	5.827634	-1.004374	1.033243
12	1	0	5.935426	-0.201729	1.765761
13	1	0	6.683449	-1.030535	0.357734
14	1	0	5.778168	-1.952806	1.578419
15	6	0	1.638190	-3.036065	-0.333367
16	8	0	2.314221	-2.918203	-1.386721
17	8	0	1.215702	-2.079149	0.394899
18	6	0	1.271869	-4.428243	0.117357
19	1	0	0.752563	-4.401108	1.076666
20	1	0	2.179942	-5.032345	0.194557
21	1	0	0.633653	-4.894596	-0.639946
22	6	0	0.004575	-0.342704	-2.357728
23	8	0	0.963214	-0.868108	-2.978962
24	8	0	0.026874	0.099236	-1.162409
25	6	0	-1.317409	-0.223004	-3.070949
26	1	0	-1.704634	0.793162	-2.953683
27	1	0	-2.030853	-0.904919	-2.595893
28	1	0	-1.211525	-0.475028	-4.126379
29	45	0	2.805968	-1.027561	-2.054594
30	45	0	1.741073	-0.130137	-0.034888
31	6	0	0.902025	0.512476	1.768850
32	6	0	0.040714	-0.544646	2.280767
33	1	0	0.628854	-1.435879	2.542276
34	6	0	1.487702	1.433896	2.720857
35	6	0	2.608484	2.207770	2.366695
36	6	0	0.942837	1.570569	4.014596
37	6	0	3.168495	3.084648	3.284587
38	1	0	3.021377	2.111409	1.370991
39	6	0	1.503582	2.451247	4.925207
40	1	0	0.065392	0.993581	4.290273
41	6	0	2.619090	3.205914	4.559863
42	1	0	4.035792	3.676012	3.008119
43	1	0	1.076374	2.552154	5.917613
44	1	0	3.061585	3.893169	5.275334
45	7	0	-1.236201	-0.563849	2.353167
46	16	0	-1.924863	-2.060160	2.784600
47	8	0	-0.893408	-3.084990	2.924885
48	8	0	-2.846722	-1.793274	3.874848
49	6	0	-2.843156	-2.352795	1.291412
50	6	0	-2.168835	-2.846864	0.178355

51	6	0	-4.191069	-2.012895	1.246827
52	6	0	-2.875132	-3.025682	-1.005971
53	1	0	-1.108697	-3.061759	0.241069
54	6	0	-4.884842	-2.192306	0.054137
55	1	0	-4.673076	-1.596680	2.123735
56	6	0	-4.229796	-2.698809	-1.065449
57	1	0	-2.366717	-3.417866	-1.882088
58	1	0	-5.929151	-1.904464	-0.010375
59	1	0	-4.776668	-2.823673	-1.995083
60	6	0	-1.838646	4.107419	-2.068087
61	6	0	-2.749056	3.069948	-1.473863
62	6	0	-2.407981	2.238669	-0.474479
63	6	0	-1.084312	2.403671	0.171287
64	6	0	-0.165555	3.495363	-0.314218
65	6	0	-0.368903	3.790715	-1.795122
66	1	0	-3.743278	2.985526	-1.907364
67	8	0	-0.788362	1.708402	1.139131
68	6	0	-3.273368	1.092978	0.060156
69	6	0	-4.651008	1.020237	-0.572347
70	6	0	-5.784167	1.329707	0.177836
71	6	0	-4.814158	0.595628	-1.892961
72	6	0	-7.055540	1.206940	-0.379215
73	1	0	-5.657683	1.639802	1.208496
74	6	0	-6.081347	0.475735	-2.453481
75	1	0	-3.940991	0.335245	-2.483359
76	6	0	-7.210237	0.778381	-1.694590
77	1	0	-7.929541	1.443673	0.221065
78	1	0	-6.188001	0.136578	-3.480137
79	1	0	-8.202059	0.679332	-2.126076
80	1	0	-0.404344	4.387166	0.285582
81	1	0	0.860233	3.200773	-0.087300
82	1	0	0.271302	4.620490	-2.112062
83	1	0	-0.070231	2.907192	-2.374050
84	1	0	-2.030782	4.180365	-3.144707
85	1	0	-2.097308	5.091850	-1.648456
86	8	0	-3.429903	1.175156	1.454956
87	1	0	-2.601702	0.841962	1.845777
88	1	0	-2.732693	0.167150	-0.200583

Zero-point correction= 0.684704 (Hartree/Particle)
Thermal correction to Energy= 0.735485
Thermal correction to Enthalpy= 0.736429
Thermal correction to Gibbs Free Energy= 0.597481
Sum of electronic and zero-point Energies= -2929.279644
Sum of electronic and thermal Energies= -2929.228863
Sum of electronic and thermal Enthalpies= -2929.227919
Sum of electronic and thermal Free Energies= -2929.366867

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2930.69233259

INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.739119	1.743859	-0.728991
2	8	0	3.958753	1.117863	-1.795829
3	8	0	2.889546	1.432096	0.168918
4	6	0	4.529553	3.003552	-0.468937
5	1	0	3.866429	3.868354	-0.579663
6	1	0	5.355643	3.091269	-1.174956
7	1	0	4.901699	3.001758	0.558527
8	6	0	3.935785	-1.921774	0.162277
9	8	0	4.195681	-1.712814	-1.050659
10	8	0	2.947228	-1.448672	0.814239
11	6	0	4.854303	-2.835989	0.933370
12	1	0	5.790123	-2.980389	0.392712
13	1	0	4.359305	-3.804625	1.058320
14	1	0	5.042805	-2.428128	1.929144
15	6	0	0.826282	-2.566147	-1.599154
16	8	0	1.742671	-2.313140	-2.424810
17	8	0	0.472983	-1.823362	-0.624395
18	6	0	0.049841	-3.846417	-1.780400
19	1	0	0.676337	-4.592661	-2.271684
20	1	0	-0.816293	-3.653381	-2.423576

21	1	0	-0.309081	-4.208132	-0.814418
22	6	0	0.555276	1.120273	-2.510210
23	8	0	1.446460	0.540540	-3.175089
24	8	0	0.389809	1.047011	-1.246465
25	6	0	-0.417741	1.987590	-3.273481
26	1	0	0.136066	2.730375	-3.854307
27	1	0	-1.118022	2.483545	-2.598981
28	1	0	-0.969672	1.364552	-3.983858
29	45	0	2.881314	-0.608191	-2.197700
30	45	0	1.632353	-0.185360	-0.135971
31	6	0	0.516245	0.210368	1.714372
32	6	0	-0.072824	-1.104224	2.026538
33	1	0	0.634309	-1.917902	2.204087
34	6	0	1.216507	0.853945	2.886836
35	6	0	2.588149	0.709031	3.098760
36	6	0	0.455971	1.574016	3.818501
37	6	0	3.188801	1.296012	4.209325
38	1	0	3.177371	0.136750	2.393417
39	6	0	1.063180	2.174537	4.915372
40	1	0	-0.621172	1.652907	3.689644
41	6	0	2.435479	2.039300	5.112741
42	1	0	4.257328	1.175725	4.362834
43	1	0	0.460393	2.733206	5.625353
44	1	0	2.911603	2.502162	5.971972
45	7	0	-1.346671	-1.271592	2.010553
46	16	0	-1.984063	-2.831676	2.094679
47	8	0	-1.005180	-3.818814	1.652404
48	8	0	-2.640310	-2.991214	3.383604
49	6	0	-3.239517	-2.599788	0.848656
50	6	0	-2.848154	-2.274856	-0.449014
51	6	0	-4.577722	-2.659523	1.214589
52	6	0	-3.827372	-2.002440	-1.396075
53	1	0	-1.792572	-2.188052	-0.687737
54	6	0	-5.549247	-2.384707	0.254108
55	1	0	-4.844259	-2.894877	2.239233
56	6	0	-5.176009	-2.050956	-1.043695
57	1	0	-3.539963	-1.725659	-2.405813
58	1	0	-6.598964	-2.413261	0.528481
59	1	0	-5.934390	-1.802025	-1.779491
60	6	0	-1.345274	4.771760	-0.165587
61	6	0	-2.327391	3.637177	-0.204739
62	6	0	-2.045056	2.390057	0.214507
63	6	0	-0.734893	2.141571	0.790234
64	6	0	0.316499	3.186153	0.893170
65	6	0	0.103022	4.276898	-0.153653
66	1	0	-3.323531	3.839215	-0.593286
67	8	0	-0.628437	0.982742	1.282413
68	6	0	-2.987425	1.184183	0.214775
69	6	0	-4.238106	1.386247	-0.614106
70	6	0	-5.489546	1.464437	-0.009360
71	6	0	-4.149339	1.433000	-2.007279
72	6	0	-6.637828	1.589449	-0.788665
73	1	0	-5.551391	1.394725	1.070616
74	6	0	-5.293945	1.558600	-2.786960
75	1	0	-3.175798	1.346892	-2.484746
76	6	0	-6.544948	1.636788	-2.176799
77	1	0	-7.610394	1.643077	-0.307752
78	1	0	-5.211866	1.585852	-3.869812
79	1	0	-7.441878	1.729748	-2.782207
80	1	0	0.245268	3.592266	1.915065
81	1	0	1.304472	2.721667	0.810572
82	1	0	0.789266	5.107278	0.035210
83	1	0	0.354035	3.862931	-1.136291
84	1	0	-1.519188	5.432856	-1.021363
85	1	0	-1.552338	5.378096	0.729832
86	8	0	-3.314533	0.854265	1.542131
87	1	0	-2.718664	0.126612	1.809998
88	1	0	-2.423740	0.361120	-0.246455

Zero-point correction= 0.687748 (Hartree/Particle)
Thermal correction to Energy= 0.738278
Thermal correction to Enthalpy= 0.739222
Thermal correction to Gibbs Free Energy= 0.600109
Sum of electronic and zero-point Energies= -2929.299669
Sum of electronic and thermal Energies= -2929.249139

Sum of electronic and thermal Enthalpies= -2929.248195
Sum of electronic and thermal Free Energies= -2929.387308
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2930.71487922

TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.559095	-0.916211	1.207226
2	6	0	0.757834	0.334950	1.825869
3	1	0	0.237047	0.638212	2.729602
4	7	0	1.549524	1.141317	1.149781
5	16	0	1.831981	2.695542	1.649232
6	8	0	3.278897	2.840079	1.770099
7	8	0	0.981880	3.000587	2.792654
8	6	0	1.305530	3.661782	0.254297
9	6	0	2.248315	4.117147	-0.660559
10	6	0	-0.047262	3.957014	0.120310
11	6	0	1.820457	4.905457	-1.725720
12	1	0	3.294566	3.865419	-0.530418
13	6	0	-0.464870	4.736622	-0.951030
14	1	0	-0.750073	3.572175	0.847561
15	6	0	0.470301	5.216665	-1.867352
16	1	0	2.544162	5.274347	-2.445573
17	1	0	-1.519310	4.963269	-1.072601
18	6	0	0.324291	-2.214963	1.855883
19	6	0	0.170677	-2.295666	3.245131
20	6	0	0.206971	-3.385959	1.094199
21	6	0	-0.114843	-3.511731	3.853871
22	1	0	0.267277	-1.404306	3.857364
23	6	0	-0.049338	-4.603191	1.712406
24	1	0	0.288842	-3.327931	0.014212
25	6	0	-0.219248	-4.673051	3.092798
26	1	0	-0.241020	-3.552913	4.931736
27	1	0	-0.129759	-5.501478	1.107278
28	1	0	-0.426698	-5.624840	3.572237
29	6	0	5.665795	-0.315722	2.092303
30	6	0	4.480821	-1.106832	1.624733
31	6	0	3.839637	-0.851319	0.474239
32	6	0	4.217080	0.320807	-0.367285
33	6	0	5.442294	1.107914	0.038558
34	6	0	6.409848	0.310323	0.910505
35	1	0	4.123323	-1.913845	2.264295
36	8	0	3.504703	0.665166	-1.294566
37	6	0	2.676429	-1.694380	0.021389
38	8	0	1.430794	-0.907910	0.025410
39	1	0	5.054686	1.967958	0.601948
40	1	0	5.914132	1.494378	-0.869651
41	1	0	7.213810	0.959523	1.270492
42	1	0	6.877087	-0.487476	0.319183
43	1	0	6.329576	-0.955079	2.684046
44	1	0	5.304877	0.473901	2.768227
45	1	0	0.142396	5.830257	-2.701176
46	6	0	2.827640	-2.292592	-1.361931
47	6	0	1.858593	-2.120597	-2.349118
48	6	0	3.958180	-3.065403	-1.628658
49	6	0	2.028392	-2.720528	-3.594344
50	1	0	0.978835	-1.522924	-2.140635
51	6	0	4.121356	-3.664444	-2.873315
52	1	0	4.717588	-3.195323	-0.861095
53	6	0	3.154999	-3.493001	-3.861180
54	1	0	1.274193	-2.575640	-4.362908
55	1	0	5.005525	-4.262979	-3.071398
56	1	0	3.282170	-3.957477	-4.834385
57	1	0	2.515546	-2.493470	0.747514
58	6	0	-2.089421	-2.036499	-1.962892
59	8	0	-3.111241	-1.332559	-2.178864
60	8	0	-1.217963	-1.836131	-1.060528
61	6	0	-1.877540	-3.253028	-2.830049
62	1	0	-0.810127	-3.449358	-2.954018
63	1	0	-2.327688	-4.118159	-2.331388
64	1	0	-2.363670	-3.120130	-3.797752
65	6	0	-0.996929	1.429391	-2.063602
66	8	0	-2.246695	1.442829	-2.237909

67	8	0	-0.385235	0.891894	-1.087506
68	6	0	-0.125556	2.054464	-3.120477
69	1	0	0.833783	2.349974	-2.694082
70	1	0	0.055639	1.302626	-3.896920
71	1	0	-0.629498	2.907369	-3.577220
72	6	0	-2.860979	2.086467	1.244484
73	8	0	-3.688156	1.921882	0.308731
74	8	0	-1.829932	1.378214	1.468133
75	6	0	-3.112172	3.222079	2.206665
76	1	0	-3.468608	4.100991	1.664622
77	1	0	-3.898821	2.919465	2.905678
78	1	0	-2.207731	3.454176	2.772034
79	6	0	-3.854484	-1.474139	1.277448
80	8	0	-4.485683	-0.886530	0.353576
81	8	0	-2.607648	-1.405246	1.500394
82	6	0	-4.665608	-2.331361	2.218062
83	1	0	-4.011373	-2.938890	2.844360
84	1	0	-5.278445	-1.682198	2.851547
85	1	0	-5.342517	-2.966416	1.641585
86	45	0	-3.451773	0.316606	-0.975778
87	45	0	-1.438935	-0.253016	0.252521
88	1	0	1.686292	0.176337	0.061898

Zero-point correction= 0.685511 (Hartree/Particle)
Thermal correction to Energy= 0.735087
Thermal correction to Enthalpy= 0.736032
Thermal correction to Gibbs Free Energy= 0.600557
Sum of electronic and zero-point Energies= -2929.294981
Sum of electronic and thermal Energies= -2929.245405
Sum of electronic and thermal Enthalpies= -2929.244461
Sum of electronic and thermal Free Energies= -2929.379936

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -2930.70917371

INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.023074	2.469951	1.946775
2	6	0	1.659020	1.244273	1.368944
3	6	0	1.059093	0.046070	1.292797
4	6	0	-0.350413	-0.121410	1.730432
5	6	0	-1.084219	1.117681	2.191248
6	6	0	-0.157222	2.132928	2.856479
7	8	0	-0.908869	-1.206967	1.662029
8	6	0	1.663956	-1.165657	0.624019
9	1	0	1.247479	-2.041774	1.133489
10	8	0	1.184472	-1.311012	-0.734754
11	6	0	3.177112	-1.290913	0.672625
12	6	0	3.865286	-1.879231	-0.389801
13	6	0	3.892347	-0.941156	1.820666
14	6	0	5.241445	-2.074261	-0.323329
15	1	0	3.312246	-2.190004	-1.269637
16	6	0	5.268063	-1.139253	1.889592
17	1	0	3.372405	-0.509411	2.670833
18	6	0	5.950063	-1.700417	0.814344
19	1	0	5.758703	-2.528068	-1.163645
20	1	0	5.806343	-0.854447	2.788948
21	1	0	7.023785	-1.853358	0.867296
22	1	0	-1.903329	0.808650	2.843748
23	1	0	-1.546906	1.552652	1.292440
24	1	0	0.224860	1.711705	3.794910
25	1	0	-0.711685	3.040204	3.116370
26	1	0	0.696823	3.094391	1.100665
27	1	0	1.775854	3.059569	2.481941
28	6	0	-0.795262	-0.484382	-1.635607
29	6	0	0.496510	-0.281005	-1.336994
30	1	0	-1.338062	0.195657	-2.280885
31	7	0	-1.500735	-1.616804	-1.226738
32	1	0	-1.131269	-2.093203	-0.406401
33	16	0	-3.165673	-1.626467	-1.308505
34	8	0	-3.508028	-1.104827	-2.619537
35	8	0	-3.563719	-2.943656	-0.854712
36	6	0	-3.754491	-0.434380	-0.112695

37	6	0	-3.939547	0.889132	-0.506298
38	6	0	-4.031049	-0.850162	1.185928
39	6	0	-4.407037	1.812764	0.423744
40	1	0	-3.755034	1.177121	-1.535860
41	6	0	-4.513618	0.078154	2.102133
42	1	0	-3.881032	-1.886847	1.463909
43	6	0	-4.697204	1.406251	1.724384
44	1	0	-4.564877	2.844882	0.126506
45	1	0	-4.745186	-0.237765	3.114551
46	6	0	1.212655	0.955107	-1.709925
47	6	0	0.543756	2.186904	-1.717056
48	6	0	2.575932	0.934886	-2.019413
49	6	0	1.213697	3.359460	-2.045926
50	1	0	-0.504927	2.225718	-1.433074
51	6	0	3.249483	2.110893	-2.330892
52	1	0	3.110468	-0.007275	-2.008799
53	6	0	2.573068	3.327454	-2.348569
54	1	0	0.677080	4.303946	-2.047675
55	1	0	4.309532	2.073193	-2.563983
56	1	0	3.100865	4.244941	-2.590594
57	1	0	2.658669	1.357920	0.954083
58	1	0	-5.074741	2.126330	2.444258

Zero-point correction= 0.472651 (Hartree/Particle)
Thermal correction to Energy= 0.500578
Thermal correction to Enthalpy= 0.501522
Thermal correction to Gibbs Free Energy= 0.413018
Sum of electronic and zero-point Energies= -1796.744667
Sum of electronic and thermal Energies= -1796.716740
Sum of electronic and thermal Enthalpies= -1796.715796
Sum of electronic and thermal Free Energies= -1796.804300

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1797.61739313

TS14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.887370	-0.468178	2.216655
2	6	0	0.278462	-0.568768	1.259257
3	6	0	0.243059	-1.489204	0.209236
4	6	0	-1.064534	-2.109207	-0.149683
5	6	0	-2.092069	-2.258215	0.962224
6	6	0	-1.591524	-1.822440	2.336784
7	8	0	-1.310583	-2.522004	-1.271492
8	6	0	1.268755	-1.614612	-0.751402
9	1	0	0.942394	-2.114783	-1.660247
10	8	0	1.202510	0.199073	-1.569846
11	6	0	2.721938	-1.694843	-0.503717
12	6	0	3.578079	-1.720093	-1.612725
13	6	0	3.280587	-1.780776	0.774120
14	6	0	4.953808	-1.775110	-1.448273
15	1	0	3.148182	-1.658071	-2.608237
16	6	0	4.660315	-1.833060	0.941087
17	1	0	2.635158	-1.826136	1.644607
18	6	0	5.501115	-1.819478	-0.166814
19	1	0	5.602978	-1.781488	-2.318910
20	1	0	5.078884	-1.890899	1.941196
21	1	0	6.578121	-1.859475	-0.034053
22	1	0	-2.428436	-3.300392	0.955259
23	1	0	-2.958495	-1.655849	0.670845
24	1	0	-0.890064	-2.563016	2.739908
25	1	0	-2.430527	-1.754549	3.037638
26	1	0	-1.619238	0.264265	1.851216
27	1	0	-0.539009	-0.110574	3.190748
28	6	0	-0.102281	1.299423	-0.045115
29	6	0	1.145248	1.055426	-0.614993
30	1	0	-0.283767	2.065317	0.697673
31	7	0	-1.239687	0.858557	-0.732781
32	1	0	-1.014401	0.380953	-1.605071
33	16	0	-2.623025	1.801999	-0.814010
34	8	0	-2.491612	2.819411	0.216403
35	8	0	-2.861021	2.134438	-2.206636
36	6	0	-3.891803	0.660922	-0.309214
37	6	0	-4.397378	0.739460	0.984217

38	6	0	-4.333841	-0.302547	-1.212008
39	6	0	-5.361806	-0.180149	1.385346
40	1	0	-4.042007	1.514201	1.655160
41	6	0	-5.294468	-1.218141	-0.797419
42	1	0	-3.929312	-0.337816	-2.217799
43	6	0	-5.805796	-1.157535	0.497740
44	1	0	-5.770979	-0.128185	2.389307
45	1	0	-5.641220	-1.980283	-1.487286
46	6	0	2.398637	1.592047	-0.017706
47	6	0	2.452553	2.155374	1.262558
48	6	0	3.576351	1.512246	-0.766375
49	6	0	3.657076	2.615460	1.782903
50	1	0	1.556146	2.223798	1.872872
51	6	0	4.779651	1.966913	-0.244866
52	1	0	3.533007	1.072490	-1.755754
53	6	0	4.825579	2.519146	1.032946
54	1	0	3.682775	3.045317	2.779849
55	1	0	5.686519	1.885700	-0.836446
56	1	0	5.766649	2.873197	1.443156
57	1	0	1.233945	-0.201862	1.616444
58	1	0	-6.555496	-1.875448	0.815531

Zero-point correction= 0.470097 (Hartree/Particle)
Thermal correction to Energy= 0.497746
Thermal correction to Enthalpy= 0.498690
Thermal correction to Gibbs Free Energy= 0.411042
Sum of electronic and zero-point Energies= -1796.706956
Sum of electronic and thermal Energies= -1796.679307
Sum of electronic and thermal Enthalpies= -1796.678363
Sum of electronic and thermal Free Energies= -1796.766011

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1797.57950209

5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.958649	0.372442	2.106505
2	6	0	-0.119120	0.439178	0.998189
3	6	0	0.009403	1.664592	0.109516
4	6	0	1.375769	2.259991	-0.080625
5	6	0	2.285999	2.236945	1.137319
6	6	0	1.579734	1.736122	2.395192
7	8	0	1.718094	2.799917	-1.114291
8	6	0	-0.993897	2.272281	-0.542131
9	1	0	-0.698427	3.064856	-1.229217
10	8	0	-1.296545	-0.917595	-1.898445
11	6	0	-2.444578	2.003410	-0.462154
12	6	0	-3.185037	1.900285	-1.645462
13	6	0	-3.117653	1.901775	0.760011
14	6	0	-4.555035	1.671151	-1.606724
15	1	0	-2.674010	1.982887	-2.600298
16	6	0	-4.488504	1.671952	0.799649
17	1	0	-2.568137	2.031339	1.687880
18	6	0	-5.210182	1.551902	-0.383554
19	1	0	-5.111602	1.583792	-2.535197
20	1	0	-4.992516	1.588178	1.757503
21	1	0	-6.280156	1.369401	-0.352503
22	1	0	2.688302	3.248469	1.257275
23	1	0	3.139931	1.590999	0.903379
24	1	0	0.804894	2.448945	2.706930
25	1	0	2.294491	1.660597	3.221229
26	1	0	1.763599	-0.305176	1.799301
27	1	0	0.518189	-0.062753	3.010407
28	6	0	-0.035162	-0.844356	0.117351
29	6	0	-1.317507	-1.076424	-0.691785
30	1	0	0.125540	-1.707107	0.772349
31	7	0	1.077461	-0.747234	-0.815076
32	1	0	0.740286	-0.620610	-1.770757
33	16	0	2.330119	-1.845868	-0.781884
34	8	0	2.095343	-2.785463	0.306975
35	8	0	2.537948	-2.290187	-2.149214
36	6	0	3.727106	-0.837369	-0.321827
37	6	0	4.347000	-1.049343	0.903786
38	6	0	4.160251	0.154873	-1.198208

39	6	0	5.421819	-0.239696	1.264359
40	1	0	3.986600	-1.836692	1.557146
41	6	0	5.231780	0.957433	-0.827500
42	1	0	3.657407	0.307068	-2.147100
43	6	0	5.860706	0.760766	0.401924
44	1	0	5.915043	-0.393358	2.218976
45	1	0	5.569840	1.742429	-1.495708
46	6	0	-2.565921	-1.475838	0.016781
47	6	0	-2.601946	-1.785276	1.381022
48	6	0	-3.742115	-1.549168	-0.733864
49	6	0	-3.800697	-2.142355	1.985548
50	1	0	-1.697765	-1.759119	1.981518
51	6	0	-4.938166	-1.910203	-0.129758
52	1	0	-3.696135	-1.308042	-1.789776
53	6	0	-4.970236	-2.201643	1.231420
54	1	0	-3.821755	-2.380031	3.044569
55	1	0	-5.848824	-1.957524	-0.718837
56	1	0	-5.906421	-2.480939	1.705775
57	1	0	-1.101343	0.449405	1.472776
58	1	0	6.695356	1.393584	0.687992

Zero-point correction= 0.472893 (Hartree/Particle)
Thermal correction to Energy= 0.500886
Thermal correction to Enthalpy= 0.501830
Thermal correction to Gibbs Free Energy= 0.412950
Sum of electronic and zero-point Energies= -1796.774424
Sum of electronic and thermal Energies= -1796.746431
Sum of electronic and thermal Enthalpies= -1796.745487
Sum of electronic and thermal Free Energies= -1796.834367

ωB97XD/6-311++G(d,p)/SMD//ωB97XD/6-31G(d)-LANL2DZ energy in toluene solvent = -1797.65084552