Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Computational Insights into Different Chemoselectivities in Rh_2(II)-Catalyzed *N*-Aryl Nitrene and Analogous Rh_2(II)/Cu(I)-Catalyzed Aryl-Substituted Carbene Involved Reactions

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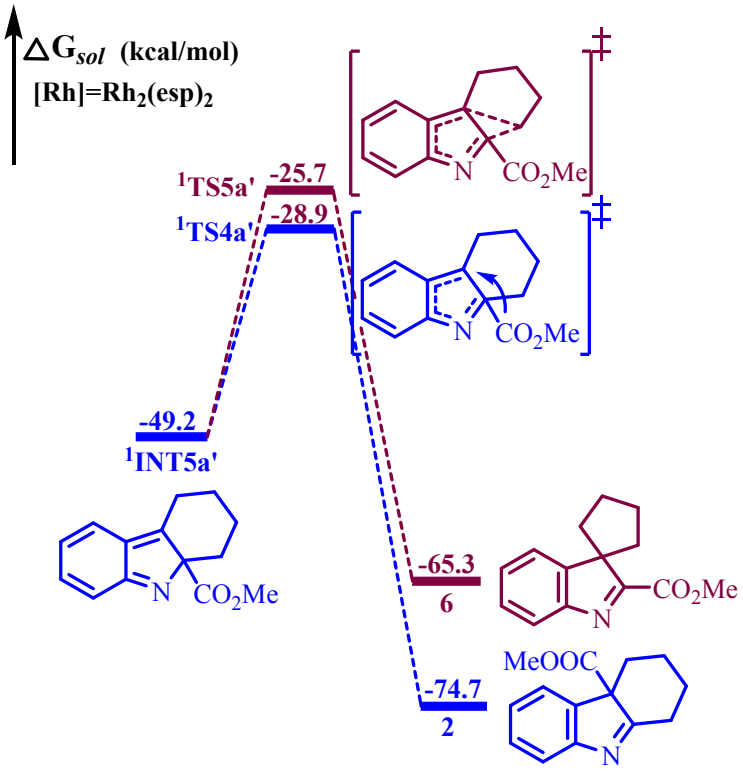

Figure S1. Energy profiles (in kcal · mol^{-1}) for the migration of the ester group and the alkyl group in the absence of the Rh_2(II) catalyst. Bond lengths are shown in Å.

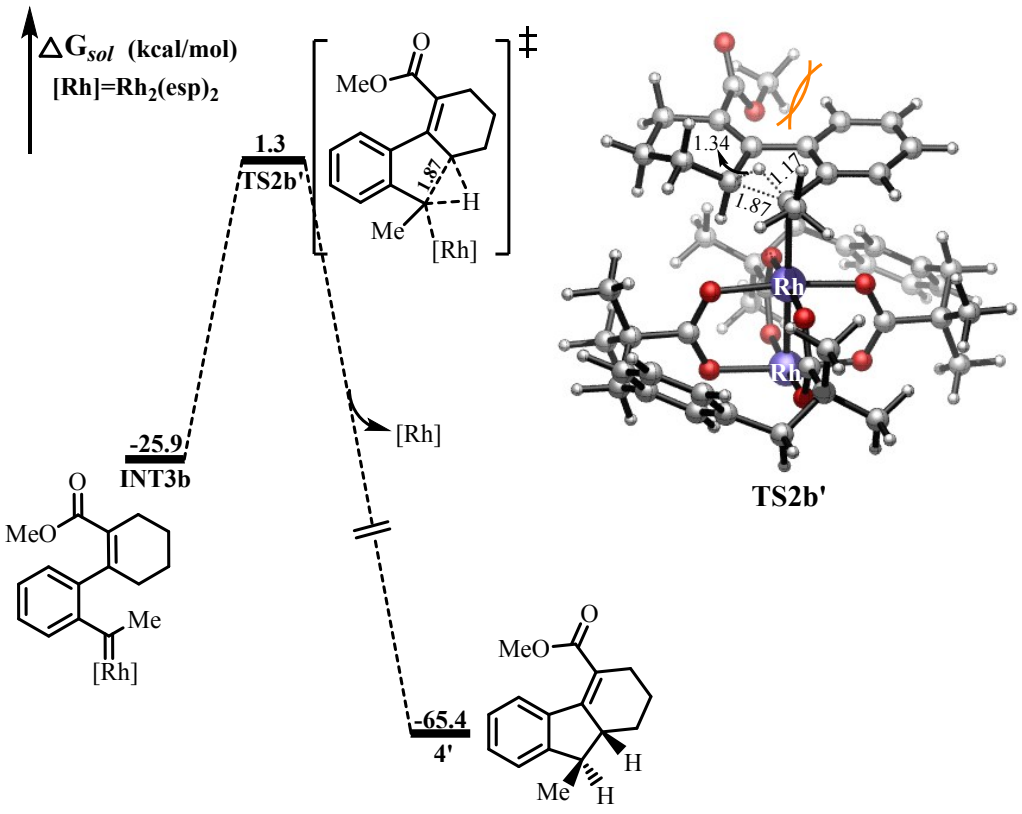

Figure S2. Energy profiles (in kcal · mol^{-1}) for the formation of the diastereoisomers product **4'** from the Rh_2(II)-carbenoid **INT3b**. Bond lengths are shown in Å.

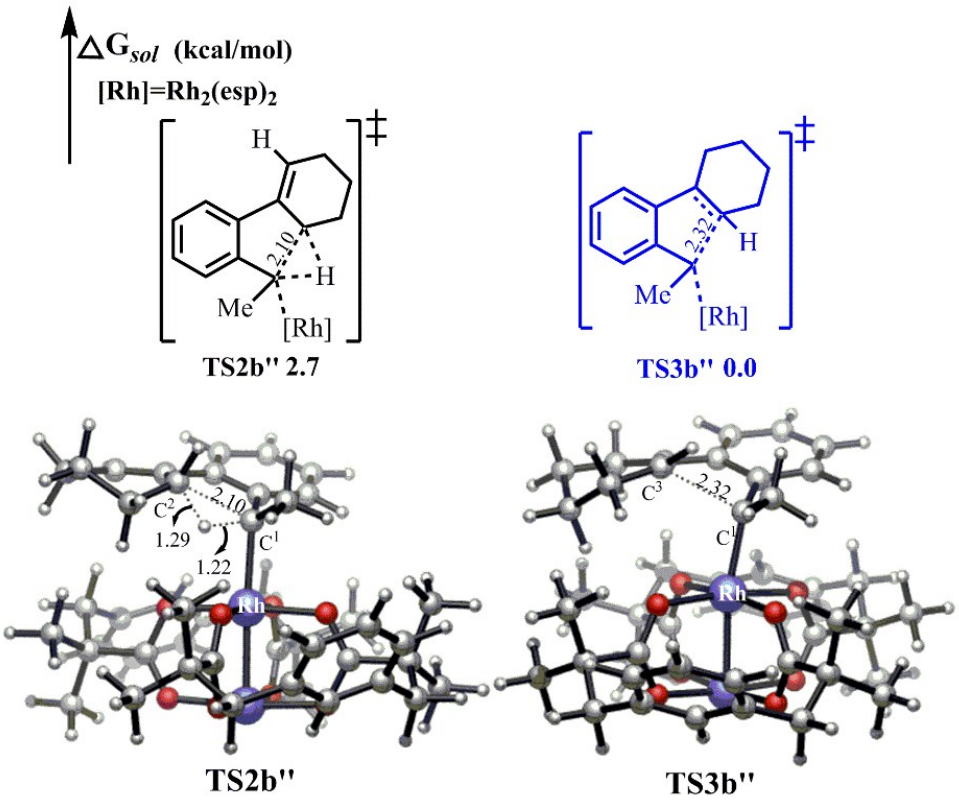

Figure S3. The energy difference between the C—H insertion and the cyclization pathway of the model substrate replacing the ester group with H. Bond lengths are shown in Å.

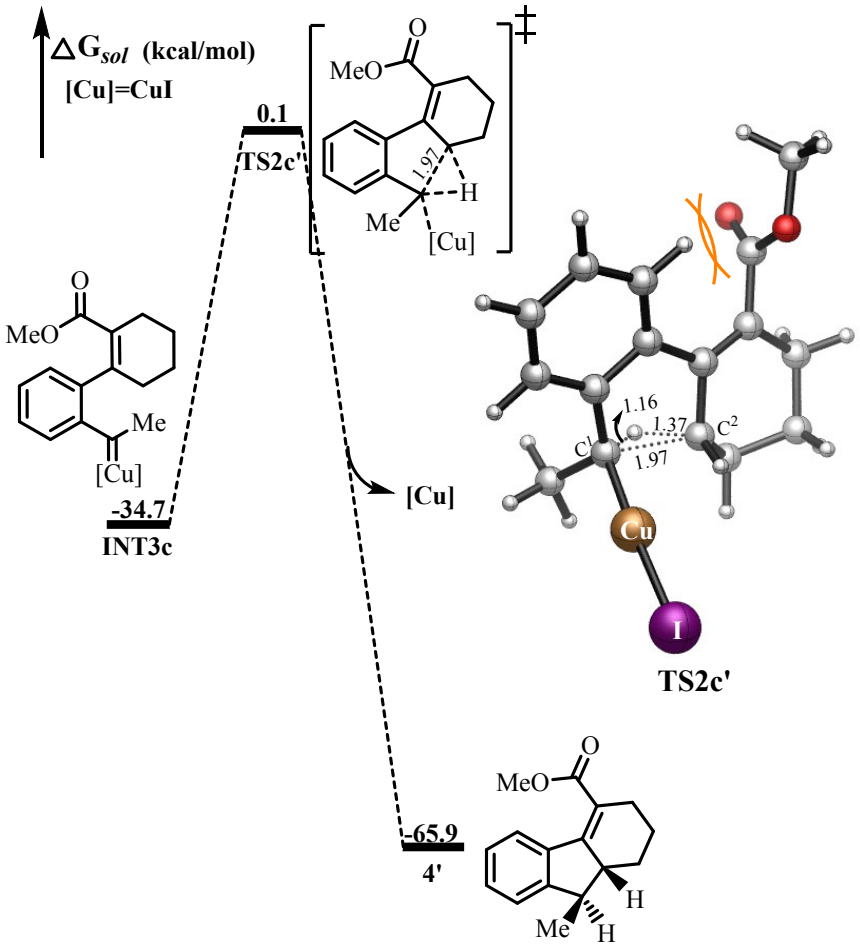

Figure S4. Energy profiles (in kcal · mol^{-1}) for the formation of the diastereoisomers product **4'** from the Cu(I)-carbenoid **INT3c**. Bond lengths are shown in Å.

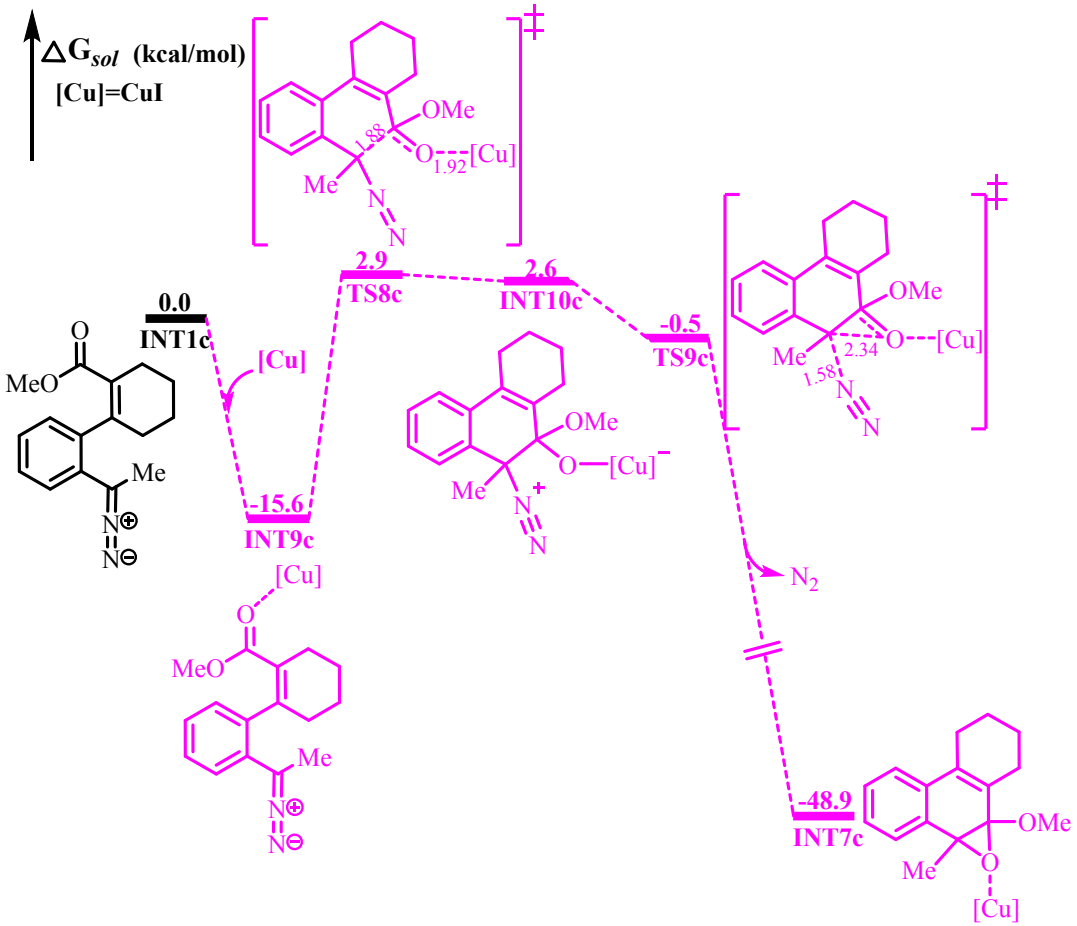

Figure S5. Energy profiles (in kcal · mol^{-1}) for the formation of **INT7c** via a noncarbene pathway. Bond lengths are shown in Å.

Cartesian Coordinates and Energies

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.085084	-1.048008	0.245741
2	6	0	1.701835	-1.012797	0.413028
3	6	0	0.876448	-0.489791	-0.593855
4	6	0	1.480834	0.025179	-1.742215
5	6	0	2.861577	0.007836	-1.905655
6	6	0	3.664286	-0.540780	-0.910304
7	1	0	3.692589	-1.465162	1.042017
8	1	0	0.843128	0.437056	-2.519509
9	1	0	3.305511	0.412111	-2.809861
10	1	0	4.743114	-0.568922	-1.027747
11	7	0	0.196558	-1.112144	2.147365
12	7	0	-0.713844	-0.814797	2.752836
13	6	0	-0.611050	-0.542089	-0.509282
14	6	0	-1.379349	0.541785	-0.318854
15	6	0	-1.209410	-1.914900	-0.736764
16	6	0	-2.888252	0.513110	-0.380575
17	6	0	-2.693297	-1.985467	-0.382624
18	1	0	-1.051618	-2.185652	-1.790930
19	6	0	-3.429621	-0.785331	-0.975265
20	1	0	-3.280402	0.651531	0.637416
21	1	0	-2.807488	-1.978891	0.709123
22	1	0	-4.506554	-0.857121	-0.791248
23	1	0	-0.635342	-2.649198	-0.157373
24	6	0	-0.803546	1.892882	-0.045281
25	8	0	-1.263412	2.924336	-0.482177
26	8	0	0.253748	1.850408	0.779703
27	6	0	0.892910	3.101033	1.024497
28	1	0	1.260795	3.531046	0.089555
29	1	0	0.198224	3.803029	1.491835
30	1	0	1.723186	2.877950	1.693714
31	1	0	-3.223837	1.382779	-0.954854
32	1	0	-3.289621	-0.777131	-2.064359
33	1	0	-3.117918	-2.927093	-0.746149
34	7	0	1.221979	-1.567384	1.631601

Zero-point correction= 0.277509 (Hartree/Particle)
Thermal correction to Energy= 0.294703
Thermal correction to Enthalpy= 0.295647
Thermal correction to Gibbs Free Energy= 0.231099
Sum of electronic and zero-point Energies= -856.615416
Sum of electronic and thermal Energies= -856.598222
Sum of electronic and thermal Enthalpies= -856.597278
Sum of electronic and thermal Free Energies= -856.661826
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -857.11730689

$Rh_2(esp)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.040985	-0.000001	-1.185049
2	45	0	-0.040985	-0.000001	1.185048
3	8	0	1.477674	-1.449891	-1.085622
4	6	0	1.843500	-1.880276	0.047403
5	8	0	1.391144	-1.474222	1.163161

6	8	0	-1.391144	-1.474222	-1.163162
7	6	0	-1.843500	-1.880276	-0.047403
8	8	0	-1.477674	-1.449891	1.085622
9	8	0	-1.391143	1.474221	-1.163161
10	6	0	-1.843502	1.880272	-0.047403
11	8	0	-1.477676	1.449887	1.085622
12	8	0	1.477676	1.449887	-1.085622
13	6	0	1.843502	1.880272	0.047402
14	8	0	1.391143	1.474221	1.163161
15	6	0	2.896057	-2.987361	0.091898
16	6	0	2.896054	2.987362	0.091897
17	6	0	3.367333	-3.342906	-1.320452
18	1	0	4.127466	-4.130705	-1.263219
19	1	0	2.536027	-3.709489	-1.929053
20	6	0	3.367326	3.342909	-1.320454
21	1	0	2.536018	3.709489	-1.929053
22	1	0	4.127456	4.130711	-1.263222
23	6	0	4.084098	2.511598	0.976024
24	1	0	4.827159	3.318384	0.980546
25	1	0	3.721788	2.396872	2.002744
26	6	0	2.248335	4.217433	0.753050
27	1	0	1.887945	3.982206	1.758263
28	1	0	2.982926	5.027251	0.823731
29	1	0	1.402878	4.579642	0.157150
30	6	0	2.248341	-4.217435	0.753049
31	1	0	2.982936	-5.027250	0.823732
32	1	0	1.887949	-3.982210	1.758262
33	1	0	1.402888	-4.579648	0.157147
34	6	0	4.084098	-2.511594	0.976028
35	1	0	3.721785	-2.396866	2.002747
36	1	0	4.827160	-3.318379	0.980553
37	6	0	-2.896057	-2.987362	-0.091898
38	6	0	-2.896054	2.987362	-0.091897
39	6	0	-4.084098	-2.511594	-0.976027
40	1	0	-4.827160	-3.318379	-0.980552
41	6	0	-4.084099	2.511598	-0.976024
42	1	0	-4.827160	3.318384	-0.980545
43	1	0	-3.721789	2.396872	-2.002744
44	6	0	-4.720311	1.220165	-0.517824
45	6	0	-5.779742	1.206809	0.391881
46	6	0	-4.221248	0.000002	-0.976957
47	6	0	-6.309815	0.000001	0.838553
48	1	0	-6.193661	2.146255	0.750104
49	6	0	-4.720311	-1.220161	-0.517826
50	1	0	-3.412563	0.000004	-1.701773
51	6	0	-5.779741	-1.206807	0.391879
52	1	0	-7.139075	0.000000	1.540084
53	1	0	-6.193660	-2.146253	0.750101
54	6	0	-2.248341	-4.217435	-0.753050
55	1	0	-1.402887	-4.579648	-0.157149
56	1	0	-2.982936	-5.027250	-0.823733
57	1	0	-1.887949	-3.982209	-1.758263
58	6	0	-3.367332	-3.342907	1.320451
59	1	0	-4.127465	-4.130706	1.263219
60	1	0	-2.536026	-3.709490	1.929052
61	1	0	-3.799306	-2.478043	1.829390
62	6	0	-2.248335	4.217433	-0.753051
63	1	0	-2.982926	5.027251	-0.823732
64	1	0	-1.402878	4.579642	-0.157152
65	1	0	-1.887946	3.982205	-1.758265
66	6	0	-3.367325	3.342910	1.320453
67	1	0	-2.536017	3.709490	1.929052
68	1	0	-4.127455	4.130712	1.263221
69	1	0	-3.799302	2.478048	1.829394
70	1	0	-3.721786	-2.396866	-2.002746
71	1	0	3.799307	-2.478042	-1.829390
72	1	0	3.799303	2.478047	-1.829393

73	6	0	4.720311	1.220165	0.517825
74	6	0	4.221248	0.000002	0.976958
75	6	0	5.779742	1.206809	-0.391879
76	6	0	4.720311	-1.220161	0.517827
77	1	0	3.412562	0.000004	1.701773
78	6	0	6.309816	0.000001	-0.838551
79	1	0	6.193662	2.146255	-0.750102
80	6	0	5.779742	-1.206807	-0.391877
81	1	0	7.139077	0.000000	-1.540081
82	1	0	6.193661	-2.146253	-0.750099

Zero-point correction= 0.686389 (Hartree/Particle)
Thermal correction to Energy= 0.726415
Thermal correction to Enthalpy= 0.727360
Thermal correction to Gibbs Free Energy= 0.619211
Sum of electronic and zero-point Energies= -2065.494325
Sum of electronic and thermal Energies= -2065.454299
Sum of electronic and thermal Enthalpies= -2065.453355
Sum of electronic and thermal Free Energies= -2065.561503
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy=-2066.68790829

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)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -109.51208290

INT1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.592463	0.595292	-2.365874
2	6	0	-2.084223	1.548142	-1.489270
3	6	0	-2.914594	2.488865	-0.872154
4	6	0	-4.276815	2.458293	-1.175444
5	6	0	-4.798511	1.508480	-2.048190
6	6	0	-3.955454	0.572255	-2.639197
7	1	0	-1.913867	-0.129073	-2.800783
8	1	0	-4.929488	3.188444	-0.705332
9	1	0	-5.863050	1.497035	-2.259934
10	1	0	-4.355046	-0.177348	-3.315197
11	7	0	-0.003310	2.518559	-1.239922
12	7	0	0.726249	3.377098	-1.242728
13	6	0	-2.393492	3.449129	0.141048
14	6	0	-2.219423	4.759964	-0.095959
15	6	0	-2.139578	2.838751	1.500872
16	6	0	-1.830871	5.749936	0.978198
17	6	0	-1.368111	3.766083	2.434264
18	1	0	-3.114950	2.574427	1.938303
19	6	0	-1.958630	5.173760	2.387334

20	1	0	-0.795103	6.072389	0.797365
21	1	0	-0.319554	3.802888	2.113048
22	1	0	-1.459358	5.834125	3.104079
23	1	0	-1.610695	1.887787	1.369337
24	6	0	-2.427770	5.372491	-1.442197
25	8	0	-2.875196	6.484071	-1.616100
26	8	0	-2.023702	4.580849	-2.449081
27	6	0	-2.254645	5.087681	-3.761604
28	1	0	-3.321988	5.258398	-3.922557
29	1	0	-1.716076	6.026617	-3.910573
30	1	0	-1.884574	4.319595	-4.439928
31	1	0	-2.450523	6.644423	0.857806
32	1	0	-3.018338	5.131388	2.672574
33	1	0	-1.378664	3.363262	3.453258
34	7	0	-0.679621	1.472777	-1.205762
35	45	0	1.310503	-2.169916	0.858715
36	45	0	0.292953	-0.291059	-0.224587
37	8	0	0.197540	-3.404724	-0.342054
38	6	0	-0.559942	-2.887921	-1.208933
39	8	0	-0.697366	-1.640824	-1.413835
40	8	0	2.760149	-2.098051	-0.600006
41	6	0	2.716508	-1.193904	-1.486812
42	8	0	1.826947	-0.295636	-1.574694
43	8	0	2.332842	-0.810162	2.017788
44	6	0	2.156919	0.431559	1.845300
45	8	0	1.364375	0.948220	0.999719
46	8	0	-0.222550	-2.145838	2.219112
47	6	0	-1.131980	-1.278787	2.103588
48	8	0	-1.174495	-0.374872	1.209605
49	6	0	-1.369100	-3.810542	-2.121769
50	6	0	-2.271281	-1.277130	3.123896
51	6	0	-1.216213	-5.270833	-1.690424
52	1	0	-1.808744	-5.912358	-2.353394
53	1	0	-0.170954	-5.586271	-1.747464
54	6	0	-2.207235	-2.526121	4.006759
55	1	0	-1.274016	-2.552233	4.575623
56	1	0	-3.044611	-2.516595	4.714538
57	6	0	-3.626827	-1.186644	2.367155
58	1	0	-4.418935	-1.135573	3.124617
59	1	0	-3.647177	-0.245407	1.807790
60	6	0	-2.102068	-0.020289	3.997574
61	1	0	-2.154432	0.890648	3.396189
62	1	0	-2.895651	0.015416	4.752349
63	1	0	-1.138735	-0.036350	4.519837
64	6	0	-0.823806	-3.626835	-3.550281
65	1	0	-1.381422	-4.263906	-4.245923
66	1	0	-0.916683	-2.586939	-3.877679
67	1	0	0.232918	-3.912172	-3.603171
68	6	0	-2.860914	-3.371165	-2.098989
69	1	0	-2.927128	-2.356931	-2.505461
70	1	0	-3.402457	-4.033214	-2.786224
71	6	0	3.821294	-1.208247	-2.544328
72	6	0	2.952104	1.374276	2.749678
73	6	0	5.199674	-1.150755	-1.827145
74	1	0	5.971609	-1.157745	-2.606653
75	6	0	4.460794	1.014216	2.645814
76	1	0	5.003059	1.696972	3.311692
77	1	0	4.599181	0.001006	3.036137
78	6	0	5.021899	1.099543	1.245697
79	6	0	5.581923	2.280054	0.752223
80	6	0	4.949970	-0.008181	0.399617
81	6	0	6.041238	2.347501	-0.559660
82	1	0	5.661429	3.149549	1.400283
83	6	0	5.380273	0.049015	-0.927168
84	1	0	4.532810	-0.936037	0.779304
85	6	0	5.935263	1.241061	-1.397339
86	1	0	6.483649	3.267305	-0.931423

87	1	0	6.289743	1.301146	-2.423536
88	6	0	3.714297	-2.541661	-3.305706
89	1	0	2.750300	-2.618579	-3.821742
90	1	0	4.506877	-2.602989	-4.059949
91	1	0	3.810674	-3.391874	-2.624882
92	6	0	3.659288	-0.038215	-3.518018
93	1	0	4.464906	-0.067797	-4.261166
94	1	0	2.702514	-0.098399	-4.044465
95	1	0	3.697583	0.923855	-3.001279
96	6	0	2.480249	1.129045	4.194418
97	1	0	3.039477	1.773490	4.881956
98	1	0	1.415054	1.365647	4.300496
99	1	0	2.633932	0.086561	4.486835
100	6	0	2.710372	2.835843	2.366202
101	1	0	1.660201	3.103561	2.506543
102	1	0	3.317561	3.486906	3.006047
103	1	0	2.970835	3.030385	1.323131
104	1	0	5.319654	-2.068605	-1.242619
105	1	0	-1.556377	-5.423705	-0.663343
106	1	0	-2.263623	-3.442189	3.414162
107	6	0	-3.881333	-2.344665	1.429985
108	6	0	-3.390320	-2.310236	0.123276
109	6	0	-4.554693	-3.490453	1.859561
110	6	0	-3.503260	-3.408184	-0.732177
111	1	0	-2.893889	-1.412547	-0.231285
112	6	0	-4.710312	-4.579262	1.007272
113	1	0	-4.957149	-3.530116	2.868918
114	6	0	-4.177855	-4.543304	-0.277797
115	1	0	-5.242742	-5.462446	1.348522
116	1	0	-4.287157	-5.402671	-0.935053

Zero-point correction= 0.964205 (Hartree/Particle)
Thermal correction to Energy= 1.023487
Thermal correction to Enthalpy= 1.024431
Thermal correction to Gibbs Free Energy= 0.871539
Sum of electronic and zero-point Energies= -2922.141029
Sum of electronic and thermal Energies= -2922.081748
Sum of electronic and thermal Enthalpies= -2922.080803
Sum of electronic and thermal Free Energies= -2922.233695
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2923.84102124

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.568775	0.644679	-2.442042
2	6	0	-1.893710	1.463093	-1.515879
3	6	0	-2.635249	2.351599	-0.700897
4	6	0	-4.024034	2.302550	-0.766965
5	6	0	-4.688552	1.387983	-1.584521
6	6	0	-3.956304	0.562718	-2.427831
7	1	0	-1.974156	0.036333	-3.113081
8	1	0	-4.594803	3.002591	-0.163350
9	1	0	-5.773182	1.353653	-1.586930
10	1	0	-4.460422	-0.121271	-3.103610
11	7	0	0.364169	2.729035	-1.291301
12	7	0	1.367728	3.183591	-1.197546
13	6	0	-1.993663	3.422429	0.112938
14	6	0	-1.980177	4.703797	-0.299549
15	6	0	-1.472660	3.020674	1.470050
16	6	0	-1.522469	5.853151	0.568406
17	6	0	-0.672050	4.123578	2.154473
18	1	0	-2.342474	2.741048	2.082742

19	6	0	-1.397163	5.461880	2.039241
20	1	0	-0.554429	6.218511	0.194183
21	1	0	0.308469	4.209375	1.669110
22	1	0	-0.867283	6.246193	2.589768
23	1	0	-0.878818	2.107087	1.372708
24	6	0	-2.489734	5.116015	-1.642967
25	8	0	-3.159126	6.106432	-1.836461
26	8	0	-2.092766	4.293348	-2.624941
27	6	0	-2.639232	4.559626	-3.914337
28	1	0	-3.729940	4.495008	-3.884145
29	1	0	-2.348334	5.555140	-4.258406
30	1	0	-2.230326	3.789697	-4.567599
31	1	0	-2.229714	6.678375	0.435093
32	1	0	-2.397762	5.374817	2.483183
33	1	0	-0.489555	3.854643	3.201060
34	7	0	-0.543230	1.196753	-1.499500
35	45	0	1.180129	-2.155102	0.926273
36	45	0	0.283948	-0.235290	-0.231435
37	8	0	-0.030184	-3.371377	-0.190936
38	6	0	-0.763536	-2.836733	-1.065548
39	8	0	-0.808332	-1.593011	-1.326951
40	8	0	2.607512	-2.254741	-0.552918
41	6	0	2.623218	-1.381042	-1.469894
42	8	0	1.810175	-0.415348	-1.580572
43	8	0	2.317820	-0.826812	2.008946
44	6	0	2.236904	0.414076	1.787175
45	8	0	1.465570	0.957494	0.934412
46	8	0	-0.333016	-1.962558	2.294438
47	6	0	-1.190624	-1.051132	2.141013
48	8	0	-1.177516	-0.174414	1.217649
49	6	0	-1.655411	-3.733090	-1.926241
50	6	0	-2.328398	-0.952659	3.159769
51	6	0	-1.648896	-5.169393	-1.398093
52	1	0	-2.296274	-5.792610	-2.026310
53	1	0	-0.639326	-5.588155	-1.418437
54	6	0	-2.383359	-2.213218	4.027918
55	1	0	-1.459171	-2.332043	4.599247
56	1	0	-3.219647	-2.134109	4.732709
57	6	0	-3.671173	-0.724778	2.410229
58	1	0	-4.446546	-0.571550	3.171288
59	1	0	-3.592946	0.200075	1.828787
60	6	0	-2.031409	0.266409	4.052500
61	1	0	-1.985625	1.186696	3.465850
62	1	0	-2.818155	0.373723	4.807622
63	1	0	-1.075900	0.140825	4.574217
64	6	0	-1.078542	-3.696016	-3.354169
65	1	0	-1.686009	-4.322340	-4.017060
66	1	0	-1.069146	-2.675231	-3.748349
67	1	0	-0.052941	-4.081674	-3.369600
68	6	0	-3.097165	-3.153165	-1.958333
69	1	0	-3.054926	-2.160698	-2.416281
70	1	0	-3.687550	-3.796081	-2.623255
71	6	0	3.705370	-1.521890	-2.542048
72	6	0	3.122586	1.325224	2.638574
73	6	0	5.095287	-1.559774	-1.846455
74	1	0	5.851060	-1.660563	-2.635268
75	6	0	4.592395	0.828215	2.544396
76	1	0	5.197002	1.485938	3.181163
77	1	0	4.643257	-0.177220	2.973789
78	6	0	5.148789	0.809919	1.139904
79	6	0	5.806456	1.916814	0.598444
80	6	0	4.972232	-0.318441	0.337708
81	6	0	6.257460	1.893906	-0.717887
82	1	0	5.968841	2.799482	1.212387
83	6	0	5.392318	-0.349148	-0.993266
84	1	0	4.479711	-1.191060	0.755791
85	6	0	6.045388	0.770808	-1.512122

86	1	0	6.776194	2.756102	-1.127233
87	1	0	6.392590	0.761078	-2.542512
88	6	0	3.472058	-2.864809	-3.257131
89	1	0	2.495649	-2.875213	-3.755101
90	1	0	4.242621	-3.017222	-4.021253
91	1	0	3.508540	-3.698219	-2.550121
92	6	0	3.626220	-0.374009	-3.551697
93	1	0	4.412052	-0.497084	-4.306457
94	1	0	2.657342	-0.366916	-4.058686
95	1	0	3.756796	0.597211	-3.068224
96	6	0	2.642775	1.189493	4.095462
97	1	0	3.260642	1.815142	4.749257
98	1	0	1.602440	1.521119	4.194466
99	1	0	2.709055	0.152537	4.436321
100	6	0	3.009046	2.782805	2.190226
101	1	0	1.988658	3.147825	2.324600
102	1	0	3.677443	3.405196	2.796689
103	1	0	3.278561	2.905798	1.138491
104	1	0	5.145084	-2.463498	-1.230572
105	1	0	-2.012364	-5.219431	-0.368657
106	1	0	-2.523222	-3.113382	3.424870
107	6	0	-4.058016	-1.871556	1.504438
108	6	0	-3.540503	-1.947700	0.210015
109	6	0	-4.877148	-2.908254	1.957230
110	6	0	-3.767477	-3.056958	-0.607658
111	1	0	-2.931924	-1.130977	-0.162126
112	6	0	-5.147511	-4.002277	1.140927
113	1	0	-5.300154	-2.860648	2.957868
114	6	0	-4.585585	-4.082851	-0.129646
115	1	0	-5.790982	-4.800294	1.500265
116	1	0	-4.783068	-4.949113	-0.756670

Zero-point correction= 0.960340 (Hartree/Particle)
Thermal correction to Energy= 1.019822
Thermal correction to Enthalpy= 1.020766
Thermal correction to Gibbs Free Energy= 0.868018
Sum of electronic and zero-point Energies= -2922.090688
Sum of electronic and thermal Energies= -2922.031205
Sum of electronic and thermal Enthalpies= -2922.030261
Sum of electronic and thermal Free Energies= -2922.183009
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2923.78609236

[1]INT2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.920925	3.207220	-1.051553
2	6	0	0.393829	2.887170	-0.585001
3	6	0	1.390289	3.935747	-0.513223
4	6	0	1.017913	5.234336	-0.841929
5	6	0	-0.278555	5.504823	-1.274006
6	6	0	-1.252207	4.499784	-1.384961
7	1	0	-1.625390	2.389513	-1.148176
8	1	0	1.744776	6.038619	-0.784775
9	1	0	-0.539829	6.525386	-1.541263
10	1	0	-2.250202	4.745389	-1.733278
11	6	0	2.741738	3.641910	0.017358
12	6	0	3.624854	2.802014	-0.550779
13	6	0	3.018069	4.316288	1.351047
14	6	0	4.937452	2.427500	0.093504
15	6	0	4.126737	3.621114	2.139580
16	1	0	3.281715	5.369865	1.172776
17	6	0	5.329913	3.356526	1.239510

18	1	0	4.835773	1.393894	0.452632
19	1	0	3.744712	2.668207	2.527301
20	1	0	6.151875	2.911820	1.810438
21	1	0	2.091448	4.329702	1.936695
22	6	0	3.349099	2.050776	-1.809372
23	8	0	3.931680	1.030635	-2.102002
24	8	0	2.419542	2.622240	-2.590470
25	6	0	1.880765	1.786927	-3.615604
26	1	0	2.675864	1.392985	-4.252674
27	1	0	1.334720	0.957010	-3.157427
28	1	0	1.206319	2.424015	-4.188022
29	1	0	5.721514	2.396157	-0.670761
30	1	0	5.699370	4.309460	0.836661
31	1	0	4.405462	4.236106	3.002146
32	7	0	0.775529	1.680123	-0.208895
33	45	0	-1.162555	-2.177645	0.484962
34	45	0	-0.200494	0.007180	-0.024519
35	8	0	-2.537136	-1.787352	-1.004031
36	6	0	-2.497327	-0.709886	-1.647457
37	8	0	-1.647271	0.229211	-1.478275
38	8	0	0.093704	-2.974170	-0.938148
39	6	0	0.834911	-2.201093	-1.606865
40	8	0	0.930184	-0.945066	-1.443797
41	8	0	0.269112	-2.382769	1.959174
42	6	0	1.084475	-1.434293	2.143857
43	8	0	1.149713	-0.369053	1.462185
44	8	0	-2.365922	-1.238155	1.860587
45	6	0	-2.264786	0.003068	2.030124
46	8	0	-1.474856	0.779121	1.395827
47	6	0	-3.532928	-0.483000	-2.752515
48	6	0	-3.138984	0.662790	3.100641
49	6	0	-4.492942	-1.671744	-2.840337
50	1	0	-5.228100	-1.491308	-3.633726
51	1	0	-3.951478	-2.592679	-3.073028
52	6	0	-4.048605	-0.374714	3.763333
53	1	0	-3.458569	-1.157908	4.246939
54	1	0	-4.666789	0.114874	4.525352
55	6	0	-3.977051	1.797926	2.448384
56	1	0	-4.610059	2.227717	3.234696
57	1	0	-3.289884	2.584817	2.119221
58	6	0	-2.199769	1.283349	4.150067
59	1	0	-1.528047	2.015303	3.692835
60	1	0	-2.788632	1.781979	4.928403
61	1	0	-1.590361	0.509784	4.630979
62	6	0	-2.771330	-0.324046	-4.080409
63	1	0	-3.479679	-0.147755	-4.897882
64	1	0	-2.071262	0.515237	-4.034752
65	1	0	-2.204622	-1.232341	-4.314429
66	6	0	-4.307487	0.833651	-2.462801
67	1	0	-3.605782	1.670710	-2.552144
68	1	0	-5.051464	0.954102	-3.260158
69	6	0	1.702697	-2.835064	-2.696790
70	6	0	2.100870	-1.575365	3.280650
71	6	0	2.765087	-3.729780	-1.994063
72	1	0	3.460788	-4.076002	-2.768608
73	6	0	3.096803	-2.708019	2.895784
74	1	0	3.889624	-2.718071	3.654445
75	1	0	2.567789	-3.664349	2.967495
76	6	0	3.686393	-2.570443	1.512762
77	6	0	4.818911	-1.792710	1.260155
78	6	0	3.059706	-3.200909	0.438314
79	6	0	5.289786	-1.637766	-0.040146
80	1	0	5.336165	-1.309968	2.086151
81	6	0	3.517873	-3.055908	-0.871816
82	1	0	2.177464	-3.808709	0.624336
83	6	0	4.643277	-2.263710	-1.101472
84	1	0	6.165945	-1.024909	-0.230823

85	1	0	5.016457	-2.132687	-2.113307
86	6	0	0.811960	-3.728958	-3.574277
87	1	0	0.056352	-3.132472	-4.098730
88	1	0	1.425175	-4.234961	-4.328790
89	1	0	0.296532	-4.483248	-2.974631
90	6	0	2.374102	-1.765393	-3.561133
91	1	0	3.027050	-2.250467	-4.296703
92	1	0	1.620251	-1.191629	-4.111120
93	1	0	2.964841	-1.062098	-2.970028
94	6	0	1.357384	-1.981433	4.561924
95	1	0	2.075726	-2.141578	5.374214
96	1	0	0.662292	-1.194167	4.875927
97	1	0	0.786388	-2.900761	4.409542
98	6	0	2.841370	-0.252215	3.503021
99	1	0	2.142052	0.541698	3.783847
100	1	0	3.571975	-0.372462	4.312031
101	1	0	3.361510	0.070849	2.598324
102	1	0	2.255168	-4.614712	-1.598801
103	1	0	-5.024510	-1.828085	-1.898735
104	1	0	-4.705760	-0.856154	3.035181
105	6	0	-4.826165	1.354806	1.280257
106	6	0	-4.276889	1.346941	-0.001544
107	6	0	-6.141728	0.915670	1.439943
108	6	0	-4.982557	0.884663	-1.111879
109	1	0	-3.257976	1.694403	-0.126562
110	6	0	-6.872315	0.471248	0.341228
111	1	0	-6.596511	0.924088	2.427448
112	6	0	-6.296888	0.450628	-0.926205
113	1	0	-7.897755	0.138328	0.473653
114	1	0	-6.872879	0.097836	-1.778227

Zero-point correction= 0.953331 (Hartree/Particle)
Thermal correction to Energy= 1.010351
Thermal correction to Enthalpy= 1.011295
Thermal correction to Gibbs Free Energy= 0.864857
Sum of electronic and zero-point Energies= -2812.644540
Sum of electronic and thermal Energies= -2812.587521
Sum of electronic and thermal Enthalpies= -2812.586577
Sum of electronic and thermal Free Energies= -2812.733015
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.30426757

^{3}INT2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.638051	2.375802	-0.568220
2	6	0	1.258250	2.730139	-0.689090
3	6	0	0.880841	4.103982	-0.876377
4	6	0	1.885446	5.055987	-0.946844
5	6	0	3.230671	4.702034	-0.807079
6	6	0	3.599092	3.362831	-0.622575
7	1	0	2.898692	1.332056	-0.432474
8	1	0	1.618128	6.099556	-1.087807
9	1	0	3.993567	5.473321	-0.846710
10	1	0	4.645248	3.089752	-0.525234
11	6	0	-0.553378	4.443639	-1.088850
12	6	0	-1.546252	4.198827	-0.210338
13	6	0	-0.836715	5.003094	-2.469601
14	6	0	-3.007700	4.379269	-0.554711
15	6	0	-2.262979	5.515637	-2.651409
16	1	0	-0.110802	5.797350	-2.685027
17	6	0	-3.251617	4.518748	-2.053819
18	1	0	-3.555332	3.523839	-0.147897

19	1	0	-2.460983	5.683884	-3.715415
20	1	0	-3.120200	3.541477	-2.537761
21	1	0	-0.623475	4.207137	-3.198555
22	6	0	-1.329906	3.680331	1.174052
23	8	0	-2.211444	3.174155	1.836611
24	8	0	-0.087286	3.862116	1.633835
25	6	0	0.224310	3.189647	2.851133
26	1	0	-0.454304	3.498997	3.650090
27	1	0	0.155703	2.108652	2.700215
28	1	0	1.249713	3.475744	3.083688
29	1	0	-3.395647	5.260435	-0.023729
30	1	0	-4.284820	4.832284	-2.235932
31	1	0	-2.374452	6.483903	-2.145523
32	7	0	0.314661	1.810854	-0.612819
33	45	0	0.076718	-2.477141	0.427738
34	45	0	0.075781	-0.131054	-0.138944
35	8	0	-1.368842	-2.734930	-1.000066
36	6	0	-1.755823	-1.748119	-1.684876
37	8	0	-1.332048	-0.554828	-1.562730
38	8	0	1.502391	-2.761913	-1.042442
39	6	0	1.881669	-1.762531	-1.718401
40	8	0	1.505193	-0.566192	-1.538006
41	8	0	1.517457	-2.072812	1.847780
42	6	0	1.888738	-0.876011	2.010965
43	8	0	1.480461	0.119717	1.339509
44	8	0	-1.366828	-2.048496	1.818551
45	6	0	-1.774195	-0.860484	1.956200
46	8	0	-1.351861	0.140924	1.295271
47	6	0	-2.802580	-1.978458	-2.775117
48	6	0	-2.842277	-0.566487	3.008969
49	6	0	-3.279142	-3.432754	-2.768419
50	1	0	-4.034827	-3.572787	-3.550415
51	1	0	-2.448216	-4.116099	-2.964569
52	6	0	-3.312158	-1.862314	3.673513
53	1	0	-2.484385	-2.362366	4.184561
54	1	0	-4.086796	-1.631094	4.414136
55	6	0	-4.023203	0.189443	2.334467
56	1	0	-4.770289	0.376537	3.116064
57	1	0	-3.654181	1.162362	1.996144
58	6	0	-2.212187	0.370719	4.055967
59	1	0	-1.938527	1.325489	3.599914
60	1	0	-2.934493	0.562142	4.857613
61	1	0	-1.322164	-0.085150	4.506841
62	6	0	-2.140414	-1.650081	-4.125679
63	1	0	-2.865830	-1.783497	-4.936146
64	1	0	-1.777067	-0.618709	-4.145333
65	1	0	-1.294001	-2.319731	-4.317230
66	6	0	-3.987001	-0.996319	-2.547601
67	1	0	-3.615569	0.024636	-2.683741
68	1	0	-4.721042	-1.185441	-3.340901
69	6	0	2.893444	-2.002656	-2.840491
70	6	0	2.931604	-0.607167	3.098729
71	6	0	4.230124	-2.461855	-2.190221
72	1	0	4.977230	-2.528730	-2.990646
73	6	0	4.246730	-1.329652	2.689815
74	1	0	5.010430	-1.060163	3.429795
75	1	0	4.082496	-2.408930	2.772506
76	6	0	4.729915	-1.009596	1.295476
77	6	0	5.541517	0.094685	1.023983
78	6	0	4.341957	-1.827213	0.233773
79	6	0	5.943994	0.366941	-0.280889
80	1	0	5.872337	0.733824	1.838791
81	6	0	4.724556	-1.562989	-1.082142
82	1	0	3.715088	-2.691711	0.436435
83	6	0	5.536215	-0.453793	-1.329525
84	1	0	6.593462	1.215129	-0.480616
85	1	0	5.861824	-0.239818	-2.344358

86	6	0	2.366811	-3.129735	-3.742417
87	1	0	1.433760	-2.831034	-4.233441
88	1	0	3.102109	-3.355017	-4.523156
89	1	0	2.175244	-4.038176	-3.165728
90	6	0	3.098299	-0.727138	-3.663540
91	1	0	3.824691	-0.920686	-4.461690
92	1	0	2.158932	-0.405209	-4.122633
93	1	0	3.463777	0.098436	-3.048200
94	6	0	2.425327	-1.210850	4.418541
95	1	0	3.175768	-1.068224	5.204325
96	1	0	1.499976	-0.720575	4.741837
97	1	0	2.226170	-2.280017	4.310952
98	6	0	3.168364	0.895075	3.272718
99	1	0	2.261640	1.386555	3.634398
100	1	0	3.960511	1.057050	4.013100
101	1	0	3.456435	1.376819	2.335213
102	1	0	4.087688	-3.472908	-1.794416
103	1	0	-3.717811	-3.707544	-1.806309
104	1	0	-3.725930	-2.562533	2.943610
105	6	0	-4.656408	-0.550160	1.180499
106	6	0	-4.144044	-0.393232	-0.108978
107	6	0	-5.728723	-1.425055	1.368889
108	6	0	-4.641666	-1.120545	-1.191875
109	1	0	-3.323712	0.300899	-0.267406
110	6	0	-6.260217	-2.132441	0.294755
111	1	0	-6.151598	-1.548967	2.362980
112	6	0	-5.715420	-1.987480	-0.977528
113	1	0	-7.101172	-2.802363	0.450300
114	1	0	-6.127102	-2.550238	-1.812005

Zero-point correction= 0.952432 (Hartree/Particle)
Thermal correction to Energy= 1.009406
Thermal correction to Enthalpy= 1.010350
Thermal correction to Gibbs Free Energy= 0.863392
Sum of electronic and zero-point Energies= -2812.673411
Sum of electronic and thermal Energies= -2812.616438
Sum of electronic and thermal Enthalpies= -2812.615493
Sum of electronic and thermal Free Energies= -2812.762451
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.32936180

^{3}TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.932752	-0.010490	-1.791465
2	6	0	-2.031075	1.094835	-1.855623
3	6	0	-2.559584	2.416233	-2.098800
4	6	0	-3.912181	2.558632	-2.374551
5	6	0	-4.766305	1.456174	-2.353749
6	6	0	-4.274644	0.180046	-2.041393
7	1	0	-2.531209	-0.989688	-1.555530
8	1	0	-4.308518	3.546524	-2.593316
9	1	0	-5.820936	1.591889	-2.573153
10	1	0	-4.947617	-0.670248	-1.998759
11	6	0	-1.617713	3.537001	-1.938507
12	6	0	-1.879391	4.648072	-1.210797
13	6	0	-0.263038	3.251929	-2.453487
14	6	0	-0.820567	5.708435	-1.013755
15	6	0	0.872339	4.189689	-2.088079
16	6	0	0.547241	5.037166	-0.859838
17	1	0	-0.812361	6.401143	-1.866590
18	1	0	1.066130	4.852595	-2.943324
19	1	0	1.328758	5.788477	-0.704738

20	6	0	-3.183893	4.891236	-0.530823
21	8	0	-3.830948	5.906712	-0.658842
22	8	0	-3.533609	3.883477	0.281459
23	6	0	-4.817231	3.998932	0.889508
24	1	0	-4.887186	4.917515	1.476924
25	1	0	-5.598357	4.003592	0.123601
26	1	0	-4.917469	3.121669	1.527571
27	1	0	-1.058755	6.310908	-0.131974
28	1	0	0.525533	4.398213	0.030608
29	1	0	1.793337	3.615656	-1.929444
30	1	0	-0.154711	2.085768	-1.924049
31	1	0	-0.256558	2.937622	-3.502427
32	7	0	-0.724353	0.908296	-1.661757
33	45	0	1.207847	-1.806025	1.333749
34	45	0	0.265776	-0.378657	-0.370131
35	8	0	2.014084	-0.120169	2.180222
36	6	0	1.804716	1.007170	1.655486
37	8	0	1.112778	1.219083	0.608580
38	8	0	-0.512817	-1.488004	2.444066
39	6	0	-1.405450	-0.729234	1.967125
40	8	0	-1.365803	-0.169776	0.832512
41	8	0	0.360226	-3.408464	0.344033
42	6	0	-0.287609	-3.198822	-0.721202
43	8	0	-0.510841	-2.062174	-1.236746
44	8	0	2.861804	-1.986950	0.132565
45	6	0	2.901241	-1.394937	-0.981596
46	8	0	1.975507	-0.671105	-1.468029
47	6	0	2.399659	2.244301	2.331352
48	6	0	4.147421	-1.568264	-1.852539
49	6	0	3.303463	1.843101	3.499448
50	1	0	3.721521	2.743968	3.964347
51	1	0	2.739485	1.292632	4.257153
52	6	0	5.226299	-2.356350	-1.106139
53	1	0	4.868570	-3.356167	-0.845823
54	1	0	6.111216	-2.460241	-1.745332
55	6	0	4.669523	-0.166386	-2.276375
56	1	0	5.549017	-0.326956	-2.912360
57	1	0	3.903141	0.310685	-2.895648
58	6	0	3.717292	-2.336003	-3.116118
59	1	0	2.935440	-1.795714	-3.657471
60	1	0	4.578069	-2.469672	-3.781093
61	1	0	3.335004	-3.329490	-2.855091
62	6	0	1.222258	3.090293	2.849924
63	1	0	1.597835	4.013210	3.306090
64	1	0	0.535648	3.352382	2.039952
65	1	0	0.657799	2.541458	3.612362
66	6	0	3.186306	3.069596	1.274683
67	1	0	2.478058	3.420975	0.518524
68	1	0	3.583912	3.956149	1.784300
69	6	0	-2.651371	-0.463584	2.813707
70	6	0	-0.863210	-4.416603	-1.446656
71	6	0	-3.406637	-1.810934	2.994218
72	1	0	-4.338190	-1.594525	3.531840
73	6	0	-1.921171	-5.074636	-0.515156
74	1	0	-2.384405	-5.895875	-1.076002
75	1	0	-1.395471	-5.519352	0.336192
76	6	0	-2.980511	-4.127260	-0.003168
77	6	0	-4.159385	-3.882091	-0.711713
78	6	0	-2.778222	-3.456363	1.203808
79	6	0	-5.100901	-2.981800	-0.220326
80	1	0	-4.347958	-4.410916	-1.642744
81	6	0	-3.703595	-2.539072	1.704452
82	1	0	-1.868531	-3.647609	1.766932
83	6	0	-4.873605	-2.309679	0.977577
84	1	0	-6.025073	-2.814156	-0.767315
85	1	0	-5.615799	-1.612354	1.358177
86	6	0	-2.202963	0.044570	4.192948

87	1	0	-1.683001	1.005076	4.102264
88	1	0	-3.076728	0.192692	4.837773
89	1	0	-1.527350	-0.667766	4.673535
90	6	0	-3.546746	0.580279	2.137136
91	1	0	-4.427614	0.762664	2.765806
92	1	0	-3.011471	1.524799	2.001099
93	1	0	-3.880335	0.251763	1.149596
94	6	0	0.275879	-5.419817	-1.689269
95	1	0	-0.120809	-6.325814	-2.161319
96	1	0	1.032933	-4.994310	-2.357714
97	1	0	0.762897	-5.695703	-0.750534
98	6	0	-1.490045	-4.008938	-2.782944
99	1	0	-0.747989	-3.540014	-3.435514
100	1	0	-1.882477	-4.899186	-3.288504
101	1	0	-2.308388	-3.297639	-2.647677
102	1	0	-2.802156	-2.456279	3.640220
103	1	0	4.128080	1.206758	3.169386
104	1	0	5.521787	-1.856137	-0.180679
105	6	0	5.026258	0.740833	-1.121972
106	6	0	4.041105	1.528404	-0.523142
107	6	0	6.321444	0.785315	-0.601672
108	6	0	4.306744	2.312276	0.601179
109	1	0	3.033755	1.508996	-0.927984
110	6	0	6.612589	1.586419	0.498466
111	1	0	7.105949	0.189499	-1.061957
112	6	0	5.610130	2.339798	1.101829
113	1	0	7.625189	1.620539	0.890197
114	1	0	5.840107	2.954724	1.968615

Zero-point correction= 0.947010 (Hartree/Particle)
Thermal correction to Energy= 1.003597
Thermal correction to Enthalpy= 1.004541
Thermal correction to Gibbs Free Energy= 0.858738
Sum of electronic and zero-point Energies= -2812.646886
Sum of electronic and thermal Energies= -2812.590299
Sum of electronic and thermal Enthalpies= -2812.589355
Sum of electronic and thermal Free Energies= -2812.735158
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.29837699

^{3}TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.957815	1.922033	0.607881
2	6	0	-1.687820	2.545571	0.612109
3	6	0	-1.561269	3.912031	1.017694
4	6	0	-2.665139	4.612706	1.458576
5	6	0	-3.919339	3.987980	1.445181
6	6	0	-4.055819	2.662424	1.017718
7	1	0	-3.055979	0.890911	0.288908
8	1	0	-2.566775	5.641027	1.793876
9	1	0	-4.795535	4.539988	1.771375
10	1	0	-5.034809	2.193292	1.014407
11	6	0	-0.135527	4.276756	1.036170
12	6	0	0.625776	3.681223	0.030865
13	6	0	0.463962	4.726808	2.342134
14	6	0	2.086449	3.381828	0.230081
15	6	0	1.993715	4.671707	2.362232
16	1	0	0.102169	5.739879	2.569734
17	6	0	2.475944	3.378629	1.702733
18	1	0	2.274919	2.416739	-0.247293
19	1	0	2.345807	4.747414	3.396177
20	1	0	2.018779	2.509622	2.194691

21	1	0	0.058680	4.083917	3.137807
22	6	0	0.243298	3.711082	-1.429765
23	8	0	0.998641	3.353207	-2.304199
24	8	0	-0.974092	4.209681	-1.668121
25	6	0	-1.405269	4.137464	-3.025403
26	1	0	-0.735742	4.708068	-3.673524
27	1	0	-1.430008	3.096479	-3.356765
28	1	0	-2.407479	4.564470	-3.034761
29	1	0	2.684858	4.114754	-0.327319
30	1	0	3.562062	3.271683	1.794780
31	1	0	2.407880	5.530730	1.818098
32	7	0	-0.535471	1.949248	0.258299
33	45	0	0.339435	-2.392061	-0.272514
34	45	0	-0.017718	-0.021395	0.044921
35	8	0	1.771763	-2.283639	1.186003
36	6	0	2.004943	-1.188068	1.764836
37	8	0	1.431214	-0.079772	1.512088
38	8	0	-1.066479	-2.722436	1.211378
39	6	0	-1.595600	-1.724847	1.779825
40	8	0	-1.381701	-0.510588	1.488698
41	8	0	-1.115390	-2.339433	-1.741873
42	6	0	-1.657999	-1.232116	-2.016797
43	8	0	-1.425982	-0.131296	-1.432937
44	8	0	1.729320	-1.899966	-1.697809
45	6	0	1.964924	-0.685793	-1.950100
46	8	0	1.401954	0.307946	-1.391102
47	6	0	3.048621	-1.177218	2.885156
48	6	0	2.994051	-0.347489	-3.028570
49	6	0	3.660036	-2.568856	3.065355
50	1	0	4.399316	-2.540322	3.874733
51	1	0	2.892393	-3.303571	3.323357
52	6	0	3.625961	-1.621207	-3.593535
53	1	0	2.867520	-2.262402	-4.051478
54	1	0	4.362415	-1.354132	-4.360838
55	6	0	4.072016	0.590389	-2.414718
56	1	0	4.798876	0.808783	-3.207047
57	1	0	3.585626	1.535836	-2.152309
58	6	0	2.257026	0.421557	-4.140589
59	1	0	1.795473	1.331389	-3.747066
60	1	0	2.965223	0.695932	-4.930996
61	1	0	1.476698	-0.203550	-4.590981
62	6	0	2.336249	-0.743742	4.178497
63	1	0	3.055675	-0.702968	5.004235
64	1	0	1.877629	0.242509	4.062778
65	1	0	1.551425	-1.459334	4.449369
66	6	0	4.149518	-0.132828	2.549825
67	1	0	3.697640	0.863595	2.582839
68	1	0	4.893356	-0.177107	3.355210
69	6	0	-2.596159	-1.996605	2.905290
70	6	0	-2.699226	-1.210460	-3.137648
71	6	0	-3.825248	-2.722936	2.287863
72	1	0	-4.574027	-2.832020	3.082216
73	6	0	-3.909435	-2.075943	-2.684577
74	1	0	-4.685152	-1.982747	-3.454745
75	1	0	-3.591355	-3.123582	-2.670217
76	6	0	-4.469801	-1.711524	-1.330073
77	6	0	-5.462673	-0.741655	-1.174527
78	6	0	-3.975220	-2.346405	-0.189550
79	6	0	-5.938767	-0.419882	0.093857
80	1	0	-5.876022	-0.248392	-2.050712
81	6	0	-4.429173	-2.026972	1.091001
82	1	0	-3.207882	-3.107839	-0.301742
83	6	0	-5.423243	-1.054115	1.221280
84	1	0	-6.727606	0.319834	0.202510
85	1	0	-5.805531	-0.803861	2.207826
86	6	0	-1.934732	-2.928672	3.932565
87	1	0	-1.073333	-2.440308	4.402251

88	1	0	-2.651499	-3.181452	4.722211
89	1	0	-1.589765	-3.852065	3.460397
90	6	0	-3.018906	-0.689340	3.582247
91	1	0	-3.733416	-0.908183	4.384801
92	1	0	-2.154681	-0.180289	4.019205
93	1	0	-3.484367	0.002669	2.876320
94	6	0	-2.078565	-1.843865	-4.392736
95	1	0	-2.822692	-1.884389	-5.196372
96	1	0	-1.228339	-1.250683	-4.747946
97	1	0	-1.726109	-2.857744	-4.187014
98	6	0	-3.137650	0.225322	-3.440604
99	1	0	-2.285789	0.823490	-3.777921
100	1	0	-3.890610	0.218151	-4.237660
101	1	0	-3.560723	0.715325	-2.560221
102	1	0	-3.513380	-3.731098	1.995670
103	1	0	4.154492	-2.909587	2.152424
104	1	0	4.127187	-2.201839	-2.815101
105	6	0	4.780545	0.025041	-1.205447
106	6	0	4.242379	0.217868	0.066876
107	6	0	5.956470	-0.720366	-1.318530
108	6	0	4.820396	-0.332006	1.211067
109	1	0	3.332509	0.796698	0.172622
110	6	0	6.559211	-1.263234	-0.187129
111	1	0	6.403554	-0.873654	-2.297787
112	6	0	5.993628	-1.075351	1.071323
113	1	0	7.476954	-1.835941	-0.286578
114	1	0	6.468219	-1.504552	1.950538

Zero-point correction= 0.951679 (Hartree/Particle)
Thermal correction to Energy= 1.007961
Thermal correction to Enthalpy= 1.008905
Thermal correction to Gibbs Free Energy= 0.864241
Sum of electronic and zero-point Energies= -2812.653828
Sum of electronic and thermal Energies= -2812.597546
Sum of electronic and thermal Enthalpies= -2812.596601
Sum of electronic and thermal Free Energies= -2812.741266
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.30821080

^{3}INT3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.796197	-2.115439	-2.489590
2	6	0	-1.572435	-2.042561	-1.297222
3	6	0	-2.962316	-2.384841	-1.351155
4	6	0	-3.514944	-2.769959	-2.560767
5	6	0	-2.733431	-2.849690	-3.717109
6	6	0	-1.371851	-2.522854	-3.673912
7	1	0	0.250370	-1.837557	-2.427335
8	1	0	-4.572621	-3.012908	-2.603585
9	1	0	-3.188996	-3.159725	-4.652571
10	1	0	-0.770752	-2.580851	-4.576240
11	6	0	-3.831614	-2.217780	-0.146038
12	6	0	-4.082841	-3.255156	0.779396
13	6	0	-4.434194	-0.980484	0.006639
14	6	0	-5.067982	-3.031531	1.895416
15	6	0	-5.351209	-0.652178	1.141478
16	6	0	-5.103818	-1.569045	2.338475
17	1	0	-6.068485	-3.337090	1.550478
18	1	0	-6.393244	-0.759054	0.797718
19	1	0	-5.876516	-1.423775	3.100155
20	6	0	-3.487145	-4.601589	0.727513
21	8	0	-3.865512	-5.523454	1.425086
22	8	0	-2.470690	-4.721002	-0.143518

23	6	0	-1.868126	-6.008978	-0.216557
24	1	0	-1.451815	-6.293882	0.753018
25	1	0	-2.600422	-6.760417	-0.523009
26	1	0	-1.077420	-5.916904	-0.960611
27	1	0	-4.825995	-3.694335	2.729844
28	1	0	-4.142326	-1.307278	2.797246
29	1	0	-5.231164	0.401691	1.413745
30	1	0	-1.618332	-1.672901	0.636662
31	1	0	-4.230347	-0.205174	-0.728304
32	7	0	-0.987092	-1.632368	-0.164430
33	45	0	1.632176	2.013695	0.219095
34	45	0	0.387628	-0.046665	0.021340
35	8	0	2.949527	1.268420	-1.166081
36	6	0	2.750722	0.127602	-1.661550
37	8	0	1.780329	-0.644979	-1.373013
38	8	0	0.485664	2.759410	-1.336002
39	6	0	-0.391503	2.012065	-1.857182
40	8	0	-0.664594	0.831447	-1.490412
41	8	0	0.238144	2.609840	1.618893
42	6	0	-0.705163	1.827895	1.928795
43	8	0	-0.909710	0.682290	1.424787
44	8	0	2.699713	1.118774	1.723418
45	6	0	2.427323	-0.063539	2.071226
46	8	0	1.520430	-0.795650	1.561880
47	6	0	3.731334	-0.390116	-2.715652
48	6	0	3.231429	-0.685208	3.215137
49	6	0	4.885601	0.596024	-2.909698
50	1	0	5.581075	0.202371	-3.660483
51	1	0	4.516176	1.565670	-3.254576
52	6	0	4.328519	0.270863	3.689070
53	1	0	3.897845	1.204727	4.060739
54	1	0	4.895140	-0.197581	4.502690
55	6	0	3.834978	-2.033548	2.729858
56	1	0	4.404401	-2.454354	3.568049
57	1	0	3.009758	-2.721341	2.519196
58	6	0	2.251619	-0.970320	4.367601
59	1	0	1.449972	-1.640786	4.045196
60	1	0	2.785656	-1.436849	5.203178
61	1	0	1.800477	-0.040451	4.732777
62	6	0	2.954118	-0.547853	-4.035028
63	1	0	3.623251	-0.921235	-4.818403
64	1	0	2.123695	-1.251691	-3.924386
65	1	0	2.549222	0.415106	-4.366621
66	6	0	4.254692	-1.785696	-2.273275
67	1	0	3.410647	-2.483278	-2.270441
68	1	0	4.957265	-2.128254	-3.043322
69	6	0	-1.202685	2.571239	-3.027519
70	6	0	-1.686308	2.308811	2.999941
71	6	0	-1.997788	3.807659	-2.520714
72	1	0	-2.621165	4.158980	-3.352357
73	6	0	-2.375936	3.602796	2.480478
74	1	0	-3.113681	3.905013	3.234229
75	1	0	-1.620424	4.393425	2.429969
76	6	0	-3.037064	3.457093	1.130319
77	6	0	-4.361890	3.034848	0.999946
78	6	0	-2.306640	3.722080	-0.028959
79	6	0	-4.926872	2.863488	-0.261098
80	1	0	-4.957463	2.851857	1.891649
81	6	0	-2.851880	3.547357	-1.302012
82	1	0	-1.279218	4.063837	0.061575
83	6	0	-4.175465	3.113192	-1.406513
84	1	0	-5.961877	2.544568	-0.351178
85	1	0	-4.624123	2.986175	-2.388757
86	6	0	-0.220503	3.026733	-4.118910
87	1	0	0.348047	2.174936	-4.509572
88	1	0	-0.771522	3.475954	-4.952984
89	1	0	0.487663	3.761894	-3.727714

90	6	0	-2.147475	1.503479	-3.588093
91	1	0	-2.716653	1.922372	-4.426635
92	1	0	-1.588524	0.634536	-3.947680
93	1	0	-2.849977	1.147850	-2.830409
94	6	0	-0.885732	2.648799	4.267646
95	1	0	-1.559592	3.033900	5.041416
96	1	0	-0.389396	1.756250	4.665222
97	1	0	-0.121814	3.402171	4.058803
98	6	0	-2.720506	1.224554	3.309734
99	1	0	-2.236928	0.326890	3.706865
100	1	0	-3.432114	1.593033	4.058065
101	1	0	-3.271559	0.936990	2.411844
102	1	0	-1.280805	4.603576	-2.293984
103	1	0	5.433187	0.759969	-1.978663
104	1	0	5.020086	0.521143	2.881053
105	6	0	4.719058	-1.917370	1.510144
106	6	0	4.156225	-1.979862	0.234123
107	6	0	6.095564	-1.709806	1.622113
108	6	0	4.923175	-1.798105	-0.918167
109	1	0	3.089055	-2.155910	0.136528
110	6	0	6.880363	-1.554881	0.483357
111	1	0	6.554851	-1.672027	2.606988
112	6	0	6.297463	-1.592175	-0.779773
113	1	0	7.951536	-1.402838	0.580817
114	1	0	6.913904	-1.463014	-1.666213

Zero-point correction= 0.951644 (Hartree/Particle)
Thermal correction to Energy= 1.008868
Thermal correction to Enthalpy= 1.009813
Thermal correction to Gibbs Free Energy= 0.860953
Sum of electronic and zero-point Energies= -2812.686508
Sum of electronic and thermal Energies= -2812.629283
Sum of electronic and thermal Enthalpies= -2812.628339
Sum of electronic and thermal Free Energies= -2812.777198
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.34804733

^{3}INT4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.851778	1.796288	-1.162587
2	6	0	1.612480	2.426240	-1.220489
3	6	0	1.486391	3.775671	-1.685521
4	6	0	2.600267	4.458771	-2.132987
5	6	0	3.856541	3.808225	-2.085530
6	6	0	3.978487	2.516858	-1.603650
7	1	0	2.948376	0.785297	-0.788177
8	1	0	2.521553	5.476326	-2.503704
9	1	0	4.739038	4.339606	-2.429423
10	1	0	4.951394	2.038494	-1.560803
11	6	0	0.111018	4.132362	-1.575693
12	6	0	-0.605426	2.988771	-0.885012
13	6	0	-0.606496	5.327231	-2.094772
14	6	0	-1.927885	2.598179	-1.582507
15	6	0	-2.114748	5.040471	-2.220260
16	1	0	-0.431643	6.204759	-1.452376
17	6	0	-2.330667	3.595592	-2.679010
18	1	0	-1.816905	1.593620	-1.997057
19	1	0	-2.566012	5.750277	-2.920709
20	1	0	-1.743795	3.414827	-3.590381
21	1	0	-0.189448	5.587218	-3.078795
22	6	0	-0.864860	3.436450	0.580331
23	8	0	-1.929479	3.812876	1.010682

24	8	0	0.278139	3.457584	1.263906
25	6	0	0.219978	3.895900	2.617606
26	1	0	-0.474425	4.731805	2.724264
27	1	0	-0.098682	3.067704	3.254524
28	1	0	1.235093	4.196802	2.875589
29	1	0	-2.714823	2.562320	-0.825468
30	1	0	-3.380629	3.425690	-2.939679
31	1	0	-2.604308	5.183395	-1.249880
32	7	0	0.395919	1.910264	-0.867333
33	45	0	-0.197936	-2.237347	0.831409
34	45	0	0.048717	-0.035184	-0.136025
35	8	0	-1.591324	-2.644966	-0.611756
36	6	0	-1.855752	-1.773992	-1.483569
37	8	0	-1.350883	-0.606858	-1.538898
38	8	0	1.251905	-2.897930	-0.484856
39	6	0	1.732203	-2.078276	-1.318297
40	8	0	1.450354	-0.844400	-1.385012
41	8	0	1.218889	-1.690216	2.233154
42	6	0	1.715627	-0.529179	2.176910
43	8	0	1.438290	0.350529	1.308908
44	8	0	-1.657700	-1.441566	2.030502
45	6	0	-1.965765	-0.222682	1.939360
46	8	0	-1.417234	0.618416	1.154338
47	6	0	-2.849175	-2.136041	-2.589793
48	6	0	-3.076037	0.307725	2.850959
49	6	0	-3.388773	-3.554030	-2.387795
50	1	0	-4.098343	-3.792249	-3.189125
51	1	0	-2.578259	-4.287629	-2.414210
52	6	0	-3.638817	-0.820521	3.718912
53	1	0	-2.863200	-1.241264	4.365178
54	1	0	-4.441425	-0.425628	4.353094
55	6	0	-4.190320	0.952615	1.979995
56	1	0	-4.960021	1.324549	2.667865
57	1	0	-3.763045	1.824370	1.473159
58	6	0	-2.474917	1.408593	3.741329
59	1	0	-2.162283	2.263215	3.136595
60	1	0	-3.226849	1.752487	4.460454
61	1	0	-1.614148	1.032368	4.307521
62	6	0	-2.103218	-2.043910	-3.932603
63	1	0	-2.789178	-2.273671	-4.755807
64	1	0	-1.691884	-1.042316	-4.086429
65	1	0	-1.278648	-2.765112	-3.969524
66	6	0	-4.005931	-1.098311	-2.588251
67	1	0	-3.594789	-0.124459	-2.875926
68	1	0	-4.711199	-1.396228	-3.374113
69	6	0	2.753644	-2.609972	-2.325584
70	6	0	2.751583	-0.147774	3.236540
71	6	0	3.999383	-3.096697	-1.531718
72	1	0	4.759717	-3.393410	-2.264734
73	6	0	3.986894	-1.075312	3.059318
74	1	0	4.748138	-0.746834	3.777849
75	1	0	3.692783	-2.091867	3.340340
76	6	0	4.560069	-1.093154	1.661985
77	6	0	5.527807	-0.175615	1.246941
78	6	0	4.101490	-2.038337	0.743232
79	6	0	6.013569	-0.207150	-0.057328
80	1	0	5.912319	0.557586	1.951442
81	6	0	4.565995	-2.076645	-0.572637
82	1	0	3.353561	-2.760599	1.059614
83	6	0	5.533393	-1.148118	-0.964606
84	1	0	6.781471	0.497837	-0.364626
85	1	0	5.923216	-1.172841	-1.979253
86	6	0	2.132860	-3.809725	-3.058784
87	1	0	1.261517	-3.497905	-3.645829
88	1	0	2.865670	-4.244839	-3.747805
89	1	0	1.812940	-4.579490	-2.351822
90	6	0	3.138833	-1.524576	-3.334944

91	1	0	3.865256	-1.931239	-4.048535
92	1	0	2.262173	-1.181558	-3.892013
93	1	0	3.579834	-0.652023	-2.846822
94	6	0	2.139999	-0.395918	4.624536
95	1	0	2.878217	-0.171963	5.403002
96	1	0	1.270063	0.250883	4.787451
97	1	0	1.818145	-1.434920	4.732017
98	6	0	3.150268	1.324009	3.096781
99	1	0	2.283660	1.973112	3.248522
100	1	0	3.905295	1.572618	3.852206
101	1	0	3.554290	1.543981	2.105877
102	1	0	3.718052	-3.995837	-0.973791
103	1	0	-3.899380	-3.655714	-1.427205
104	1	0	-4.042753	-1.632703	3.109932
105	6	0	-4.810481	0.026369	0.961960
106	6	0	-4.225471	-0.096279	-0.297564
107	6	0	-5.946503	-0.735396	1.243288
108	6	0	-4.723567	-0.968049	-1.265587
109	1	0	-3.346797	0.495605	-0.525861
110	6	0	-6.468990	-1.599457	0.284926
111	1	0	-6.426771	-0.647241	2.214857
112	6	0	-5.860844	-1.718675	-0.961945
113	1	0	-7.357804	-2.182069	0.510096
114	1	0	-6.274056	-2.395985	-1.705566

Zero-point correction= 0.953812 (Hartree/Particle)
Thermal correction to Energy= 1.010099
Thermal correction to Enthalpy= 1.011043
Thermal correction to Gibbs Free Energy= 0.867068
Sum of electronic and zero-point Energies= -2812.702084
Sum of electronic and thermal Energies= -2812.645797
Sum of electronic and thermal Enthalpies= -2812.644852
Sum of electronic and thermal Free Energies= -2812.788828
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.35787155

[1]INT5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.267175	1.835534	3.089195
2	6	0	0.525214	2.521559	2.061523
3	6	0	0.276851	3.958096	2.201200
4	6	0	0.804812	4.679015	3.329070
5	6	0	1.509196	3.993630	4.259685
6	6	0	1.730754	2.565965	4.132702
7	1	0	1.442892	0.772760	2.988872
8	1	0	0.627568	5.746111	3.422798
9	1	0	1.917441	4.504822	5.125796
10	1	0	2.294433	2.068911	4.917605
11	6	0	-0.445614	4.337932	1.117996
12	6	0	-0.661510	3.108005	0.274154
13	6	0	-0.843226	5.672722	0.600904
14	6	0	-0.072706	3.359036	-1.138512
15	6	0	-0.150756	5.878489	-0.766141
16	1	0	-1.930084	5.703359	0.451454
17	6	0	-0.461447	4.723256	-1.720200
18	1	0	0.933038	5.949678	-0.604751
19	1	0	-0.574454	6.466603	1.304698
20	6	0	-2.180230	2.843163	0.223732
21	8	0	-2.924114	3.409988	-0.543048
22	8	0	-2.551429	1.993958	1.168681
23	6	0	-3.885236	1.487942	1.122029
24	1	0	-4.543788	2.175834	0.589722

25	1	0	-3.854457	0.518105	0.622667
26	1	0	-4.207695	1.366665	2.155938
27	1	0	-0.478758	6.829851	-1.198290
28	45	0	0.250376	-2.193838	-0.843181
29	45	0	0.093644	0.009099	0.145274
30	8	0	1.815109	-2.611794	0.411684
31	6	0	2.180285	-1.728889	1.231336
32	8	0	1.652254	-0.578528	1.359346
33	8	0	-1.054206	-2.833282	0.614098
34	6	0	-1.504524	-2.006324	1.461646
35	8	0	-1.218671	-0.774553	1.518639
36	8	0	-1.298886	-1.646827	-2.073240
37	6	0	-1.822111	-0.500631	-1.973189
38	8	0	-1.472957	0.396033	-1.144526
39	8	0	1.566739	-1.414554	-2.215283
40	6	0	1.860254	-0.189954	-2.154159
41	8	0	1.404094	0.638654	-1.305232
42	6	0	3.336914	-2.045593	2.182380
43	6	0	2.823925	0.387237	-3.193237
44	6	0	3.970955	-3.393351	1.829465
45	1	0	4.805807	-3.595407	2.511119
46	1	0	3.242227	-4.202784	1.924831
47	6	0	3.395728	-0.721828	-4.078778
48	1	0	2.598110	-1.238416	-4.619472
49	1	0	4.086901	-0.287439	-4.810958
50	6	0	3.955349	1.160449	-2.459041
51	1	0	4.619479	1.573409	-3.228704
52	1	0	3.503683	2.006618	-1.930962
53	6	0	2.023931	1.384500	-4.051361
54	1	0	1.604275	2.185266	-3.434792
55	1	0	2.676779	1.832274	-4.809213
56	1	0	1.201062	0.879198	-4.569908
57	6	0	2.760319	-2.103806	3.608909
58	1	0	3.557958	-2.339898	4.322298
59	1	0	2.310427	-1.149306	3.898409
60	1	0	1.993810	-2.882893	3.687948
61	6	0	4.381793	-0.896400	2.110928
62	1	0	3.906632	0.024758	2.464945
63	1	0	5.183578	-1.142035	2.818650
64	6	0	-2.467698	-2.565785	2.512849
65	6	0	-2.955082	-0.192488	-2.955900
66	6	0	-3.646542	-3.274984	1.788364
67	1	0	-4.321581	-3.657426	2.564147
68	6	0	-4.048991	-1.288957	-2.811337
69	1	0	-4.852609	-1.038715	-3.514914
70	1	0	-3.620636	-2.243429	-3.133311
71	6	0	-4.613635	-1.441108	-1.417000
72	6	0	-5.766803	-0.765648	-1.009616
73	6	0	-3.967605	-2.267963	-0.495052
74	6	0	-6.246198	-0.910672	0.290009
75	1	0	-6.294358	-0.128449	-1.715185
76	6	0	-4.416286	-2.404731	0.820433
77	1	0	-3.086293	-2.818183	-0.808998
78	6	0	-5.571132	-1.717586	1.202807
79	1	0	-7.150821	-0.391042	0.593276
80	1	0	-5.948210	-1.822806	2.217350
81	6	0	-1.693355	-3.612045	3.334325
82	1	0	-0.855847	-3.144847	3.865262
83	1	0	-2.355616	-4.065542	4.080617
84	1	0	-1.296535	-4.401266	2.689992
85	6	0	-2.981223	-1.459366	3.435625
86	1	0	-3.642123	-1.893391	4.195424
87	1	0	-2.154277	-0.953160	3.940838
88	1	0	-3.541767	-0.705786	2.879203
89	6	0	-2.360303	-0.273490	-4.373808
90	1	0	-3.146400	-0.097587	-5.116779
91	1	0	-1.587794	0.491775	-4.513295

92	1	0	-1.913034	-1.253808	-4.558561
93	6	0	-3.544671	1.197234	-2.725083
94	1	0	-2.783502	1.975776	-2.818170
95	1	0	-4.325716	1.388480	-3.470568
96	1	0	-3.986898	1.296015	-1.732692
97	1	0	-3.244490	-4.140878	1.252772
98	1	0	4.348158	-3.402908	0.804162
99	1	0	3.935722	-1.466620	-3.489034
100	6	0	4.750962	0.322954	-1.485059
101	6	0	4.304227	0.166281	-0.171324
102	6	0	5.913797	-0.342886	-1.878225
103	6	0	4.959476	-0.671724	0.732804
104	1	0	3.409886	0.692310	0.148693
105	6	0	6.599258	-1.155225	-0.979942
106	1	0	6.284418	-0.222849	-2.893431
107	6	0	6.121074	-1.325374	0.315694
108	1	0	7.507951	-1.661739	-1.292532
109	1	0	6.653131	-1.971254	1.010087
110	7	0	0.022293	2.024756	0.962860
111	1	0	-1.526986	4.725880	-1.964420
112	1	0	0.090435	4.863201	-2.657215
113	1	0	1.015467	3.290877	-1.029173
114	1	0	-0.379114	2.541376	-1.794208

Zero-point correction= 0.957401 (Hartree/Particle)
Thermal correction to Energy= 1.013055
Thermal correction to Enthalpy= 1.014000
Thermal correction to Gibbs Free Energy= 0.873319
Sum of electronic and zero-point Energies= -2812.753197
Sum of electronic and thermal Energies= -2812.697542
Sum of electronic and thermal Enthalpies= -2812.696598
Sum of electronic and thermal Free Energies= -2812.837278
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.41392319

^{1}INT5a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.669199	1.501429	0.827843
2	6	0	1.432006	0.808883	0.535766
3	6	0	1.459788	-0.323567	-0.403838
4	6	0	2.704759	-0.742917	-0.995539
5	6	0	3.829892	-0.060651	-0.680996
6	6	0	3.805323	1.069096	0.234394
7	1	0	2.654191	2.344071	1.510715
8	1	0	2.727472	-1.584248	-1.682203
9	1	0	4.783062	-0.348389	-1.114144
10	1	0	4.745155	1.574460	0.439296
11	6	0	0.188643	-0.785088	-0.481101
12	6	0	-0.628667	0.077801	0.459916
13	6	0	-0.383749	-2.023389	-1.070957
14	6	0	-1.172038	-0.864644	1.577720
15	6	0	-0.905495	-2.906614	0.086508
16	1	0	-1.224096	-1.766120	-1.725445
17	6	0	-1.838297	-2.126944	1.018018
18	1	0	-0.045716	-3.279922	0.658483
19	1	0	0.363278	-2.562953	-1.662421
20	6	0	-1.807101	0.728312	-0.272879
21	8	0	-2.601674	0.109339	-0.947607
22	8	0	-1.884502	2.041439	-0.074822
23	6	0	-2.980750	2.688062	-0.721805
24	1	0	-2.920067	2.555365	-1.804714
25	1	0	-3.930948	2.281707	-0.366638
26	1	0	-2.891179	3.741173	-0.458272
27	1	0	-1.424606	-3.778508	-0.325719

28	7	0	0.264312	1.062679	1.040575
29	1	0	-2.752026	-1.857859	0.479605
30	1	0	-2.133028	-2.764058	1.859893
31	1	0	-0.301443	-1.138597	2.185278
32	1	0	-1.851900	-0.299719	2.223390

Zero-point correction= 0.269484 (Hartree/Particle)
Thermal correction to Energy= 0.282656
Thermal correction to Enthalpy= 0.283601
Thermal correction to Gibbs Free Energy= 0.230252
Sum of electronic and zero-point Energies= -747.201295
Sum of electronic and thermal Energies= -747.188123
Sum of electronic and thermal Enthalpies= -747.187178
Sum of electronic and thermal Free Energies= -747.240527
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -747.67009358

^{1}TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.876101	1.787103	1.200704
2	6	0	-1.597385	2.376098	1.350387
3	6	0	-1.473751	3.754233	1.688411
4	6	0	-2.619265	4.552005	1.897541
5	6	0	-3.851017	3.959591	1.772468
6	6	0	-3.970187	2.585552	1.421323
7	1	0	-2.976001	0.744297	0.924754
8	1	0	-2.522380	5.603037	2.154084
9	1	0	-4.752656	4.541285	1.938552
10	1	0	-4.961298	2.152791	1.318627
11	6	0	-0.087334	4.036310	1.690321
12	6	0	0.554013	2.774560	1.341232
13	6	0	0.660923	5.194421	2.289858
14	6	0	1.989874	2.489273	1.712595
15	6	0	2.167723	4.912511	2.448726
16	1	0	0.494211	6.114718	1.718966
17	6	0	2.438169	3.451581	2.822439
18	1	0	2.040464	1.448768	2.040945
19	1	0	2.569943	5.581904	3.216381
20	1	0	1.911151	3.204308	3.754534
21	1	0	0.211931	5.357982	3.278429
22	6	0	0.542364	3.802919	-0.172757
23	8	0	1.589927	4.272229	-0.524152
24	8	0	-0.539993	3.621249	-0.894561
25	6	0	-0.398028	3.686061	-2.316233
26	1	0	-0.225338	2.672433	-2.682159
27	1	0	-1.343038	4.074805	-2.693585
28	1	0	0.427781	4.345901	-2.587301
29	1	0	2.638282	2.598235	0.839971
30	1	0	3.506676	3.306011	3.012139
31	1	0	2.684742	5.142335	1.512830
32	7	0	-0.378716	1.797734	1.172967
33	45	0	0.214801	-2.163920	-0.997760
34	45	0	-0.031568	-0.065000	0.174405
35	8	0	1.666842	-2.668593	0.355801
36	6	0	1.930985	-1.886903	1.308552
37	8	0	1.406858	-0.742232	1.494776
38	8	0	-1.166461	-2.966091	0.316598
39	6	0	-1.647582	-2.224198	1.220637
40	8	0	-1.409465	-0.988340	1.364900
41	8	0	-1.278777	-1.522915	-2.277969
42	6	0	-1.783575	-0.376120	-2.110679
43	8	0	-1.453308	0.451647	-1.209813

44	8	0	1.618969	-1.225762	-2.167163
45	6	0	1.931431	-0.022477	-1.960782
46	8	0	1.404514	0.738708	-1.084737
47	6	0	2.954965	-2.343204	2.351576
48	6	0	3.025328	0.589702	-2.844912
49	6	0	3.500029	-3.730345	2.003187
50	1	0	4.230338	-4.037296	2.761482
51	1	0	2.695326	-4.470338	1.978494
52	6	0	3.571789	-0.455640	-3.820597
53	1	0	2.784008	-0.818178	-4.486852
54	1	0	4.363218	-0.005608	-4.431861
55	6	0	4.159209	1.157605	-1.947237
56	1	0	4.909638	1.597052	-2.616424
57	1	0	3.742410	1.976885	-1.351265
58	6	0	2.410477	1.763642	-3.624548
59	1	0	2.100837	2.559240	-2.942504
60	1	0	3.150993	2.174771	-4.319809
61	1	0	1.542695	1.438176	-4.210875
62	6	0	2.244506	-2.385568	3.715629
63	1	0	2.954011	-2.682060	4.496587
64	1	0	1.826018	-1.408254	3.971868
65	1	0	1.429014	-3.117715	3.705616
66	6	0	4.104550	-1.299919	2.419755
67	1	0	3.694011	-0.361110	2.807649
68	1	0	4.831336	-1.662929	3.157112
69	6	0	-2.609599	-2.864877	2.223937
70	6	0	-2.891794	0.048411	-3.080345
71	6	0	-3.865566	-3.349128	1.445728
72	1	0	-4.583370	-3.728774	2.183372
73	6	0	-4.062992	-0.965793	-2.959344
74	1	0	-4.858085	-0.628014	-3.635877
75	1	0	-3.714824	-1.936672	-3.325939
76	6	0	-4.602230	-1.125854	-1.558027
77	6	0	-5.592591	-0.284797	-1.044327
78	6	0	-4.083451	-2.123954	-0.733441
79	6	0	-6.037278	-0.439856	0.265553
80	1	0	-6.024390	0.487508	-1.675907
81	6	0	-4.507045	-2.286073	0.586771
82	1	0	-3.318064	-2.787236	-1.127028
83	6	0	-5.495106	-1.431227	1.079619
84	1	0	-6.820226	0.207792	0.651145
85	1	0	-5.850068	-1.550358	2.100267
86	6	0	-1.914396	-4.083566	2.851339
87	1	0	-1.033987	-3.774916	3.426429
88	1	0	-2.602222	-4.593466	3.535545
89	1	0	-1.592094	-4.790791	2.082758
90	6	0	-2.996907	-1.865152	3.317558
91	1	0	-3.683839	-2.345193	4.024821
92	1	0	-2.113347	-1.528993	3.867861
93	1	0	-3.483447	-0.978447	2.903980
94	6	0	-2.327030	-0.016825	-4.508938
95	1	0	-3.105834	0.251859	-5.231792
96	1	0	-1.495374	0.687242	-4.631855
97	1	0	-1.961505	-1.020599	-4.740954
98	6	0	-3.376815	1.467456	-2.774324
99	1	0	-2.578807	2.192743	-2.944046
100	1	0	-4.212801	1.720023	-3.437671
101	1	0	-3.702129	1.574417	-1.737097
102	1	0	-3.571288	-4.193559	0.813778
103	1	0	3.987562	-3.735921	1.025412
104	1	0	3.985388	-1.318490	-3.293495
105	6	0	4.811226	0.149924	-1.031814
106	6	0	4.257380	-0.092926	0.224026
107	6	0	5.948602	-0.567769	-1.407122
108	6	0	4.788510	-1.040780	1.098374
109	1	0	3.376133	0.462892	0.522050
110	6	0	6.503276	-1.507447	-0.542634

111	1	0	6.404130	-0.386628	-2.377693
112	6	0	5.926629	-1.745580	0.702124
113	1	0	7.392556	-2.056110	-0.839600
114	1	0	6.364674	-2.481570	1.372048

Zero-point correction= 0.955613 (Hartree/Particle)
Thermal correction to Energy= 1.011062
Thermal correction to Enthalpy= 1.012006
Thermal correction to Gibbs Free Energy= 0.871864
Sum of electronic and zero-point Energies= -2812.719834
Sum of electronic and thermal Energies= -2812.664385
Sum of electronic and thermal Enthalpies= -2812.663441
Sum of electronic and thermal Free Energies= -2812.803583
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.37831395

^{1}TS4a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.754990	-0.297630	1.282783
2	6	0	1.382370	-0.341927	0.922805
3	6	0	1.015807	-0.648136	-0.426952
4	6	0	1.999723	-0.917483	-1.404528
5	6	0	3.316047	-0.894132	-1.021241
6	6	0	3.687017	-0.580873	0.319616
7	1	0	3.036510	-0.049924	2.300807
8	1	0	1.717071	-1.146226	-2.428415
9	1	0	4.096434	-1.112699	-1.743980
10	1	0	4.743094	-0.565506	0.574522
11	6	0	-0.391640	-0.580514	-0.459424
12	6	0	-0.765179	-0.207666	0.915607
13	6	0	-1.366735	-1.148719	-1.454139
14	6	0	-2.145348	-0.527568	1.452152
15	6	0	-2.786845	-1.309542	-0.873754
16	1	0	-1.393816	-0.558276	-2.376607
17	6	0	-2.768467	-1.658209	0.618418
18	1	0	-2.030250	-0.819491	2.498830
19	1	0	-3.310501	-2.089410	-1.437059
20	1	0	-2.198664	-2.584132	0.776980
21	1	0	-0.970271	-2.135002	-1.727655
22	6	0	-0.887503	1.266194	-0.112946
23	8	0	-1.971408	1.627015	-0.493572
24	8	0	0.191195	2.030210	-0.031161
25	6	0	0.003903	3.386093	-0.438607
26	1	0	-0.740560	3.874825	0.194405
27	1	0	0.977776	3.858561	-0.320108
28	1	0	-0.322178	3.430098	-1.480788
29	1	0	-2.795866	0.351100	1.416234
30	1	0	-3.789038	-1.848291	0.967562
31	1	0	-3.343600	-0.378807	-1.012655
32	7	0	0.325246	-0.103422	1.725293

Zero-point correction= 0.267476 (Hartree/Particle)
Thermal correction to Energy= 0.281338
Thermal correction to Enthalpy= 0.282283
Thermal correction to Gibbs Free Energy= 0.227311
Sum of electronic and zero-point Energies= -747.168007
Sum of electronic and thermal Energies= -747.154145
Sum of electronic and thermal Enthalpies= -747.153200
Sum of electronic and thermal Free Energies= -747.208172
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -747.63468614

^{1}TS5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.904826	1.403124	1.668914
2	6	0	1.685104	2.118255	1.664403
3	6	0	1.696539	3.529863	1.821166
4	6	0	2.901221	4.235890	2.025355
5	6	0	4.072247	3.520256	2.061890
6	6	0	4.063584	2.112438	1.876373
7	1	0	2.913279	0.333638	1.501816
8	1	0	2.899252	5.315306	2.150458
9	1	0	5.017378	4.029264	2.223681
10	1	0	5.007182	1.575399	1.884555
11	6	0	0.354070	3.958723	1.672122
12	6	0	-0.386550	2.743127	1.411680
13	6	0	-0.198391	5.339544	1.868402
14	6	0	-0.123822	3.585043	-0.260177
15	6	0	-0.816224	5.830339	0.540711
16	1	0	-0.940050	5.345045	2.674190
17	6	0	-0.073011	5.078046	-0.558350
18	1	0	0.721224	3.000781	-0.619252
19	1	0	-0.726669	6.915110	0.433336
20	1	0	0.972325	5.407183	-0.598808
21	1	0	0.623474	5.993245	2.175500
22	6	0	-1.864565	2.666705	1.677298
23	8	0	-2.695291	3.375147	1.150237
24	8	0	-2.125528	1.812120	2.656326
25	6	0	-3.480857	1.805174	3.117399
26	1	0	-3.496146	1.100388	3.946950
27	1	0	-3.767283	2.804394	3.454739
28	1	0	-4.155696	1.482478	2.322070
29	1	0	-0.522984	5.256707	-1.542413
30	1	0	-1.875547	5.566028	0.510679
31	7	0	0.419150	1.643718	1.461258
32	45	0	-0.134972	-1.972217	-1.318579
33	45	0	0.047688	-0.135998	0.243658
34	8	0	-1.543462	-0.868439	-2.324948
35	6	0	-1.879584	0.267072	-1.897397
36	8	0	-1.383265	0.847758	-0.877329
37	8	0	1.354901	-1.058109	-2.434464
38	6	0	1.825322	0.045771	-2.037534
39	8	0	1.474642	0.658576	-0.985887
40	8	0	1.248595	-2.985622	-0.177631
41	6	0	1.703989	-2.432437	0.864888
42	8	0	1.419626	-1.264633	1.263913
43	8	0	-1.603689	-2.747528	-0.128208
44	6	0	-1.917145	-2.153384	0.941068
45	8	0	-1.410149	-1.069431	1.367143
46	6	0	-2.954406	1.038215	-2.669142
47	6	0	-2.988950	-2.796444	1.825091
48	6	0	-3.568285	0.156419	-3.760086
49	1	0	-4.346145	0.719332	-4.289752
50	1	0	-2.810614	-0.154054	-4.484431
51	6	0	-3.594766	-4.025646	1.144300
52	1	0	-2.829405	-4.781942	0.951037
53	1	0	-4.359841	-4.464394	1.796197
54	6	0	-4.082522	-1.740635	2.138367
55	1	0	-4.822365	-2.218900	2.792492
56	1	0	-3.611302	-0.936756	2.711116
57	6	0	-2.307556	-3.205871	3.143233
58	1	0	-1.852366	-2.341010	3.634514
59	1	0	-3.043907	-3.651685	3.821819
60	1	0	-1.524708	-3.950384	2.958884
61	6	0	-2.276160	2.258910	-3.317385
62	1	0	-3.009093	2.820533	-3.907315
63	1	0	-1.857024	2.931212	-2.563254

64	1	0	-1.468465	1.945870	-3.988681
65	6	0	-4.042735	1.535428	-1.678634
66	1	0	-3.581396	2.224041	-0.963329
67	1	0	-4.770519	2.113838	-2.261516
68	6	0	2.913722	0.703263	-2.888827
69	6	0	2.689971	-3.241910	1.710064
70	6	0	4.121651	-0.271735	-2.970998
71	1	0	4.909570	0.232489	-3.544369
72	6	0	3.943404	-3.536708	0.837986
73	1	0	4.669891	-4.057096	1.474438
74	1	0	3.650217	-4.231676	0.044302
75	6	0	4.574760	-2.312351	0.217911
76	6	0	5.573976	-1.585910	0.869994
77	6	0	4.142626	-1.872848	-1.034559
78	6	0	6.115196	-0.447424	0.279089
79	1	0	5.939788	-1.922200	1.837077
80	6	0	4.659341	-0.722568	-1.633004
81	1	0	3.374905	-2.438102	-1.555534
82	6	0	5.656656	-0.012797	-0.961247
83	1	0	6.906423	0.099805	0.784766
84	1	0	6.084010	0.877234	-1.416432
85	6	0	2.352940	0.915234	-4.304617
86	1	0	1.500062	1.603739	-4.286476
87	1	0	3.124200	1.349933	-4.950696
88	1	0	2.020583	-0.030732	-4.740437
89	6	0	3.337371	2.046327	-2.285768
90	1	0	4.143791	2.480420	-2.888886
91	1	0	2.500778	2.752486	-2.282563
92	1	0	3.685574	1.938370	-1.255353
93	6	0	2.020328	-4.574858	2.082601
94	1	0	2.723259	-5.200443	2.644507
95	1	0	1.141066	-4.404046	2.714163
96	1	0	1.701802	-5.117522	1.188833
97	6	0	3.075065	-2.482200	2.982360
98	1	0	2.191421	-2.258280	3.586537
99	1	0	3.758634	-3.096449	3.580540
100	1	0	3.570310	-1.534315	2.758042
101	1	0	3.811456	-1.148838	-3.548228
102	1	0	-4.018184	-0.746074	-3.339497
103	1	0	-4.058079	-3.767399	0.188758
104	6	0	-4.769226	-1.162494	0.922529
105	6	0	-4.180937	-0.104276	0.226452
106	6	0	-5.978531	-1.677035	0.450633
107	6	0	-4.751407	0.430482	-0.929796
108	1	0	-3.240479	0.301032	0.584154
109	6	0	-6.571458	-1.146539	-0.691518
110	1	0	-6.457741	-2.496386	0.981162
111	6	0	-5.961308	-0.101608	-1.379737
112	1	0	-7.515192	-1.549890	-1.047548
113	1	0	-6.427926	0.305218	-2.273679
114	1	0	-1.063142	3.147176	-0.594428

Zero-point correction= 0.955634 (Hartree/Particle)
Thermal correction to Energy= 1.011018
Thermal correction to Enthalpy= 1.011962
Thermal correction to Gibbs Free Energy= 0.872097
Sum of electronic and zero-point Energies= -2812.711517
Sum of electronic and thermal Energies= -2812.656134
Sum of electronic and thermal Enthalpies= -2812.655189
Sum of electronic and thermal Free Energies= -2812.795054
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.37083949

^{1}TS5a'

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

1	6	0	-2.601667	-1.915946	0.301170
2	6	0	-1.432890	-1.146106	0.077359
3	6	0	-1.556971	0.216102	-0.332338
4	6	0	-2.825077	0.810936	-0.514984
5	6	0	-3.940460	0.038973	-0.306080
6	6	0	-3.821440	-1.319460	0.101546
7	1	0	-2.513392	-2.949806	0.618341
8	1	0	-2.915184	1.849097	-0.824292
9	1	0	-4.929957	0.461861	-0.450174
10	1	0	-4.729462	-1.895060	0.259550
11	6	0	-0.234131	0.700545	-0.454781
12	6	0	0.583080	-0.441138	-0.060871
13	6	0	0.221120	2.024333	-0.986228
14	6	0	0.529861	0.744679	1.455616
15	6	0	1.126627	2.704488	0.055716
16	1	0	0.756092	1.881319	-1.929417
17	6	0	0.590761	2.266285	1.416766
18	1	0	-0.305200	0.313429	2.003313
19	1	0	1.123875	3.792645	-0.056021
20	1	0	-0.417050	2.673450	1.559713
21	1	0	-0.661818	2.642215	-1.181461
22	6	0	2.033185	-0.583329	-0.404133
23	8	0	2.615782	0.121655	-1.199431
24	8	0	2.612452	-1.565523	0.283887
25	6	0	3.989018	-1.791364	-0.017951
26	1	0	4.294062	-2.619959	0.619710
27	1	0	4.110930	-2.053100	-1.071585
28	1	0	4.582425	-0.899235	0.198328
29	1	0	1.222433	2.630648	2.235433
30	1	0	2.156225	2.357465	-0.074189
31	7	0	-0.147960	-1.544204	0.230844
32	1	0	1.469782	0.321428	1.816350

Zero-point correction= 0.267455 (Hartree/Particle)
Thermal correction to Energy= 0.281403
Thermal correction to Enthalpy= 0.282347
Thermal correction to Gibbs Free Energy= 0.226507
Sum of electronic and zero-point Energies= -747.159833
Sum of electronic and thermal Energies= -747.145885
Sum of electronic and thermal Enthalpies= -747.144941
Sum of electronic and thermal Free Energies= -747.200781
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -747.62888728

^{3}TS6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.013887	1.652446	-0.418601
2	6	0	-1.866498	2.446035	-0.278947
3	6	0	-1.971915	3.848269	-0.112120
4	6	0	-3.245753	4.418929	-0.109365
5	6	0	-4.382105	3.626164	-0.248873
6	6	0	-4.268552	2.245306	-0.385664
7	1	0	-2.899384	0.584426	-0.554464
8	1	0	-3.359862	5.492375	0.004483
9	1	0	-5.362169	4.093838	-0.245811
10	1	0	-5.151189	1.622183	-0.483616
11	6	0	-0.775532	4.685628	0.150407
12	6	0	0.414538	4.598921	-0.495211
13	6	0	-0.967758	5.701686	1.262042
14	6	0	1.598275	5.501742	-0.191809
15	6	0	0.338309	6.236989	1.838796

16	1	0	-1.564529	6.539933	0.873417
17	6	0	1.249461	6.686915	0.703989
18	1	0	2.376172	4.889850	0.286405
19	1	0	0.832684	5.448232	2.420066
20	1	0	2.170041	7.136941	1.089267
21	1	0	-1.574688	5.236662	2.046016
22	6	0	0.633415	3.649130	-1.598254
23	8	0	0.046110	2.568719	-1.793286
24	8	0	1.564986	4.013806	-2.454964
25	6	0	1.922543	3.043014	-3.454779
26	1	0	1.132529	2.973942	-4.205435
27	1	0	2.845101	3.415483	-3.896632
28	1	0	2.063121	2.070107	-2.979457
29	1	0	2.030326	5.856634	-1.131261
30	1	0	0.737800	7.458608	0.113496
31	1	0	0.125507	7.061571	2.526986
32	45	0	0.270480	-2.307955	0.283716
33	45	0	0.046012	0.123973	0.046107
34	8	0	1.707957	-2.083498	1.714560
35	6	0	2.075023	-0.937449	2.120411
36	8	0	1.591272	0.151068	1.723852
37	8	0	-1.178687	-2.266782	1.751242
38	6	0	-1.716435	-1.157990	2.038388
39	8	0	-1.433345	-0.042639	1.515757
40	8	0	-1.113864	-2.758555	-1.159808
41	6	0	-1.628458	-1.807448	-1.835080
42	8	0	-1.370735	-0.595489	-1.676737
43	8	0	1.717742	-2.237959	-1.159376
44	6	0	2.073746	-1.142388	-1.674180
45	8	0	1.587452	-0.000684	-1.403827
46	6	0	3.180959	-0.882547	3.181114
47	6	0	3.180231	-1.194463	-2.734444
48	6	0	3.743870	-2.274802	3.473846
49	1	0	4.540261	-2.200239	4.224756
50	1	0	2.963498	-2.935257	3.861698
51	6	0	3.753999	-2.609319	-2.852703
52	1	0	2.981031	-3.317107	-3.163346
53	1	0	4.554811	-2.617694	-3.602291
54	6	0	4.293171	-0.179163	-2.355086
55	1	0	5.034009	-0.189087	-3.164688
56	1	0	3.855832	0.824159	-2.329814
57	6	0	2.553966	-0.787482	-4.080063
58	1	0	2.103729	0.207129	-4.030937
59	1	0	3.319149	-0.788767	-4.864866
60	1	0	1.769682	-1.495616	-4.369480
61	6	0	2.558274	-0.289817	4.457634
62	1	0	3.318198	-0.209104	5.243662
63	1	0	2.143932	0.704078	4.264952
64	1	0	1.753052	-0.933241	4.830332
65	6	0	4.295154	0.079252	2.683056
66	1	0	3.850612	1.070967	2.551262
67	1	0	5.041055	0.158680	3.484185
68	6	0	-2.802531	-1.165200	3.117877
69	6	0	-2.641016	-2.215744	-2.914018
70	6	0	-3.910764	-2.171186	2.701910
71	1	0	-4.695508	-2.126304	3.467627
72	6	0	-3.781268	-3.031397	-2.244880
73	1	0	-4.526284	-3.253427	-3.019643
74	1	0	-3.365238	-3.987299	-1.911367
75	6	0	-4.444840	-2.348075	-1.071603
76	6	0	-5.548952	-1.507164	-1.232707
77	6	0	-3.948486	-2.552659	0.217413
78	6	0	-6.131562	-0.890728	-0.128069
79	1	0	-5.965175	-1.350030	-2.224836
80	6	0	-4.507852	-1.929773	1.334639
81	1	0	-3.096311	-3.211630	0.352648
82	6	0	-5.611758	-1.094434	1.147602

83	1	0	-7.005567	-0.257887	-0.260797
84	1	0	-6.075859	-0.615017	2.006086
85	6	0	-2.158159	-1.652968	4.426936
86	1	0	-1.371575	-0.962974	4.752819
87	1	0	-2.914267	-1.704442	5.218896
88	1	0	-1.714912	-2.644375	4.298962
89	6	0	-3.382893	0.238383	3.313091
90	1	0	-4.162977	0.208012	4.083458
91	1	0	-2.606759	0.939038	3.633378
92	1	0	-3.818257	0.628006	2.389015
93	6	0	-1.922435	-3.117225	-3.931199
94	1	0	-2.628513	-3.458161	-4.697665
95	1	0	-1.116929	-2.569286	-4.433641
96	1	0	-1.487447	-3.991433	-3.439215
97	6	0	-3.198211	-0.976111	-3.618539
98	1	0	-2.395843	-0.408557	-4.097930
99	1	0	-3.918693	-1.279876	-4.387994
100	1	0	-3.700181	-0.304366	-2.916976
101	1	0	-3.484956	-3.179096	2.733256
102	1	0	4.156211	-2.738554	2.574441
103	1	0	4.163660	-2.958164	-1.902251
104	6	0	4.974183	-0.467934	-1.036273
105	6	0	4.406981	-0.031616	0.163130
106	6	0	6.156873	-1.208973	-0.985968
107	6	0	4.971439	-0.349462	1.401035
108	1	0	3.492586	0.554195	0.136309
109	6	0	6.744906	-1.516355	0.236782
110	1	0	6.617146	-1.549177	-1.910652
111	6	0	6.152701	-1.094177	1.422919
112	1	0	7.667501	-2.089232	0.265474
113	1	0	6.610728	-1.343905	2.377030
114	7	0	-0.592357	1.905853	-0.230595

Zero-point correction= 0.951999 (Hartree/Particle)
Thermal correction to Energy= 1.008673
Thermal correction to Enthalpy= 1.009617
Thermal correction to Gibbs Free Energy= 0.863321
Sum of electronic and zero-point Energies= -2812.592589
Sum of electronic and thermal Energies= -2812.535915
Sum of electronic and thermal Enthalpies= -2812.534971
Sum of electronic and thermal Free Energies= -2812.681267
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.24980259

^{1}TS7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.533796	2.147744	2.994367
2	6	0	-0.850034	0.799150	2.747839
3	6	0	-2.150388	0.308387	3.029688
4	6	0	-3.071446	1.174654	3.618449
5	6	0	-2.770554	2.514230	3.825641
6	6	0	-1.506283	2.999986	3.490352
7	1	0	0.466468	2.494930	2.761124
8	1	0	-4.039434	0.788257	3.911591
9	1	0	-3.509915	3.171834	4.271178
10	1	0	-1.260071	4.044621	3.658033
11	6	0	-2.325092	-1.152040	2.834374
12	6	0	-3.348326	-1.851765	2.291420
13	6	0	-1.076536	-1.856435	3.286811
14	6	0	-3.248885	-3.356915	2.124993
15	6	0	-0.958802	-3.356746	3.097424
16	6	0	-1.806508	-3.806786	1.919759

17	1	0	-3.681531	-3.859205	3.002341
18	1	0	-1.307847	-3.847325	4.017001
19	1	0	-1.758579	-4.894299	1.799297
20	6	0	-4.636308	-1.303059	1.758974
21	8	0	-5.525871	-2.024806	1.357212
22	8	0	-4.726817	0.027586	1.733859
23	6	0	-5.921354	0.553583	1.156026
24	1	0	-6.034388	0.201876	0.128230
25	1	0	-6.792005	0.252525	1.744469
26	1	0	-5.795054	1.635632	1.174273
27	1	0	-3.874127	-3.652570	1.279990
28	1	0	-1.412474	-3.345038	1.007228
29	1	0	0.093943	-3.632357	2.972352
30	1	0	-0.223099	-1.345191	2.668296
31	1	0	-0.811431	-1.540175	4.302130
32	45	0	0.534422	-0.007313	0.300467
33	45	0	1.256294	0.370639	-1.986857
34	8	0	2.019288	1.322906	0.823255
35	6	0	2.763676	1.859505	-0.051948
36	8	0	2.692460	1.660224	-1.297499
37	8	0	-0.729794	1.571681	0.031697
38	6	0	-0.791566	2.183549	-1.081848
39	8	0	-0.080805	1.934836	-2.092456
40	8	0	-0.842532	-1.328057	-0.469378
41	6	0	-0.969518	-1.447365	-1.735063
42	8	0	-0.233442	-0.890570	-2.590086
43	8	0	1.842112	-1.570052	0.416859
44	6	0	2.530320	-1.863818	-0.608725
45	8	0	2.498817	-1.254206	-1.716781
46	6	0	3.830628	2.839649	0.438865
47	6	0	3.467868	-3.067664	-0.504411
48	6	0	3.804792	2.959844	1.964626
49	1	0	4.594089	3.647757	2.289892
50	1	0	2.844859	3.356567	2.308494
51	6	0	3.416609	-3.679754	0.897932
52	1	0	2.409225	-4.038836	1.128683
53	1	0	4.105573	-4.531045	0.950187
54	6	0	4.909041	-2.604597	-0.860831
55	1	0	5.565266	-3.477657	-0.757058
56	1	0	4.921920	-2.312094	-1.915683
57	6	0	3.008780	-4.104599	-1.544890
58	1	0	3.019362	-3.681041	-2.552881
59	1	0	3.675396	-4.974016	-1.521351
60	1	0	1.992358	-4.452049	-1.326171
61	6	0	3.533572	4.207694	-0.200143
62	1	0	4.295069	4.933336	0.106998
63	1	0	3.531891	4.140356	-1.291417
64	1	0	2.556884	4.585234	0.124093
65	6	0	5.218721	2.345265	-0.058662
66	1	0	5.230128	2.404495	-1.151766
67	1	0	5.967524	3.055457	0.313496
68	6	0	-1.798166	3.332756	-1.132981
69	6	0	-2.086863	-2.362635	-2.242346
70	6	0	-3.141804	2.866354	-0.505438
71	1	0	-3.811331	3.735873	-0.497948
72	6	0	-3.389991	-2.067608	-1.454318
73	1	0	-4.136462	-2.814649	-1.748879
74	1	0	-3.184156	-2.219136	-0.392157
75	6	0	-3.936438	-0.676864	-1.678377
76	6	0	-4.947837	-0.433983	-2.611020
77	6	0	-3.398681	0.406734	-0.982702
78	6	0	-5.387443	0.864641	-2.851606
79	1	0	-5.391112	-1.266377	-3.151926
80	6	0	-3.803636	1.719395	-1.233302
81	1	0	-2.655642	0.226289	-0.215329
82	6	0	-4.810102	1.936754	-2.176173
83	1	0	-6.178850	1.042638	-3.574085

84	1	0	-5.146997	2.950686	-2.378947
85	6	0	-1.217969	4.463803	-0.262246
86	1	0	-0.249750	4.798131	-0.652169
87	1	0	-1.899603	5.321851	-0.267184
88	1	0	-1.084493	4.128694	0.770929
89	6	0	-1.992883	3.820319	-2.569948
90	1	0	-2.721153	4.639793	-2.582968
91	1	0	-1.051771	4.186230	-2.988817
92	1	0	-2.360919	3.020598	-3.218051
93	6	0	-1.649815	-3.816017	-1.979861
94	1	0	-2.409332	-4.503036	-2.368968
95	1	0	-0.703603	-4.033895	-2.487676
96	1	0	-1.523622	-4.014638	-0.912966
97	6	0	-2.294607	-2.163918	-3.747167
98	1	0	-1.395449	-2.436935	-4.305265
99	1	0	-3.120648	-2.800775	-4.084980
100	1	0	-2.538254	-1.126347	-3.987546
101	1	0	-2.958618	2.584338	0.537245
102	1	0	3.960101	1.993101	2.449011
103	1	0	3.697460	-2.954083	1.664920
104	6	0	5.423198	-1.462546	-0.015847
105	6	0	5.182764	-0.145244	-0.410374
106	6	0	6.110167	-1.685512	1.179427
107	6	0	5.572534	0.941646	0.374070
108	1	0	4.665411	0.038458	-1.347440
109	6	0	6.528762	-0.613535	1.962052
110	1	0	6.323080	-2.703898	1.495501
111	6	0	6.256599	0.692496	1.565762
112	1	0	7.071036	-0.796878	2.885248
113	1	0	6.582478	1.526039	2.183287
114	7	0	0.163459	0.007074	2.248071

Zero-point correction= 0.951061 (Hartree/Particle)
Thermal correction to Energy= 1.006647
Thermal correction to Enthalpy= 1.007591
Thermal correction to Gibbs Free Energy= 0.866441
Sum of electronic and zero-point Energies= -2812.625622
Sum of electronic and thermal Energies= -2812.570036
Sum of electronic and thermal Enthalpies= -2812.569092
Sum of electronic and thermal Free Energies= -2812.710242
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.28182113

^{1}TS8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.753760	2.239506	2.783099
2	6	0	0.250575	2.540135	1.794799
3	6	0	1.047308	3.757024	1.955869
4	6	0	0.900719	4.507525	3.128595
5	6	0	-0.027671	4.135242	4.083492
6	6	0	-0.851860	2.999869	3.917350
7	1	0	-1.372057	1.365012	2.616800
8	1	0	1.488919	5.407804	3.274717
9	1	0	-0.145101	4.747393	4.973441
10	1	0	-1.580647	2.750106	4.682362
11	6	0	2.012651	4.034006	0.927488
12	6	0	1.772921	3.676179	-0.370543
13	6	0	3.385989	4.502972	1.374885
14	6	0	2.876341	3.461764	-1.364316
15	6	0	4.383821	4.644271	0.225129
16	6	0	4.257113	3.450864	-0.720145
17	6	0	0.409463	3.645228	-0.999960

18	8	0	0.207022	3.171296	-2.094908
19	8	0	-0.522156	4.281986	-0.277824
20	6	0	-1.871383	4.062466	-0.690896
21	1	0	-2.027254	4.423039	-1.710372
22	1	0	-2.097126	2.994082	-0.643919
23	1	0	-2.485920	4.623472	0.012912
24	45	0	-0.572273	-2.293667	-0.628267
25	45	0	-0.138230	-0.031356	0.164413
26	8	0	0.726176	-2.994596	0.803168
27	6	0	1.277914	-2.164514	1.571764
28	8	0	1.088903	-0.906145	1.563023
29	8	0	-2.110420	-2.389376	0.746017
30	6	0	-2.356943	-1.390129	1.474526
31	8	0	-1.725099	-0.288370	1.458656
32	8	0	-1.799789	-1.452842	-2.043233
33	6	0	-1.970647	-0.200302	-2.070722
34	8	0	-1.457920	0.633099	-1.263248
35	8	0	0.996775	-2.058890	-1.926799
36	6	0	1.620289	-0.963485	-1.951200
37	8	0	1.375404	0.047191	-1.220063
38	6	0	2.246619	-2.677115	2.639730
39	6	0	2.762377	-0.796355	-2.955411
40	6	0	2.498725	-4.176316	2.465696
41	1	0	3.201766	-4.521370	3.233337
42	1	0	1.568559	-4.741685	2.568601
43	6	0	3.054164	-2.117013	-3.671591
44	1	0	2.174709	-2.463949	-4.220428
45	1	0	3.874227	-1.972740	-4.385394
46	6	0	4.022614	-0.281306	-2.204511
47	1	0	4.818752	-0.159553	-2.949715
48	1	0	3.801353	0.710724	-1.800815
49	6	0	2.314926	0.264913	-3.978084
50	1	0	2.014291	1.195098	-3.487669
51	1	0	3.131916	0.477498	-4.677338
52	1	0	1.460194	-0.099868	-4.558959
53	6	0	1.597285	-2.410419	4.010289
54	1	0	2.263035	-2.752809	4.810753
55	1	0	1.400444	-1.343362	4.150177
56	1	0	0.649807	-2.953555	4.103326
57	6	0	3.571551	-1.867452	2.552474
58	1	0	3.346441	-0.820886	2.781167
59	1	0	4.231699	-2.241249	3.345429
60	6	0	-3.512409	-1.527376	2.470170
61	6	0	-2.868149	0.334266	-3.189765
62	6	0	-4.800841	-1.897478	1.682543
63	1	0	-5.616570	-1.978239	2.412001
64	6	0	-4.261854	-0.345663	-3.066477
65	1	0	-4.900007	0.073881	-3.854242
66	1	0	-4.142194	-1.413116	-3.277569
67	6	0	-4.917627	-0.170197	-1.716376
68	6	0	-5.762939	0.908191	-1.444535
69	6	0	-4.651825	-1.081061	-0.692041
70	6	0	-6.309783	1.074072	-0.175251
71	1	0	-5.999204	1.617519	-2.234169
72	6	0	-5.173452	-0.919361	0.592715
73	1	0	-4.008158	-1.931404	-0.897141
74	6	0	-6.012604	0.169483	0.839945
75	1	0	-6.975178	1.909919	0.022263
76	1	0	-6.443236	0.303104	1.829614
77	6	0	-3.168638	-2.683209	3.425934
78	1	0	-2.260396	-2.459324	3.997401
79	1	0	-3.988052	-2.834727	4.137841
80	1	0	-3.006391	-3.612277	2.873120
81	6	0	-3.710933	-0.236647	3.268968
82	1	0	-4.562420	-0.353467	3.949652
83	1	0	-2.824991	-0.013156	3.872407
84	1	0	-3.904744	0.617210	2.614358

85	6	0	-2.226823	-0.077584	-4.526828
86	1	0	-2.864756	0.243122	-5.358339
87	1	0	-1.248038	0.400323	-4.646913
88	1	0	-2.093707	-1.161245	-4.581963
89	6	0	-2.992870	1.856532	-3.130452
90	1	0	-2.007795	2.330436	-3.148082
91	1	0	-3.573163	2.207226	-3.992511
92	1	0	-3.507658	2.176746	-2.220942
93	1	0	-4.656603	-2.890636	1.245609
94	1	0	2.918484	-4.401096	1.482257
95	1	0	3.339254	-2.902282	-2.967102
96	6	0	4.492568	-1.185190	-1.088323
97	6	0	3.934558	-1.072405	0.187576
98	6	0	5.450271	-2.176446	-1.313339
99	6	0	4.271697	-1.955435	1.215998
100	1	0	3.200414	-0.294166	0.376410
101	6	0	5.823796	-3.042195	-0.290057
102	1	0	5.904069	-2.270795	-2.297037
103	6	0	5.231941	-2.938141	0.964876
104	1	0	6.575389	-3.804943	-0.473004
105	1	0	5.516609	-3.625615	1.757897
106	7	0	0.576040	1.711496	0.837256
107	1	0	3.771719	3.787596	2.113581
108	1	0	3.282747	5.459471	1.903908
109	1	0	5.396950	4.725863	0.631761
110	1	0	4.183778	5.568953	-0.332211
111	1	0	5.029957	3.476786	-1.494862
112	1	0	4.395003	2.518161	-0.156563
113	1	0	2.816123	4.225300	-2.152529
114	1	0	2.652798	2.510128	-1.857493

Zero-point correction= 0.953189 (Hartree/Particle)
Thermal correction to Energy= 1.009133
Thermal correction to Enthalpy= 1.010077
Thermal correction to Gibbs Free Energy= 0.867122
Sum of electronic and zero-point Energies= -2812.645817
Sum of electronic and thermal Energies= -2812.589873
Sum of electronic and thermal Enthalpies= -2812.588929
Sum of electronic and thermal Free Energies= -2812.731884
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.30420689

^{1}TS9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.280735	2.470346	0.313207
2	6	0	0.918152	2.809922	0.203371
3	6	0	0.540922	4.177033	0.095140
4	6	0	1.535468	5.154299	0.095625
5	6	0	2.879440	4.798366	0.186320
6	6	0	3.252782	3.459668	0.281366
7	1	0	2.560769	1.429722	0.411843
8	1	0	1.267466	6.204144	0.022740
9	1	0	3.638462	5.575409	0.182462
10	1	0	4.299372	3.179957	0.350211
11	6	0	-0.881717	4.553626	-0.089695
12	6	0	-1.912784	4.071790	0.640278
13	6	0	-1.125288	5.552681	-1.205259
14	6	0	-3.354972	4.498032	0.435182
15	6	0	-2.576093	5.596809	-1.674659
16	1	0	-0.819697	6.552211	-0.862433
17	6	0	-3.502597	5.718225	-0.470320
18	1	0	-3.899681	3.645724	0.003803

19	1	0	-2.808721	4.677158	-2.226763
20	1	0	-4.546958	5.818060	-0.783594
21	1	0	-0.458083	5.302327	-2.037263
22	6	0	-1.692671	3.131063	1.760978
23	8	0	-0.845837	2.235954	1.836881
24	8	0	-2.523820	3.319962	2.775977
25	6	0	-2.396202	2.412047	3.877870
26	1	0	-1.449060	2.580739	4.395169
27	1	0	-3.238238	2.633980	4.531532
28	1	0	-2.433031	1.382027	3.519483
29	1	0	-3.817528	4.692082	1.406661
30	1	0	-3.247685	6.626716	0.091624
31	1	0	-2.715584	6.434190	-2.366449
32	45	0	0.393156	-2.506473	-0.401728
33	45	0	0.133626	-0.116406	0.006930
34	8	0	-1.028448	-2.321193	-1.876354
35	6	0	-1.541399	-1.192209	-2.106574
36	8	0	-1.253846	-0.106357	-1.512317
37	8	0	1.848883	-2.032866	-1.794768
38	6	0	2.106291	-0.816092	-2.009383
39	8	0	1.578993	0.169440	-1.411752
40	8	0	1.773541	-2.500383	1.151874
41	6	0	2.015831	-1.423304	1.764193
42	8	0	1.516469	-0.287778	1.498593
43	8	0	-1.097844	-2.818535	0.974270
44	6	0	-1.624623	-1.834058	1.556715
45	8	0	-1.310488	-0.612447	1.391880
46	6	0	-2.588996	-1.080800	-3.218483
47	6	0	-2.725185	-2.109534	2.586704
48	6	0	-2.969889	-2.464804	-3.748416
49	1	0	-3.725295	-2.361129	-4.536833
50	1	0	-2.098007	-2.973393	-4.168297
51	6	0	-3.122434	-3.587652	2.575299
52	1	0	-2.268353	-4.221128	2.828387
53	1	0	-3.915064	-3.760407	3.313525
54	6	0	-3.949294	-1.202147	2.280996
55	1	0	-4.700771	-1.393907	3.057460
56	1	0	-3.636933	-0.157559	2.379783
57	6	0	-2.156909	-1.738422	3.968463
58	1	0	-1.812054	-0.700617	3.989042
59	1	0	-2.924294	-1.872802	4.739579
60	1	0	-1.306674	-2.381884	4.221213
61	6	0	-1.962789	-0.241175	-4.347159
62	1	0	-2.682334	-0.118489	-5.164972
63	1	0	-1.670816	0.748159	-3.982851
64	1	0	-1.073219	-0.737764	-4.751350
65	6	0	-3.832977	-0.325782	-2.671554
66	1	0	-3.521358	0.686596	-2.395281
67	1	0	-4.548481	-0.235249	-3.498749
68	6	0	3.158113	-0.488112	-3.072067
69	6	0	3.011487	-1.478488	2.925918
70	6	0	4.518686	-1.071827	-2.596561
71	1	0	5.278187	-0.770938	-3.328997
72	6	0	4.395865	-1.893920	2.352380
73	1	0	5.118026	-1.855927	3.177569
74	1	0	4.329690	-2.937013	2.026212
75	6	0	4.874587	-1.043877	1.199169
76	6	0	5.618963	0.121175	1.398149
77	6	0	4.552033	-1.412557	-0.108018
78	6	0	6.020436	0.893717	0.311489
79	1	0	5.897754	0.416167	2.406741
80	6	0	4.933222	-0.643413	-1.208696
81	1	0	3.978105	-2.320652	-0.272746
82	6	0	5.676464	0.517717	-0.984290
83	1	0	6.617628	1.787151	0.474927
84	1	0	5.998739	1.121856	-1.828818
85	6	0	2.753816	-1.180361	-4.383351

86	1	0	1.803223	-0.781821	-4.755661
87	1	0	3.517773	-1.004216	-5.149355
88	1	0	2.640554	-2.257917	-4.238947
89	6	0	3.258756	1.024619	-3.288970
90	1	0	4.019448	1.234924	-4.050522
91	1	0	2.303591	1.432211	-3.632876
92	1	0	3.527302	1.550003	-2.369156
93	6	0	2.541898	-2.555908	3.916151
94	1	0	3.266160	-2.653745	4.733068
95	1	0	1.573625	-2.285845	4.353050
96	1	0	2.436081	-3.524220	3.420265
97	6	0	3.097761	-0.122456	3.632318
98	1	0	2.123872	0.167121	4.037705
99	1	0	3.814142	-0.185649	4.460349
100	1	0	3.418156	0.669496	2.951030
101	1	0	4.450316	-2.164131	-2.629706
102	1	0	-3.376740	-3.099673	-2.957451
103	1	0	-3.487550	-3.897361	1.593280
104	6	0	-4.554118	-1.416550	0.912727
105	6	0	-4.032251	-0.746116	-0.195279
106	6	0	-5.603930	-2.316364	0.716163
107	6	0	-4.495874	-0.993605	-1.489199
108	1	0	-3.225284	-0.033882	-0.052083
109	6	0	-6.101674	-2.549597	-0.562148
110	1	0	-6.031054	-2.838791	1.568930
111	6	0	-5.545330	-1.899210	-1.659460
112	1	0	-6.922918	-3.246324	-0.704616
113	1	0	-5.927388	-2.096283	-2.658282
114	7	0	-0.100837	1.883860	0.124039

Zero-point correction= 0.954020 (Hartree/Particle)
Thermal correction to Energy= 1.009795
Thermal correction to Enthalpy= 1.010740
Thermal correction to Gibbs Free Energy= 0.868302
Sum of electronic and zero-point Energies= -2812.631184
Sum of electronic and thermal Energies= -2812.575408
Sum of electronic and thermal Enthalpies= -2812.574464
Sum of electronic and thermal Free Energies= -2812.716902
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2814.28893467

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.925826	-0.976118	-0.945264
2	6	0	-1.574296	-0.818074	-0.679160
3	6	0	-1.139727	-0.032686	0.395507
4	6	0	-2.038325	0.622844	1.217209
5	6	0	-3.401918	0.467338	0.952930
6	6	0	-3.835641	-0.321520	-0.113058
7	1	0	-3.254704	-1.589850	-1.777302
8	1	0	-1.694084	1.243117	2.040143
9	1	0	-4.131545	0.966552	1.583266
10	1	0	-4.900390	-0.427278	-0.299258
11	6	0	0.368677	-0.089181	0.388276
12	6	0	0.581240	-0.980309	-0.830824
13	6	0	1.011370	-0.774951	1.611155
14	6	0	1.964769	-1.425913	-1.162927
15	6	0	2.471531	-1.143207	1.320751
16	1	0	0.939048	-0.105392	2.472652
17	6	0	2.601605	-2.054748	0.094699
18	1	0	1.937434	-2.131864	-1.996567
19	1	0	2.900993	-1.639155	2.197933

20	1	0	2.102361	-3.010332	0.300589
21	1	0	0.433789	-1.679386	1.836074
22	6	0	0.915763	1.325023	0.227162
23	8	0	1.245355	2.036494	1.146234
24	8	0	0.940450	1.706359	-1.055104
25	6	0	1.343515	3.056737	-1.287555
26	1	0	0.657928	3.748363	-0.792454
27	1	0	2.355264	3.224598	-0.910891
28	1	0	1.307966	3.189776	-2.367988
29	1	0	2.556660	-0.553700	-1.471881
30	1	0	3.655231	-2.279646	-0.102049
31	1	0	3.052215	-0.223936	1.166105
32	7	0	-0.494433	-1.400870	-1.391544

Zero-point correction= 0.269750 (Hartree/Particle)
Thermal correction to Energy= 0.283853
Thermal correction to Enthalpy= 0.284797
Thermal correction to Gibbs Free Energy= 0.228509
Sum of electronic and zero-point Energies= -747.239711
Sum of electronic and thermal Energies= -747.225608
Sum of electronic and thermal Enthalpies= -747.224664
Sum of electronic and thermal Free Energies= -747.280952
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -747.70899956

6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.383028	-2.232966	0.004252
2	6	0	-1.311127	-1.351663	-0.001749
3	6	0	-1.492117	0.034973	-0.028591
4	6	0	-2.769551	0.569992	-0.051553
5	6	0	-3.857045	-0.306939	-0.044364
6	6	0	-3.666602	-1.690012	-0.016454
7	1	0	-2.214749	-3.304617	0.023439
8	1	0	-2.929588	1.644682	-0.078297
9	1	0	-4.866586	0.092900	-0.062670
10	1	0	-4.529346	-2.349164	-0.013272
11	6	0	-0.127756	0.675314	-0.012176
12	6	0	0.710052	-0.592513	0.001413
13	6	0	0.143035	1.619591	-1.234222
14	6	0	0.106630	1.574795	1.244352
15	6	0	0.617779	2.953914	-0.640315
16	1	0	0.872038	1.192060	-1.926643
17	6	0	-0.061687	3.006541	0.728681
18	1	0	-0.574221	1.312881	2.058450
19	1	0	0.369755	3.805234	-1.281538
20	1	0	-1.126489	3.250974	0.618018
21	1	0	-0.791946	1.755019	-1.787012
22	6	0	2.201374	-0.545919	-0.008870
23	8	0	2.826603	0.493007	-0.073017
24	8	0	2.763896	-1.750440	0.056305
25	6	0	4.190606	-1.755197	0.040789
26	1	0	4.478122	-2.804102	0.099220
27	1	0	4.566318	-1.304106	-0.881043
28	1	0	4.585867	-1.199622	0.894948
29	1	0	0.378865	3.746510	1.403703
30	1	0	1.703900	2.927971	-0.507821
31	7	0	0.059675	-1.701333	0.012580
32	1	0	1.132960	1.442712	1.598996

Zero-point correction= 0.269398 (Hartree/Particle)
Thermal correction to Energy= 0.283688

Thermal correction to Enthalpy= 0.284632
Thermal correction to Gibbs Free Energy= 0.227716
Sum of electronic and zero-point Energies= -747.226286
Sum of electronic and thermal Energies= -747.211997
Sum of electronic and thermal Enthalpies= -747.211052
Sum of electronic and thermal Free Energies= -747.267969
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -747.69321810

INT1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.104802	-0.020935	-0.429637
2	6	0	1.805586	-0.449799	-0.123602
3	6	0	0.724839	0.128367	-0.822539
4	6	0	0.975491	1.130375	-1.761072
5	6	0	2.268347	1.555497	-2.044487
6	6	0	3.337154	0.964000	-1.381102
7	1	0	3.949247	-0.455128	0.096397
8	1	0	0.130452	1.567082	-2.286427
9	1	0	2.437323	2.330774	-2.785323
10	1	0	4.356097	1.273473	-1.594009
11	6	0	1.642686	-1.477261	0.915588
12	7	0	0.549704	-1.535552	1.614937
13	7	0	-0.399537	-1.623272	2.243772
14	6	0	-0.677823	-0.357720	-0.676696
15	6	0	-1.663883	0.364151	-0.120160
16	6	0	-0.943309	-1.708796	-1.308588
17	6	0	-3.113116	-0.064286	-0.120615
18	6	0	-2.302476	-2.292023	-0.928963
19	1	0	-0.865792	-1.592011	-2.399520
20	6	0	-3.385480	-1.224803	-1.074863
21	1	0	-3.391768	-0.348571	0.904477
22	1	0	-2.270548	-2.638225	0.112052
23	1	0	-4.377529	-1.644406	-0.877636
24	1	0	-0.133661	-2.393386	-1.027427
25	6	0	2.752215	-2.411941	1.330252
26	1	0	3.220886	-2.856033	0.445954
27	1	0	3.533724	-1.899058	1.905661
28	1	0	2.362782	-3.223434	1.950633
29	6	0	-1.421442	1.680756	0.540561
30	8	0	-2.199771	2.608674	0.502902
31	8	0	-0.268568	1.718836	1.225520
32	6	0	0.054165	2.974437	1.815240
33	1	0	0.126871	3.750115	1.048649
34	1	0	-0.705429	3.265027	2.545105
35	1	0	1.018413	2.828678	2.301281
36	1	0	-3.727492	0.806795	-0.370529
37	1	0	-3.392786	-0.855915	-2.109288
38	1	0	-2.521796	-3.164198	-1.554304

Zero-point correction= 0.317827 (Hartree/Particle)
Thermal correction to Energy= 0.336695
Thermal correction to Enthalpy= 0.337640
Thermal correction to Gibbs Free Energy= 0.270118
Sum of electronic and zero-point Energies= -879.849347
Sum of electronic and thermal Energies= -879.830479
Sum of electronic and thermal Enthalpies= -879.829535
Sum of electronic and thermal Free Energies= -879.897057
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -880.39968702

INT2b

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.886526	0.458152	-2.052125
2	6	0	-1.997404	1.425392	-1.564118
3	6	0	-2.517423	2.485128	-0.801330
4	6	0	-3.895921	2.539873	-0.567408
5	6	0	-4.766383	1.578808	-1.063570
6	6	0	-4.250808	0.526301	-1.810303
7	1	0	-2.502706	-0.393257	-2.605879
8	1	0	-4.280891	3.368769	0.020042
9	1	0	-5.831027	1.650762	-0.865050
10	1	0	-4.901838	-0.254238	-2.191417
11	6	0	-0.526823	1.270011	-1.832359
12	7	0	-0.304400	0.507215	-2.935178
13	7	0	-0.058011	-0.170693	-3.793116
14	6	0	-1.707843	3.532084	-0.118431
15	6	0	-1.601733	4.820102	-0.492809
16	6	0	-1.094100	3.170769	1.211634
17	6	0	-0.914157	5.770754	0.453917
18	6	0	-1.585457	4.128419	2.311279
19	1	0	-1.296184	2.128833	1.458408
20	6	0	-1.454907	5.610923	1.889648
21	1	0	0.166153	5.560930	0.449702
22	1	0	-1.021631	3.929791	3.229732
23	1	0	-0.798471	6.153568	2.577914
24	1	0	-0.005248	3.251948	1.130645
25	6	0	0.461725	2.437709	-1.846362
26	1	0	0.088674	3.263046	-2.460917
27	1	0	0.642839	2.788034	-0.832931
28	1	0	1.423079	2.085072	-2.230325
29	6	0	-2.150430	5.393181	-1.747554
30	8	0	-2.413337	6.566888	-1.899642
31	8	0	-2.301800	4.483148	-2.726518
32	6	0	-2.881583	4.973146	-3.931679
33	1	0	-3.876462	5.383582	-3.741668
34	1	0	-2.255300	5.753833	-4.371104
35	1	0	-2.945464	4.111884	-4.596359
36	1	0	-1.043538	6.798829	0.109192
37	1	0	-2.433501	6.098964	1.941626
38	1	0	-2.632231	3.893443	2.535462
39	45	0	1.111524	-1.949394	1.239305
40	45	0	0.253700	-0.298981	-0.299143
41	8	0	0.098252	-3.374907	0.158950
42	6	0	-0.531034	-3.037795	-0.878558
43	8	0	-0.654693	-1.845467	-1.311039
44	8	0	2.693478	-2.183261	-0.073578
45	6	0	2.761965	-1.474703	-1.117605
46	8	0	1.913336	-0.597651	-1.466937
47	8	0	2.083332	-0.417293	2.217084
48	6	0	2.008026	0.761211	1.763534
49	8	0	1.311862	1.121671	0.766985
50	8	0	-0.547404	-1.655072	2.408147
51	6	0	-1.436981	-0.846092	2.024562
52	8	0	-1.371449	-0.121169	0.981504
53	6	0	-1.190574	-4.133597	-1.718308
54	6	0	-2.695740	-0.705264	2.888755
55	6	0	-0.996198	-5.504272	-1.065848
56	1	0	-1.468105	-6.274333	-1.687483
57	1	0	0.066388	-5.742000	-0.966904
58	6	0	-2.669640	-1.716552	4.038176
59	1	0	-1.824099	-1.527870	4.705444
60	1	0	-3.595624	-1.630183	4.618944
61	6	0	-3.955423	-0.896797	1.999654
62	1	0	-4.829986	-0.740043	2.643834
63	1	0	-3.961635	-0.106055	1.241928
64	6	0	-2.731330	0.724553	3.457848
65	1	0	-2.892146	1.459549	2.664959

66	1	0	-3.552960	0.812516	4.177319
67	1	0	-1.798861	0.970468	3.978986
68	6	0	-0.523813	-4.114598	-3.105465
69	1	0	-0.977265	-4.878521	-3.746957
70	1	0	-0.639091	-3.139329	-3.587009
71	1	0	0.546825	-4.333901	-3.023843
72	6	0	-2.701253	-3.807587	-1.880754
73	1	0	-2.793275	-2.884047	-2.462911
74	1	0	-3.145956	-4.612582	-2.478819
75	6	0	3.952503	-1.719228	-2.046195
76	6	0	2.807200	1.834696	2.511804
77	6	0	5.262304	-1.658841	-1.211881
78	1	0	6.094099	-1.862196	-1.897658
79	6	0	4.269731	1.340061	2.695536
80	1	0	4.794167	2.092599	3.297267
81	1	0	4.248737	0.413103	3.276604
82	6	0	5.004295	1.112889	1.394649
83	6	0	5.748307	2.127401	0.787180
84	6	0	4.905192	-0.119028	0.746918
85	6	0	6.355602	1.914455	-0.446672
86	1	0	5.853505	3.088935	1.283792
87	6	0	5.481375	-0.341153	-0.505705
88	1	0	4.351008	-0.921702	1.222830
89	6	0	6.214945	0.690592	-1.094771
90	1	0	6.938999	2.707053	-0.906602
91	1	0	6.682602	0.532722	-2.063722
92	6	0	3.791484	-3.138299	-2.621588
93	1	0	2.867832	-3.216588	-3.206581
94	1	0	4.632245	-3.368515	-3.285575
95	1	0	3.760236	-3.885164	-1.823297
96	6	0	3.978845	-0.698449	-3.186865
97	1	0	4.842458	-0.895521	-3.832750
98	1	0	3.072357	-0.768612	-3.794723
99	1	0	4.057102	0.324210	-2.808496
100	6	0	2.154245	1.994552	3.897092
101	1	0	2.687513	2.757557	4.475157
102	1	0	1.109533	2.312994	3.797589
103	1	0	2.176358	1.052616	4.452422
104	6	0	2.786379	3.175181	1.771781
105	1	0	1.786913	3.616954	1.779842
106	1	0	3.462004	3.877934	2.273233
107	1	0	3.106240	3.070325	0.732373
108	1	0	5.238262	-2.470286	-0.477949
109	1	0	-1.441471	-5.539575	-0.068741
110	1	0	-2.583715	-2.741617	3.670419
111	6	0	-4.049254	-2.240680	1.319395
112	6	0	-3.440044	-2.421842	0.078417
113	6	0	-4.706246	-3.325551	1.903575
114	6	0	-3.443784	-3.654537	-0.574346
115	1	0	-2.942342	-1.576899	-0.383821
116	6	0	-4.738155	-4.558355	1.258115
117	1	0	-5.196631	-3.203505	2.866356
118	6	0	-4.108008	-4.724910	0.027677
119	1	0	-5.256724	-5.395639	1.716471
120	1	0	-4.133438	-5.691856	-0.469096

Zero-point correction= 1.005466 (Hartree/Particle)
Thermal correction to Energy= 1.066103
Thermal correction to Enthalpy= 1.067047
Thermal correction to Gibbs Free Energy= 0.913199
Sum of electronic and zero-point Energies= -2945.373930
Sum of electronic and thermal Energies= -2945.313293
Sum of electronic and thermal Enthalpies= -2945.312349
Sum of electronic and thermal Free Energies= -2945.466196
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2947.11945975

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.603326	1.263413	1.960211
2	6	0	1.475681	1.945504	1.482063
3	6	0	1.666292	3.178610	0.831926
4	6	0	2.964106	3.688285	0.707877
5	6	0	4.066200	3.013474	1.212841
6	6	0	3.881243	1.785930	1.841382
7	1	0	2.474553	0.285973	2.414214
8	1	0	3.093710	4.639850	0.200399
9	1	0	5.059890	3.437199	1.106034
10	1	0	4.729042	1.222578	2.218173
11	6	0	0.132733	1.292940	1.553666
12	7	0	0.180853	0.460566	3.099066
13	7	0	0.038429	-0.332719	3.853897
14	6	0	0.595644	3.920006	0.113116
15	6	0	0.059287	5.101349	0.468355
16	6	0	0.173893	3.364261	-1.225353
17	6	0	-0.878284	5.764074	-0.508512
18	6	0	0.337143	4.421571	-2.331048
19	1	0	0.723955	2.450815	-1.453590
20	6	0	-0.277739	5.782915	-1.928567
21	1	0	-1.828029	5.208229	-0.525340
22	1	0	-0.120709	4.039466	-3.250212
23	1	0	-1.055396	6.081795	-2.639018
24	1	0	-0.878085	3.066158	-1.168264
25	6	0	-1.106126	2.125024	1.790066
26	1	0	-0.947947	2.970495	2.466261
27	1	0	-1.424678	2.500566	0.815482
28	1	0	-1.920725	1.483290	2.137346
29	6	0	0.337874	5.822013	1.735960
30	8	0	0.159591	7.010595	1.894037
31	8	0	0.783775	5.018710	2.718932
32	6	0	1.117175	5.674540	3.938618
33	1	0	1.888410	6.430663	3.771687
34	1	0	0.236408	6.157079	4.370078
35	1	0	1.488052	4.891698	4.599905
36	1	0	-1.106165	6.779075	-0.176446
37	1	0	0.491495	6.561174	-1.961958
38	1	0	1.405533	4.540488	-2.543819
39	45	0	-0.494035	-2.236931	-1.231787
40	45	0	-0.137028	-0.352127	0.282678
41	8	0	0.886773	-3.282037	-0.113285
42	6	0	1.387065	-2.759693	0.913169
43	8	0	1.155619	-1.575870	1.333765
44	8	0	-1.949509	-2.861387	0.113039
45	6	0	-2.216007	-2.172464	1.134269
46	8	0	-1.653030	-1.078213	1.458405
47	8	0	-1.853623	-1.047889	-2.239793
48	6	0	-2.103172	0.115238	-1.820100
49	8	0	-1.539669	0.684112	-0.833523
50	8	0	1.027582	-1.490684	-2.402384
51	6	0	1.645805	-0.456925	-2.036563
52	8	0	1.376297	0.244404	-1.006576
53	6	0	2.341065	-3.601718	1.764926
54	6	0	2.815847	0.025521	-2.904313
55	6	0	2.563967	-4.972720	1.121332
56	1	0	3.242461	-5.565058	1.746685
57	1	0	1.619771	-5.515110	1.023783
58	6	0	3.095951	-0.980219	-4.024339
59	1	0	2.235448	-1.068712	-4.693103
60	1	0	3.957990	-0.641923	-4.611799
61	6	0	4.071243	0.235713	-2.012705

62	1	0	4.864992	0.627679	-2.661279
63	1	0	3.839757	1.010689	-1.273523
64	6	0	2.429589	1.385001	-3.514926
65	1	0	2.352668	2.156726	-2.744461
66	1	0	3.195181	1.696689	-4.234139
67	1	0	1.472282	1.324417	-4.045275
68	6	0	1.697751	-3.775191	3.151877
69	1	0	2.349430	-4.380482	3.791947
70	1	0	1.534536	-2.808321	3.636637
71	1	0	0.732622	-4.287924	3.071224
72	6	0	3.686584	-2.842240	1.926140
73	1	0	3.497960	-1.923808	2.493160
74	1	0	4.343388	-3.470124	2.541118
75	6	0	-3.291240	-2.714251	2.079655
76	6	0	-3.163847	0.908085	-2.595018
77	6	0	-4.572864	-3.020261	1.255507
78	1	0	-5.319283	-3.424684	1.950550
79	6	0	-4.443388	0.035565	-2.730569
80	1	0	-5.157504	0.601106	-3.342095
81	1	0	-4.183397	-0.870879	-3.285618
82	6	0	-5.075010	-0.339383	-1.410231
83	6	0	-6.056365	0.456598	-0.814673
84	6	0	-4.646896	-1.484005	-0.736455
85	6	0	-6.577024	0.119382	0.431016
86	1	0	-6.416817	1.343254	-1.330613
87	6	0	-5.136489	-1.822698	0.526731
88	1	0	-3.900029	-2.119666	-1.201663
89	6	0	-6.114468	-1.008901	1.102316
90	1	0	-7.347477	0.739095	0.881057
91	1	0	-6.520044	-1.263365	2.078725
92	6	0	-2.753240	-4.029962	2.670707
93	1	0	-1.838057	-3.850636	3.247076
94	1	0	-3.497454	-4.466987	3.346042
95	1	0	-2.527496	-4.751906	1.881007
96	6	0	-3.586975	-1.721861	3.206991
97	1	0	-4.368339	-2.129043	3.859440
98	1	0	-2.694768	-1.544218	3.814278
99	1	0	-3.929971	-0.760447	2.815742
100	6	0	-2.588987	1.172023	-3.998551
101	1	0	-3.306191	1.747151	-4.595036
102	1	0	-1.660187	1.751579	-3.934237
103	1	0	-2.373019	0.233198	-4.515912
104	6	0	-3.494973	2.237822	-1.912204
105	1	0	-2.651396	2.930944	-1.965104
106	1	0	-4.341553	2.710612	-2.423824
107	1	0	-3.760393	2.099651	-0.861250
108	1	0	-4.334190	-3.809447	0.535874
109	1	0	2.999939	-4.879200	0.123870
110	1	0	3.313537	-1.974191	-3.626887
111	6	0	4.552786	-1.005456	-1.299996
112	6	0	4.004052	-1.337712	-0.062053
113	6	0	5.516834	-1.853652	-1.848990
114	6	0	4.366760	-2.498033	0.622020
115	1	0	3.265085	-0.673326	0.370216
116	6	0	5.905922	-3.006683	-1.172681
117	1	0	5.966241	-1.609711	-2.808581
118	6	0	5.332594	-3.330583	0.053929
119	1	0	6.661269	-3.657586	-1.603769
120	1	0	5.638168	-4.235306	0.574116

Zero-point correction= 1.003025 (Hartree/Particle)
Thermal correction to Energy= 1.063628
Thermal correction to Enthalpy= 1.064572
Thermal correction to Gibbs Free Energy= 0.911004
Sum of electronic and zero-point Energies= -2945.361087
Sum of electronic and thermal Energies= -2945.300484
Sum of electronic and thermal Enthalpies= -2945.299540

Sum of electronic and thermal Free Energies= -2945.453108
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2947.10518524

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.969640	2.580709	-2.022858
2	6	0	0.279746	2.429273	-1.402448
3	6	0	0.974069	3.569126	-0.934160
4	6	0	0.391366	4.823265	-1.106792
5	6	0	-0.826696	4.966369	-1.765760
6	6	0	-1.506114	3.844337	-2.230901
7	1	0	-1.498745	1.689949	-2.342997
8	1	0	0.902225	5.695251	-0.708795
9	1	0	-1.254291	5.955847	-1.896897
10	1	0	-2.467289	3.948275	-2.724316
11	6	0	0.822871	1.087849	-1.255611
12	6	0	2.195045	3.428973	-0.101970
13	6	0	3.396984	3.983834	-0.345300
14	6	0	2.065310	2.629947	1.174239
15	6	0	4.468243	3.838658	0.706006
16	6	0	2.588912	3.406665	2.397412
17	1	0	1.033523	2.308898	1.334476
18	6	0	3.909629	4.154249	2.105108
19	1	0	4.849859	2.806413	0.690491
20	1	0	2.713383	2.697401	3.223462
21	1	0	4.666698	3.911627	2.857695
22	1	0	2.649814	1.708643	1.060763
23	6	0	2.196765	0.810145	-1.728233
24	1	0	2.733501	1.677763	-2.120346
25	1	0	2.763261	0.305270	-0.934893
26	1	0	2.090657	0.040720	-2.510050
27	6	0	3.756265	4.743324	-1.571606
28	8	0	4.621541	5.590433	-1.616439
29	8	0	3.049191	4.365098	-2.650652
30	6	0	3.317707	5.092891	-3.845891
31	1	0	3.136396	6.160030	-3.695254
32	1	0	4.355621	4.950274	-4.157272
33	1	0	2.633426	4.690828	-4.592446
34	1	0	5.307834	4.496656	0.471039
35	1	0	3.743999	5.234996	2.164494
36	1	0	1.820825	4.119451	2.716368
37	45	0	-1.229058	-2.138980	0.964258
38	45	0	-0.138262	-0.342308	-0.327078
39	8	0	-2.884778	-1.892022	-0.242244
40	6	0	-2.852508	-1.052241	-1.173375
41	8	0	-1.864743	-0.294853	-1.462999
42	8	0	-0.436718	-3.437846	-0.453717
43	6	0	0.278298	-2.998738	-1.392854
44	8	0	0.584466	-1.778506	-1.591386
45	8	0	0.501658	-2.231443	2.099865
46	6	0	1.469902	-1.474117	1.832343
47	8	0	1.501461	-0.607307	0.899979
48	8	0	-1.933586	-0.662544	2.227506
49	6	0	-1.653196	0.541405	2.006170
50	8	0	-0.929967	0.977648	1.047579
51	6	0	-4.080272	-0.917888	-2.079836
52	6	0	-2.192775	1.605576	2.967388
53	6	0	-5.202387	-1.841475	-1.599678
54	1	0	-6.073928	-1.729828	-2.255625
55	1	0	-4.883481	-2.887017	-1.622984
56	6	0	-3.118568	0.968010	4.006376
57	1	0	-2.580280	0.229616	4.606728
58	1	0	-3.505427	1.744512	4.677132

59	6	0	-2.936386	2.700463	2.151299
60	1	0	-3.291339	3.453102	2.866495
61	1	0	-2.210798	3.190759	1.493192
62	6	0	-0.990177	2.255749	3.674626
63	1	0	-0.339850	2.769092	2.961250
64	1	0	-1.343755	2.989949	4.407278
65	1	0	-0.395692	1.505629	4.208653
66	6	0	-3.650350	-1.311619	-3.504362
67	1	0	-4.500937	-1.222223	-4.189523
68	1	0	-2.842183	-0.668217	-3.864351
69	1	0	-3.302307	-2.350422	-3.532250
70	6	0	-4.553054	0.563112	-2.094045
71	1	0	-3.776107	1.169746	-2.571801
72	1	0	-5.438033	0.612190	-2.740900
73	6	0	0.815792	-4.019695	-2.399473
74	6	0	2.712952	-1.600105	2.720632
75	6	0	1.603987	-5.112576	-1.623917
76	1	0	1.980547	-5.829593	-2.364045
77	6	0	3.189368	-3.079852	2.687668
78	1	0	4.071320	-3.152669	3.336247
79	1	0	2.405298	-3.700249	3.132584
80	6	0	3.515282	-3.591775	1.304360
81	6	0	4.797020	-3.473574	0.761697
82	6	0	2.509999	-4.163509	0.522582
83	6	0	5.055516	-3.905946	-0.535624
84	1	0	5.597686	-3.046843	1.361183
85	6	0	2.744454	-4.578941	-0.789369
86	1	0	1.514219	-4.274468	0.941736
87	6	0	4.034393	-4.450147	-1.309294
88	1	0	6.057666	-3.819500	-0.946018
89	1	0	4.240405	-4.783006	-2.323764
90	6	0	-0.397040	-4.676354	-3.082230
91	1	0	-0.979304	-3.933466	-3.639460
92	1	0	-0.056913	-5.439331	-3.791577
93	1	0	-1.053627	-5.147666	-2.345945
94	6	0	1.701705	-3.346644	-3.451063
95	1	0	2.070124	-4.100919	-4.156487
96	1	0	1.138417	-2.596966	-4.014325
97	1	0	2.562326	-2.851036	-2.994422
98	6	0	2.289154	-1.246265	4.157111
99	1	0	3.146091	-1.341644	4.833531
100	1	0	1.927820	-0.212489	4.212800
101	1	0	1.491410	-1.908216	4.504255
102	6	0	3.832138	-0.659620	2.267782
103	1	0	3.543121	0.386243	2.404520
104	1	0	4.729003	-0.840444	2.871750
105	1	0	4.088653	-0.811059	1.216270
106	1	0	0.899588	-5.648920	-0.980350
107	1	0	-5.502668	-1.607583	-0.575547
108	1	0	-3.963846	0.461846	3.534376
109	6	0	-4.091077	2.180978	1.327913
110	6	0	-3.859388	1.704616	0.037393
111	6	0	-5.389974	2.119906	1.836712
112	6	0	-4.873868	1.135789	-0.733422
113	1	0	-2.856250	1.770294	-0.369101
114	6	0	-6.420505	1.579118	1.073302
115	1	0	-5.594676	2.498836	2.835077
116	6	0	-6.164096	1.082850	-0.201562
117	1	0	-7.428661	1.541147	1.476002
118	1	0	-6.971940	0.654583	-0.790090

Zero-point correction= 0.994189 (Hartree/Particle)
Thermal correction to Energy= 1.053016
Thermal correction to Enthalpy= 1.053960
Thermal correction to Gibbs Free Energy= 0.903002
Sum of electronic and zero-point Energies= -2835.911061
Sum of electronic and thermal Energies= -2835.852233

Sum of electronic and thermal Enthalpies= -2835.851289
Sum of electronic and thermal Free Energies= -2836.002248
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2837.61766675

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.865999	1.370645	3.394008
2	6	0	-1.088609	0.102128	2.848624
3	6	0	-2.381985	-0.448980	2.853888
4	6	0	-3.424684	0.257685	3.460958
5	6	0	-3.196547	1.511280	4.007693
6	6	0	-1.918359	2.072812	3.961507
7	1	0	0.125690	1.809015	3.338302
8	1	0	-4.411282	-0.184629	3.528282
9	1	0	-4.011579	2.048286	4.482667
10	1	0	-1.742900	3.058722	4.381750
11	6	0	0.031603	-0.635352	2.234051
12	6	0	-2.454253	-1.803872	2.272326
13	6	0	-3.486589	-2.484960	1.733326
14	6	0	-1.099580	-2.435422	2.321196
15	6	0	-3.366269	-3.927448	1.287863
16	6	0	-0.872887	-3.657825	1.452928
17	6	0	-2.057992	-4.596718	1.700919
18	1	0	0.081441	-4.128114	1.704882
19	1	0	-2.095192	-4.862127	2.765429
20	1	0	-0.729595	-2.564806	3.338686
21	6	0	1.230206	-0.944730	3.092522
22	1	0	1.814099	-0.020336	3.158512
23	1	0	0.972541	-1.266394	4.109759
24	1	0	1.874109	-1.682285	2.605972
25	6	0	-4.855114	-1.933633	1.486090
26	8	0	-5.859390	-2.611804	1.521166
27	8	0	-4.847021	-0.646420	1.136769
28	6	0	-6.104259	-0.074737	0.781856
29	1	0	-6.531148	-0.602981	-0.073703
30	1	0	-6.800684	-0.125945	1.623073
31	1	0	-5.884526	0.957894	0.513653
32	1	0	-1.921086	-5.528780	1.143588
33	1	0	-0.834506	-3.360910	0.400301
34	45	0	1.286221	0.840937	-1.912340
35	45	0	0.567049	0.008514	0.261638
36	8	0	0.029146	2.457894	-1.626306
37	6	0	-0.640101	2.525777	-0.561139
38	8	0	-0.608473	1.685676	0.392892
39	8	0	2.782337	1.871273	-0.918578
40	6	0	2.860186	1.790159	0.338296
41	8	0	2.098728	1.104088	1.087263
42	8	0	2.453405	-0.878972	-2.021660
43	6	0	2.457581	-1.714044	-1.075484
44	8	0	1.795376	-1.618318	0.004503
45	8	0	-0.293339	-0.211775	-2.722408
46	6	0	-1.037353	-0.907244	-1.985901
47	8	0	-0.907881	-1.055389	-0.724431
48	6	0	-1.563706	3.726832	-0.341344
49	6	0	-2.195080	-1.665817	-2.642629
50	6	0	-1.668175	4.571497	-1.612567
51	1	0	-2.341445	5.418956	-1.435623
52	1	0	-0.689115	4.961258	-1.903705
53	6	0	-2.332797	-1.270732	-4.114861
54	1	0	-1.428134	-1.525092	-4.673571
55	1	0	-3.179786	-1.806894	-4.559451
56	6	0	-3.500186	-1.368078	-1.858139
57	1	0	-4.299087	-1.973983	-2.304528

58	1	0	-3.359472	-1.711644	-0.829470
59	6	0	-1.887265	-3.170066	-2.539473
60	1	0	-1.816343	-3.490384	-1.496092
61	1	0	-2.684242	-3.746793	-3.022346
62	1	0	-0.942766	-3.411468	-3.039960
63	6	0	-0.950510	4.560980	0.798592
64	1	0	-1.572907	5.442063	0.992814
65	1	0	-0.881714	3.971299	1.717750
66	1	0	0.053532	4.909301	0.530205
67	6	0	-2.959698	3.219718	0.116185
68	1	0	-2.838598	2.693830	1.069352
69	1	0	-3.579713	4.105305	0.305344
70	6	0	3.971013	2.593304	1.020477
71	6	0	3.338062	-2.955273	-1.245087
72	6	0	5.336420	2.136532	0.432881
73	1	0	6.120902	2.702396	0.950911
74	6	0	4.806124	-2.488948	-1.458553
75	1	0	5.425316	-3.390656	-1.544999
76	1	0	4.859476	-1.964891	-2.418121
77	6	0	5.342296	-1.592507	-0.366798
78	6	0	5.981135	-2.112548	0.761285
79	6	0	5.176744	-0.209517	-0.460828
80	6	0	6.430130	-1.265310	1.770222
81	1	0	6.136463	-3.185482	0.845608
82	6	0	5.601217	0.653930	0.550837
83	1	0	4.692670	0.205998	-1.339998
84	6	0	6.238363	0.109362	1.668072
85	1	0	6.936350	-1.678339	2.638188
86	1	0	6.593371	0.767490	2.457602
87	6	0	3.756058	4.077482	0.678790
88	1	0	2.805353	4.438067	1.088327
89	1	0	4.561508	4.680681	1.113036
90	1	0	3.744534	4.231500	-0.403425
91	6	0	3.936399	2.398463	2.538449
92	1	0	4.740792	2.981729	3.002166
93	1	0	2.983476	2.739985	2.954346
94	1	0	4.068699	1.348475	2.811778
95	6	0	2.867193	-3.699890	-2.505898
96	1	0	3.506199	-4.571956	-2.685458
97	1	0	1.836977	-4.055205	-2.385708
98	1	0	2.906089	-3.047831	-3.382497
99	6	0	3.229485	-3.877264	-0.027571
100	1	0	2.201064	-4.227436	0.104733
101	1	0	3.873528	-4.752780	-0.171938
102	1	0	3.533788	-3.369373	0.890931
103	1	0	5.367555	2.428422	-0.621766
104	1	0	-2.058058	3.987581	-2.450256
105	1	0	-2.503928	-0.197567	-4.227377
106	6	0	-3.903086	0.087145	-1.841761
107	6	0	-3.344716	0.951606	-0.898901
108	6	0	-4.818418	0.602811	-2.760921
109	6	0	-3.646673	2.313664	-0.878625
110	1	0	-2.668460	0.553312	-0.151018
111	6	0	-5.153530	1.954186	-2.739127
112	1	0	-5.272268	-0.057716	-3.496141
113	6	0	-4.566619	2.806588	-1.808311
114	1	0	-5.872652	2.344526	-3.453757
115	1	0	-4.822053	3.863671	-1.802296
116	1	0	-0.377731	-1.637633	1.636345
117	1	0	-4.226544	-4.476449	1.683442
118	1	0	-3.473352	-3.960248	0.193828

Zero-point correction= 0.992897 (Hartree/Particle)
Thermal correction to Energy= 1.050251
Thermal correction to Enthalpy= 1.051195
Thermal correction to Gibbs Free Energy= 0.906368
Sum of electronic and zero-point Energies= -2835.902414

Sum of electronic and thermal Energies= -2835.845061
Sum of electronic and thermal Enthalpies= -2835.844117
Sum of electronic and thermal Free Energies= -2835.988944
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2837.60909394

TS2b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.804426	-0.845994	-3.280363
2	6	0	-1.629975	0.338099	-2.566707
3	6	0	-2.745420	1.026905	-2.049030
4	6	0	-4.023825	0.499016	-2.244196
5	6	0	-4.190065	-0.691517	-2.941088
6	6	0	-3.083590	-1.354833	-3.468805
7	1	0	-0.938704	-1.374688	-3.664437
8	1	0	-4.895293	0.998975	-1.844714
9	1	0	-5.185982	-1.100864	-3.075732
10	1	0	-3.218363	-2.280222	-4.021350
11	6	0	-0.308765	0.933819	-2.266082
12	6	0	-2.370115	2.320173	-1.440506
13	6	0	-3.118673	3.371028	-1.057043
14	6	0	-0.872336	2.476080	-1.374612
15	6	0	-2.539762	4.732387	-0.716101
16	6	0	-0.365411	3.876750	-1.700782
17	6	0	-1.010964	4.776642	-0.643424
18	1	0	-2.909345	5.432251	-1.477114
19	1	0	-0.660469	4.196845	-2.708374
20	1	0	-0.662149	5.807148	-0.762137
21	6	0	-4.610434	3.386059	-1.016446
22	8	0	-5.300712	4.160594	-1.637521
23	8	0	-5.101100	2.503389	-0.131922
24	6	0	-6.522389	2.473277	-0.006077
25	1	0	-6.895944	3.437463	0.347312
26	1	0	-6.989510	2.242254	-0.967173
27	1	0	-6.731810	1.688613	0.720101
28	1	0	-2.960231	5.081692	0.235440
29	1	0	-0.680638	4.438856	0.346803
30	1	0	0.725208	3.903400	-1.625556
31	6	0	0.854001	0.863433	-3.268683
32	1	0	0.579489	1.203252	-4.276720
33	1	0	1.704424	1.445585	-2.903353
34	1	0	1.201407	-0.169907	-3.329000
35	1	0	-0.476141	2.197022	-0.405856
36	1	0	-0.532210	2.036158	-2.591599
37	45	0	1.289849	-1.217187	1.609663
38	45	0	0.515008	-0.117640	-0.411469
39	8	0	0.363523	-2.927434	0.956612
40	6	0	-0.208784	-2.927151	-0.166667
41	8	0	-0.300213	-1.932001	-0.953105
42	8	0	2.973602	-1.779426	0.552409
43	6	0	3.096450	-1.423645	-0.655038
44	8	0	2.267550	-0.723497	-1.309387
45	8	0	2.159236	0.589887	2.137328
46	6	0	2.064962	1.584885	1.368362
47	8	0	1.448354	1.604706	0.257265
48	8	0	-0.459645	-0.606646	2.520724
49	6	0	-1.296944	0.062014	1.860471
50	8	0	-1.166384	0.412873	0.643336
51	6	0	-0.844714	-4.230645	-0.656063
52	6	0	-2.582014	0.527799	2.545470
53	6	0	-0.669285	-5.340525	0.382873
54	1	0	-1.132048	-6.263492	0.013399
55	1	0	0.390316	-5.535549	0.570483
56	6	0	-2.639943	0.019917	3.987356

57	1	0	-1.797785	0.403211	4.570535
58	1	0	-3.570466	0.358715	4.458212
59	6	0	-3.798298	0.023670	1.717685
60	1	0	-4.703307	0.354525	2.243997
61	1	0	-3.786933	0.530478	0.749179
62	6	0	-2.583955	2.067636	2.526630
63	1	0	-2.551391	2.443567	1.499909
64	1	0	-3.496240	2.444365	3.002625
65	1	0	-1.723972	2.465333	3.078718
66	6	0	-0.147156	-4.624511	-1.969584
67	1	0	-0.590815	-5.544462	-2.367246
68	1	0	-0.249969	-3.833825	-2.718483
69	1	0	0.920736	-4.808126	-1.804645
70	6	0	-2.348723	-3.973374	-0.952651
71	1	0	-2.414804	-3.278747	-1.794649
72	1	0	-2.783961	-4.927237	-1.276923
73	6	0	4.355116	-1.891489	-1.390554
74	6	0	2.739128	2.880180	1.831697
75	6	0	5.602078	-1.410933	-0.596671
76	1	0	6.489716	-1.745918	-1.147722
77	6	0	4.236712	2.584571	2.125386
78	1	0	4.695502	3.523256	2.460363
79	1	0	4.286197	1.880950	2.962156
80	6	0	5.000054	2.022873	0.948661
81	6	0	5.653289	2.853091	0.034656
82	6	0	5.032866	0.643579	0.737912
83	6	0	6.304407	2.310117	-1.069143
84	1	0	5.657585	3.929112	0.192451
85	6	0	5.660847	0.082426	-0.375562
86	1	0	4.542884	-0.011535	1.451961
87	6	0	6.303060	0.933844	-1.277318
88	1	0	6.819954	2.962489	-1.768352
89	1	0	6.809999	0.515395	-2.143548
90	6	0	4.340529	-3.430075	-1.404484
91	1	0	3.472918	-3.804972	-1.959652
92	1	0	5.244708	-3.807815	-1.895204
93	1	0	4.297477	-3.831166	-0.388257
94	6	0	4.379665	-1.359916	-2.825991
95	1	0	5.293828	-1.699492	-3.327212
96	1	0	3.520329	-1.730543	-3.392610
97	1	0	4.352921	-0.267680	-2.852054
98	6	0	2.052344	3.313727	3.138786
99	1	0	2.519745	4.227554	3.522728
100	1	0	0.989256	3.522853	2.969391
101	1	0	2.130347	2.532103	3.899136
102	6	0	2.597286	3.984107	0.781544
103	1	0	1.544638	4.233740	0.622166
104	1	0	3.111603	4.888765	1.126432
105	1	0	3.026091	3.684675	-0.178156
106	1	0	5.607633	-1.922934	0.370722
107	1	0	-1.132926	-5.073791	1.335481
108	1	0	-2.603885	-1.071358	4.028896
109	6	0	-3.835700	-1.470981	1.507109
110	6	0	-3.187578	-2.031447	0.404876
111	6	0	-4.479159	-2.323322	2.407309
112	6	0	-3.131831	-3.412763	0.210060
113	1	0	-2.702242	-1.376664	-0.312613
114	6	0	-4.458423	-3.701109	2.212688
115	1	0	-5.000394	-1.904205	3.264890
116	6	0	-3.783438	-4.244085	1.123517
117	1	0	-4.969835	-4.354857	2.913614
118	1	0	-3.763587	-5.321656	0.978411

Zero-point correction= 0.993903 (Hartree/Particle)
Thermal correction to Energy= 1.051385
Thermal correction to Enthalpy= 1.052329
Thermal correction to Gibbs Free Energy= 0.907423

Sum of electronic and zero-point Energies= -2835.867150
Sum of electronic and thermal Energies= -2835.809668
Sum of electronic and thermal Enthalpies= -2835.808723
Sum of electronic and thermal Free Energies= -2835.953630
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2837.57873656

TS2b''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.179751	-1.534840	3.376044
2	6	0	1.238012	-0.189297	3.005070
3	6	0	2.451992	0.508358	3.105773
4	6	0	3.600669	-0.148965	3.546495
5	6	0	3.538221	-1.489350	3.906278
6	6	0	2.325164	-2.176226	3.829112
7	1	0	0.247846	-2.081242	3.266653
8	1	0	4.536240	0.395624	3.634948
9	1	0	4.430188	-1.996884	4.259882
10	1	0	2.276215	-3.223580	4.112267
11	6	0	0.057758	0.486165	2.428676
12	6	0	2.348206	1.927781	2.739204
13	6	0	3.331069	2.766086	2.388711
14	6	0	0.925254	2.371819	2.743041
15	6	0	3.096830	4.206066	2.020521
16	6	0	0.626761	3.624441	1.936170
17	6	0	1.671481	4.679938	2.328954
18	1	0	-0.389355	3.975061	2.136572
19	1	0	1.579941	4.892196	3.401853
20	1	0	0.475475	2.386124	3.736599
21	6	0	-1.217685	0.533365	3.227459
22	1	0	-1.678678	-0.457008	3.149725
23	1	0	-1.060361	0.763710	4.289268
24	1	0	-1.926007	1.238746	2.784021
25	1	0	1.463277	5.616071	1.800509
26	1	0	0.699147	3.395524	0.868953
27	45	0	-0.705834	-0.649244	-1.960283
28	45	0	-0.263999	-0.005683	0.346618
29	8	0	0.689678	-2.153472	-1.737458
30	6	0	1.268849	-2.282193	-0.625506
31	8	0	1.067577	-1.566541	0.405467
32	8	0	-2.159736	-1.927158	-1.220664
33	6	0	-2.354651	-1.990609	0.025080
34	8	0	-1.735956	-1.323343	0.909753
35	8	0	-2.037119	0.947440	-1.997400
36	6	0	-2.209803	1.665767	-0.974786
37	8	0	-1.633440	1.514158	0.147263
38	8	0	0.806959	0.646312	-2.504453
39	6	0	1.420035	1.308476	-1.629471
40	8	0	1.179187	1.288775	-0.376558
41	6	0	2.290272	-3.408433	-0.446986
42	6	0	2.541734	2.246313	-2.088807
43	6	0	2.574749	-4.099422	-1.781848
44	1	0	3.315027	-4.895019	-1.634017
45	1	0	1.664147	-4.544630	-2.191684
46	6	0	2.847409	2.030260	-3.573222
47	1	0	1.973372	2.261144	-4.188005
48	1	0	3.670091	2.688740	-3.877233
49	6	0	3.800159	1.999687	-1.211957
50	1	0	4.560163	2.729694	-1.519097
51	1	0	3.536968	2.212328	-0.171184
52	6	0	2.058756	3.691249	-1.871455
53	1	0	1.867406	3.890949	-0.813604
54	1	0	2.821749	4.396082	-2.221157
55	1	0	1.136779	3.884676	-2.431378

56	6	0	1.682297	-4.414239	0.548437
57	1	0	2.385402	-5.237117	0.721605
58	1	0	1.467312	-3.929377	1.505258
59	1	0	0.752500	-4.839937	0.153822
60	6	0	3.588208	-2.825526	0.180254
61	1	0	3.343565	-2.433248	1.172064
62	1	0	4.284383	-3.662290	0.320673
63	6	0	-3.430173	-2.964692	0.513862
64	6	0	-3.200850	2.826002	-1.102884
65	6	0	-4.778061	-2.588333	-0.164305
66	1	0	-5.538270	-3.284698	0.211357
67	6	0	-4.581681	2.245706	-1.520545
68	1	0	-5.284684	3.085806	-1.584288
69	1	0	-4.481947	1.826476	-2.526704
70	6	0	-5.120133	1.186587	-0.587270
71	6	0	-5.916009	1.513997	0.512790
72	6	0	-4.796496	-0.154592	-0.800417
73	6	0	-6.361992	0.521192	1.380141
74	1	0	-6.192994	2.551238	0.685921
75	6	0	-5.216225	-1.161524	0.070709
76	1	0	-4.188167	-0.420597	-1.660149
77	6	0	-6.011282	-0.808274	1.163490
78	1	0	-6.990706	0.784391	2.226236
79	1	0	-6.362661	-1.579378	1.844968
80	6	0	-3.024461	-4.377699	0.061120
81	1	0	-2.078503	-4.677394	0.526750
82	1	0	-3.792170	-5.100452	0.359923
83	1	0	-2.902099	-4.421590	-1.024357
84	6	0	-3.555182	-2.923851	2.039100
85	1	0	-4.331750	-3.626928	2.362954
86	1	0	-2.613069	-3.212359	2.515184
87	1	0	-3.821049	-1.924853	2.394235
88	6	0	-2.697447	3.755242	-2.220486
89	1	0	-3.408254	4.575824	-2.370955
90	1	0	-1.726990	4.192163	-1.957268
91	1	0	-2.584551	3.210462	-3.161506
92	6	0	-3.306369	3.604465	0.210860
93	1	0	-2.341266	4.045733	0.478240
94	1	0	-4.035940	4.415575	0.100386
95	1	0	-3.623779	2.960451	1.034713
96	1	0	-4.677008	-2.765724	-1.239701
97	1	0	2.963717	-3.395620	-2.521961
98	1	0	3.135588	0.996422	-3.776307
99	6	0	4.355457	0.598625	-1.313069
100	6	0	3.843981	-0.413610	-0.498706
101	6	0	5.338962	0.272341	-2.249409
102	6	0	4.246565	-1.743349	-0.641904
103	1	0	3.097330	-0.165785	0.249470
104	6	0	5.780179	-1.040801	-2.378694
105	1	0	5.756150	1.050663	-2.884041
106	6	0	5.229493	-2.044254	-1.587236
107	1	0	6.549633	-1.285133	-3.105532
108	1	0	5.564203	-3.072293	-1.704363
109	1	0	0.336909	1.559058	1.925050
110	1	0	3.820559	4.843545	2.543428
111	1	0	3.311010	4.332114	0.949272
112	1	0	4.354625	2.399825	2.338716

Zero-point correction= 0.949661 (Hartree/Particle)
Thermal correction to Energy= 1.002431
Thermal correction to Enthalpy= 1.003375
Thermal correction to Gibbs Free Energy= 0.868014
Sum of electronic and zero-point Energies= -2608.139582
Sum of electronic and thermal Energies= -2608.086811
Sum of electronic and thermal Enthalpies= -2608.085867
Sum of electronic and thermal Free Energies= -2608.221229
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2609.73670881

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.347521	-1.003234	-2.984997
2	6	0	1.674511	-1.691208	-1.956959
3	6	0	2.404716	-2.581035	-1.141123
4	6	0	3.805037	-2.650471	-1.238465
5	6	0	4.456827	-1.911210	-2.203868
6	6	0	3.721643	-1.103248	-3.088084
7	1	0	1.795739	-0.337646	-3.639799
8	1	0	4.365126	-3.311731	-0.584709
9	1	0	5.536318	-1.968445	-2.297761
10	1	0	4.244941	-0.531819	-3.849198
11	6	0	0.272763	-1.445191	-1.665623
12	6	0	1.582418	-3.369990	-0.270814
13	6	0	0.257839	-3.573790	-0.632086
14	6	0	2.136271	-3.864836	1.035068
15	6	0	-0.777616	-3.889874	0.422520
16	6	0	1.091079	-4.508284	1.946460
17	1	0	2.933650	-4.583698	0.797076
18	6	0	-0.224034	-3.740405	1.835320
19	1	0	-1.614680	-3.206549	0.261463
20	1	0	1.465431	-4.523620	2.975648
21	1	0	-0.059669	-2.678159	2.050235
22	1	0	2.625405	-3.028152	1.539486
23	6	0	-0.637439	-1.416376	-2.853489
24	1	0	-0.316725	-2.060393	-3.678677
25	1	0	-1.670357	-1.633152	-2.573802
26	1	0	-0.641154	-0.375086	-3.202330
27	6	0	-0.156303	-4.081795	-1.981594
28	8	0	-1.306971	-4.346416	-2.249841
29	8	0	0.862192	-4.337752	-2.819598
30	6	0	0.488599	-4.890980	-4.078115
31	1	0	-0.011662	-5.852927	-3.941681
32	1	0	-0.182894	-4.217421	-4.617368
33	1	0	1.421894	-5.017714	-4.625866
34	1	0	-1.164144	-4.905097	0.268168
35	1	0	-0.952725	-4.117895	2.560646
36	1	0	0.925467	-5.553049	1.653082
37	45	0	-0.590816	1.950714	1.213640
38	45	0	-0.187146	-0.018012	-0.196767
39	8	0	0.846447	2.952966	0.132305
40	6	0	1.377640	2.378466	-0.851085
41	8	0	1.149200	1.182655	-1.228013
42	8	0	-1.981984	2.583541	-0.174955
43	6	0	-2.219309	1.848830	-1.172806
44	8	0	-1.672402	0.730663	-1.418043
45	8	0	-2.008107	0.828380	2.206007
46	6	0	-2.260366	-0.350390	1.830193
47	8	0	-1.657437	-0.979593	0.906234
48	8	0	0.879216	1.241554	2.455986
49	6	0	1.519364	0.199461	2.163310
50	8	0	1.271904	-0.579408	1.182496
51	6	0	2.368572	3.171448	-1.707440
52	6	0	2.682864	-0.182382	3.089238
53	6	0	2.636702	4.544466	-1.086728
54	1	0	3.340655	5.100853	-1.717170
55	1	0	1.712493	5.122396	-1.004157
56	6	0	2.998778	0.967619	4.051658
57	1	0	2.141098	1.184443	4.693101
58	1	0	3.846676	0.686564	4.688355
59	6	0	3.933486	-0.545090	2.241078
60	1	0	4.699193	-0.918809	2.932568

61	1	0	3.675646	-1.364031	1.563359
62	6	0	2.238066	-1.405570	3.911399
63	1	0	1.976627	-2.251296	3.273231
64	1	0	3.042864	-1.715741	4.587399
65	1	0	1.360583	-1.158911	4.519618
66	6	0	1.732366	3.340976	-3.098834
67	1	0	2.405759	3.908070	-3.751471
68	1	0	1.533970	2.368782	-3.560471
69	1	0	0.786480	3.889966	-3.029581
70	6	0	3.683841	2.360029	-1.857477
71	1	0	3.455981	1.439249	-2.400096
72	1	0	4.361020	2.953366	-2.485044
73	6	0	-3.239623	2.369229	-2.190121
74	6	0	-3.373860	-1.079082	2.595312
75	6	0	-4.552898	2.731398	-1.442750
76	1	0	-5.258635	3.117396	-2.189028
77	6	0	-4.632514	-0.169004	2.653204
78	1	0	-5.380771	-0.691589	3.262357
79	1	0	-4.367687	0.752635	3.180099
80	6	0	-5.211194	0.167054	1.299054
81	6	0	-6.183721	-0.634269	0.696079
82	6	0	-4.738142	1.278376	0.601067
83	6	0	-6.649563	-0.336383	-0.580845
84	1	0	-6.577646	-1.496119	1.229172
85	6	0	-5.171284	1.575616	-0.692503
86	1	0	-3.997642	1.918393	1.070118
87	6	0	-6.140257	0.757011	-1.275705
88	1	0	-7.411236	-0.961507	-1.038228
89	1	0	-6.499826	0.978681	-2.277854
90	6	0	-2.652277	3.650109	-2.809345
91	1	0	-1.716411	3.432918	-3.337521
92	1	0	-3.358859	4.071641	-3.533443
93	1	0	-2.447664	4.399621	-2.039736
94	6	0	-3.499079	1.332766	-3.286139
95	1	0	-4.242565	1.721940	-3.992004
96	1	0	-2.582233	1.114785	-3.841818
97	1	0	-3.873114	0.393741	-2.870407
98	6	0	-2.856856	-1.301602	4.028688
99	1	0	-3.613043	-1.830515	4.620027
100	1	0	-1.945194	-1.910757	4.022228
101	1	0	-2.631987	-0.349035	4.516554
102	6	0	-3.718025	-2.425409	1.955583
103	1	0	-2.892204	-3.131578	2.058187
104	1	0	-4.590746	-2.856989	2.459848
105	1	0	-3.949541	-2.323522	0.892525
106	1	0	-4.334584	3.547059	-0.746321
107	1	0	3.063992	4.452486	-0.085086
108	1	0	3.255933	1.884063	3.516143
109	6	0	4.486561	0.605554	1.432706
110	6	0	3.950793	0.897038	0.177352
111	6	0	5.497798	1.427282	1.936146
112	6	0	4.359147	2.017007	-0.551410
113	1	0	3.184200	0.247192	-0.233263
114	6	0	5.940708	2.526790	1.207984
115	1	0	5.935391	1.208001	2.907118
116	6	0	5.366964	2.826194	-0.023932
117	1	0	6.730277	3.158062	1.605642
118	1	0	5.703546	3.696740	-0.581978

Zero-point correction= 0.995225 (Hartree/Particle)
Thermal correction to Energy= 1.052258
Thermal correction to Enthalpy= 1.053202
Thermal correction to Gibbs Free Energy= 0.910948
Sum of electronic and zero-point Energies= -2835.900964
Sum of electronic and thermal Energies= -2835.843931
Sum of electronic and thermal Enthalpies= -2835.842987
Sum of electronic and thermal Free Energies= -2835.985241

TS3b''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.254243	-0.684273	3.422229
2	6	0	1.620182	0.451306	2.887888
3	6	0	2.368730	1.627716	2.679859
4	6	0	3.760851	1.613155	2.849552
5	6	0	4.383676	0.463055	3.299252
6	6	0	3.626261	-0.676886	3.604980
7	1	0	1.682345	-1.587453	3.608424
8	1	0	4.342378	2.508657	2.652375
9	1	0	5.460216	0.446616	3.436189
10	1	0	4.123848	-1.571701	3.966960
11	6	0	0.226592	0.427664	2.464257
12	6	0	1.564218	2.780434	2.339799
13	6	0	0.244706	2.734299	2.686587
14	6	0	2.145646	3.934257	1.571999
15	6	0	-0.784558	3.671389	2.134469
16	6	0	1.119073	5.023940	1.239739
17	1	0	2.970642	4.361855	2.157763
18	6	0	-0.244800	4.413197	0.913369
19	1	0	-1.668860	3.083938	1.870890
20	1	0	1.488997	5.627488	0.403701
21	1	0	-0.151551	3.697905	0.086497
22	1	0	2.599750	3.543480	0.658125
23	6	0	-0.757665	-0.115552	3.458292
24	1	0	-0.499290	0.093881	4.503011
25	1	0	-1.774189	0.217569	3.233799
26	1	0	-0.775019	-1.203727	3.312510
27	1	0	-1.090814	4.384529	2.914075
28	1	0	-0.946010	5.194660	0.600781
29	1	0	1.009129	5.703509	2.095071
30	45	0	-0.576342	-0.890052	-1.779852
31	45	0	-0.187838	0.009800	0.472582
32	8	0	0.855407	-2.320377	-1.400716
33	6	0	1.403030	-2.343378	-0.269557
34	8	0	1.167561	-1.536959	0.688905
35	8	0	-1.986909	-2.158105	-0.956554
36	6	0	-2.226178	-2.081000	0.279042
37	8	0	-1.668814	-1.285854	1.096368
38	8	0	-1.976268	0.606791	-2.008711
39	6	0	-2.225348	1.407526	-1.065404
40	8	0	-1.643186	1.432106	0.064136
41	8	0	0.894110	0.379520	-2.434129
42	6	0	1.504832	1.124332	-1.625544
43	8	0	1.253014	1.243935	-0.380261
44	6	0	2.425460	-3.445429	0.021898
45	6	0	2.636690	1.990244	-2.193011
46	6	0	2.716306	-4.258844	-1.241530
47	1	0	3.451466	-5.039657	-1.012622
48	1	0	1.807547	-4.736156	-1.617498
49	6	0	2.955343	1.581333	-3.634791
50	1	0	2.088585	1.734617	-4.282571
51	1	0	3.783777	2.193421	-4.011785
52	6	0	3.895593	1.852374	-1.292782
53	1	0	4.649721	2.552269	-1.674440
54	1	0	3.639566	2.168680	-0.277733
55	6	0	2.148507	3.450473	-2.187814
56	1	0	1.869182	3.781520	-1.185827
57	1	0	2.936888	4.111479	-2.565548
58	1	0	1.272497	3.562720	-2.836461
59	6	0	1.815680	-4.357363	1.102151

60	1	0	2.517766	-5.161049	1.351443
61	1	0	1.594176	-3.792635	2.013096
62	1	0	0.887341	-4.817043	0.744571
63	6	0	3.725120	-2.809468	0.586466
64	1	0	3.484841	-2.326201	1.536962
65	1	0	4.421651	-3.629866	0.801672
66	6	0	-3.266772	-3.052948	0.844155
67	6	0	-3.312962	2.453142	-1.345864
68	6	0	-4.575825	-2.920639	0.017208
69	1	0	-5.298848	-3.635200	0.430298
70	6	0	-4.580407	1.729726	-1.881245
71	1	0	-5.320990	2.504144	-2.117354
72	1	0	-4.320586	1.229809	-2.819004
73	6	0	-5.169672	0.727896	-0.916012
74	6	0	-6.138235	1.095570	0.021141
75	6	0	-4.714994	-0.591303	-0.920629
76	6	0	-6.618690	0.167177	0.939832
77	1	0	-6.520725	2.113533	0.028924
78	6	0	-5.165255	-1.529505	0.010477
79	1	0	-3.977175	-0.891585	-1.657862
80	6	0	-6.129125	-1.136072	0.941020
81	1	0	-7.378025	0.460855	1.659087
82	1	0	-6.501488	-1.855997	1.666112
83	6	0	-2.706610	-4.474937	0.661394
84	1	0	-1.772891	-4.600524	1.221784
85	1	0	-3.427481	-5.211500	1.034244
86	1	0	-2.505764	-4.682054	-0.393344
87	6	0	-3.526838	-2.782509	2.327841
88	1	0	-4.283764	-3.482519	2.701094
89	1	0	-2.614347	-2.922031	2.915082
90	1	0	-3.884640	-1.763186	2.494198
91	6	0	-2.769116	3.383393	-2.445820
92	1	0	-3.515094	4.148386	-2.689411
93	1	0	-1.859374	3.893001	-2.106971
94	1	0	-2.532226	2.821332	-3.353480
95	6	0	-3.651607	3.276108	-0.102250
96	1	0	-2.803184	3.893935	0.197668
97	1	0	-4.491001	3.945409	-0.325480
98	1	0	-3.931506	2.640699	0.741788
99	1	0	-4.361694	-3.231204	-1.010320
100	1	0	3.115914	-3.627687	-2.039041
101	1	0	3.241117	0.529462	-3.702914
102	6	0	4.466764	0.454559	-1.240579
103	6	0	3.950815	-0.477450	-0.338417
104	6	0	5.476989	0.050275	-2.116140
105	6	0	4.380114	-1.806704	-0.333189
106	1	0	3.184128	-0.166520	0.364647
107	6	0	5.941338	-1.261056	-2.100036
108	1	0	5.896947	0.766510	-2.818481
109	6	0	5.389239	-2.187079	-1.220054
110	1	0	6.730455	-1.564828	-2.782007
111	1	0	5.743462	-3.215295	-1.221341
112	1	0	-0.047073	2.169776	3.568161

Zero-point correction= 0.950690 (Hartree/Particle)
Thermal correction to Energy= 1.003552
Thermal correction to Enthalpy= 1.004497
Thermal correction to Gibbs Free Energy= 0.870533
Sum of electronic and zero-point Energies= -2608.149371
Sum of electronic and thermal Energies= -2608.096508
Sum of electronic and thermal Enthalpies= -2608.095564
Sum of electronic and thermal Free Energies= -2608.229528
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2609.74349585

INT4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.963475	-1.152676	-0.361618
2	6	0	1.615240	-0.632394	-0.341125
3	6	0	1.373588	0.688243	0.267620
4	6	0	2.485540	1.425838	0.820161
5	6	0	3.724620	0.886193	0.770275
6	6	0	3.964453	-0.417382	0.173537
7	1	0	3.162431	-2.123851	-0.805705
8	1	0	2.315425	2.398633	1.273052
9	1	0	4.572179	1.425052	1.183913
10	1	0	4.981763	-0.798444	0.164778
11	6	0	0.453999	-1.142070	-0.827777
12	6	0	0.055805	0.988329	0.177636
13	6	0	-0.642642	-0.129849	-0.543743
14	6	0	-0.722277	2.200988	0.580751
15	6	0	-1.311667	0.425778	-1.829459
16	6	0	-2.067104	2.236805	-0.167754
17	1	0	-0.901162	2.203410	1.664204
18	6	0	-1.882999	1.852356	-1.639693
19	1	0	-0.557716	0.433079	-2.621994
20	1	0	-2.510182	3.235138	-0.089991
21	1	0	-1.198486	2.578218	-2.096085
22	1	0	-0.146011	3.108098	0.354485
23	6	0	0.210149	-2.415837	-1.565825
24	1	0	-0.617449	-2.983257	-1.125544
25	1	0	-0.067784	-2.219745	-2.610295
26	1	0	1.100212	-3.051570	-1.571305
27	6	0	-1.675383	-0.854259	0.322063
28	8	0	-2.566923	-1.544571	-0.116333
29	8	0	-1.456363	-0.684390	1.633373
30	6	0	-2.320859	-1.423058	2.494677
31	1	0	-3.364683	-1.152165	2.318503
32	1	0	-2.199748	-2.496533	2.329279
33	1	0	-2.020983	-1.157822	3.508060
34	1	0	-2.091768	-0.280898	-2.127217
35	1	0	-2.835735	1.943643	-2.171119
36	1	0	-2.777636	1.548676	0.308299

Zero-point correction= 0.309175 (Hartree/Particle)
Thermal correction to Energy= 0.325373
Thermal correction to Enthalpy= 0.326317
Thermal correction to Gibbs Free Energy= 0.265787
Sum of electronic and zero-point Energies= -770.423226
Sum of electronic and thermal Energies= -770.407028
Sum of electronic and thermal Enthalpies= -770.406084
Sum of electronic and thermal Free Energies= -770.466614
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -770.93735837

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.843857	1.185932	-1.213335
2	6	0	1.792145	2.109986	-1.230365
3	6	0	2.097613	3.473969	-1.472947
4	6	0	3.422111	3.834736	-1.743250
5	6	0	4.444627	2.893026	-1.755485
6	6	0	4.153481	1.563526	-1.484597
7	1	0	2.628107	0.150432	-0.997178
8	1	0	3.666456	4.878628	-1.914776
9	1	0	5.464557	3.206929	-1.957368
10	1	0	4.936095	0.811802	-1.461180

11	6	0	0.401309	1.634814	-0.963589
12	6	0	1.112254	4.591760	-1.405955
13	6	0	0.312674	4.832215	-0.346558
14	6	0	1.098873	5.521297	-2.603973
15	6	0	-0.586311	6.043535	-0.213595
16	6	0	-0.121364	6.438168	-2.640617
17	1	0	2.013956	6.129230	-2.603919
18	6	0	-0.312100	7.101615	-1.279825
19	1	0	-1.632392	5.709891	-0.281145
20	1	0	-1.015796	5.852072	-2.891068
21	1	0	-1.134464	7.823650	-1.304127
22	1	0	1.151777	4.905308	-3.509506
23	6	0	-0.699367	2.169404	-1.828854
24	1	0	-0.519950	3.129416	-2.319018
25	1	0	-0.835755	1.402056	-2.601823
26	1	0	-1.640722	2.202885	-1.272965
27	6	0	0.280949	3.874493	0.773576
28	8	0	0.269735	2.649188	0.664364
29	8	0	0.247225	4.447852	1.966684
30	6	0	0.312889	3.601255	3.125787
31	1	0	1.316918	3.693436	3.545617
32	1	0	-0.424493	3.982634	3.832451
33	1	0	0.106596	2.564536	2.859787
34	1	0	-0.466529	6.467953	0.788193
35	1	0	0.597505	7.658814	-1.019502
36	1	0	0.002211	7.187237	-3.429630
37	45	0	-0.607018	-2.409137	0.832793
38	45	0	-0.074601	-0.217458	-0.169467
39	8	0	-2.015429	-2.632059	-0.662355
40	6	0	-2.151006	-1.742583	-1.540576
41	8	0	-1.515183	-0.639321	-1.597697
42	8	0	0.784328	-3.257780	-0.449407
43	6	0	1.359444	-2.516894	-1.290074
44	8	0	1.216256	-1.260393	-1.398524
45	8	0	0.865219	-1.973477	2.242595
46	6	0	1.503674	-0.888657	2.161583
47	8	0	1.340589	0.015271	1.287238
48	8	0	-2.001984	-1.420930	1.987334
49	6	0	-2.183176	-0.184590	1.850617
50	8	0	-1.519178	0.591489	1.088773
51	6	0	-3.152702	-1.989906	-2.674289
52	6	0	-3.283201	0.469211	2.701318
53	6	0	-3.919100	-3.293911	-2.441531
54	1	0	-4.638267	-3.448747	-3.255102
55	1	0	-3.234898	-4.146185	-2.415020
56	6	0	-4.065575	-0.596074	3.473760
57	1	0	-3.411707	-1.136790	4.162933
58	1	0	-4.864044	-0.116609	4.053249
59	6	0	-4.226979	1.303494	1.793587
60	1	0	-4.961617	1.789102	2.448786
61	1	0	-3.634820	2.097466	1.325875
62	6	0	-2.601570	1.431389	3.688187
63	1	0	-2.117348	2.250295	3.150472
64	1	0	-3.345714	1.856402	4.371731
65	1	0	-1.847091	0.910876	4.289655
66	6	0	-2.350941	-2.080104	-3.984926
67	1	0	-3.030757	-2.248810	-4.828070
68	1	0	-1.789046	-1.159003	-4.165480
69	1	0	-1.641815	-2.914932	-3.949818
70	6	0	-4.124837	-0.781629	-2.769617
71	1	0	-3.545042	0.103407	-3.052675
72	1	0	-4.824888	-0.988235	-3.588934
73	6	0	2.329076	-3.186629	-2.269489
74	6	0	2.586773	-0.628983	3.214811
75	6	0	3.459488	-3.863084	-1.443483
76	1	0	4.178174	-4.286681	-2.156358
77	6	0	3.650803	-1.756792	3.110636

78	1	0	4.434113	-1.538213	3.847572
79	1	0	3.177600	-2.697827	3.408894
80	6	0	4.260167	-1.919571	1.737993
81	6	0	5.398344	-1.210132	1.348386
82	6	0	3.667968	-2.786211	0.818063
83	6	0	5.919918	-1.364712	0.067056
84	1	0	5.885435	-0.543189	2.055519
85	6	0	4.166639	-2.942287	-0.476833
86	1	0	2.786123	-3.347062	1.115149
87	6	0	5.305783	-2.221264	-0.843236
88	1	0	6.817335	-0.822982	-0.220251
89	1	0	5.723095	-2.344548	-1.839882
90	6	0	1.558034	-4.276217	-3.032752
91	1	0	0.763762	-3.833629	-3.644657
92	1	0	2.237517	-4.817694	-3.700930
93	1	0	1.101530	-4.988863	-2.340928
94	6	0	2.907770	-2.170537	-3.257393
95	1	0	3.579585	-2.682409	-3.956873
96	1	0	2.111806	-1.688135	-3.831848
97	1	0	3.471223	-1.383705	-2.749363
98	6	0	1.928369	-0.698779	4.602130
99	1	0	2.683558	-0.559598	5.384495
100	1	0	1.174230	0.089480	4.714657
101	1	0	1.437435	-1.663826	4.752260
102	6	0	3.229104	0.745397	3.007504
103	1	0	2.480292	1.537577	3.093927
104	1	0	4.000615	0.910681	3.769645
105	1	0	3.684054	0.835097	2.018060
106	1	0	3.020445	-4.698638	-0.888938
107	1	0	-4.462514	-3.274734	-1.493780
108	1	0	-4.515562	-1.328289	2.799426
109	6	0	-4.936332	0.509386	0.723585
110	6	0	-4.309189	0.289854	-0.502409
111	6	0	-6.198093	-0.049920	0.936436
112	6	0	-4.887506	-0.499545	-1.497084
113	1	0	-3.329875	0.723335	-0.676858
114	6	0	-6.802927	-0.818308	-0.053861
115	1	0	-6.707446	0.116379	1.882647
116	6	0	-6.150083	-1.047360	-1.261780
117	1	0	-7.787033	-1.245186	0.117727
118	1	0	-6.622970	-1.657130	-2.027885

Zero-point correction= 0.995625 (Hartree/Particle)
Thermal correction to Energy= 1.052694
Thermal correction to Enthalpy= 1.053638
Thermal correction to Gibbs Free Energy= 0.909844
Sum of electronic and zero-point Energies= -2835.900533
Sum of electronic and thermal Energies= -2835.843463
Sum of electronic and thermal Enthalpies= -2835.842519
Sum of electronic and thermal Free Energies= -2835.986313
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2837.60580725

INT5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.974256	1.371243	-0.210756
2	6	0	1.948700	2.315396	-0.310700
3	6	0	2.303791	3.690202	-0.320825
4	6	0	3.658706	4.045382	-0.198124
5	6	0	4.652840	3.088750	-0.075649
6	6	0	4.307442	1.743152	-0.100268
7	1	0	2.723422	0.322482	-0.217967
8	1	0	3.940598	5.092806	-0.177754
9	1	0	5.688861	3.394864	0.034301

10	1	0	5.064923	0.969885	-0.021411
11	6	0	0.495517	1.893579	-0.418099
12	6	0	1.346035	4.810379	-0.499032
13	6	0	0.118566	4.910986	0.075933
14	6	0	1.832552	5.942205	-1.387101
15	6	0	-0.802124	6.111143	-0.052421
16	6	0	0.717439	6.854064	-1.889296
17	1	0	2.559258	6.546937	-0.827676
18	6	0	-0.133356	7.313675	-0.711413
19	1	0	-1.679765	5.807303	-0.641177
20	1	0	0.091472	6.312551	-2.610578
21	1	0	-0.897068	8.030632	-1.028547
22	1	0	2.385264	5.502033	-2.223424
23	6	0	-0.169914	2.364586	-1.701453
24	1	0	0.119425	3.360553	-2.055451
25	1	0	0.124749	1.641248	-2.467485
26	1	0	-1.259230	2.307313	-1.622820
27	6	0	-0.369876	3.841617	0.922471
28	8	0	-0.120988	2.610454	0.812657
29	8	0	-1.146641	4.204039	1.908413
30	6	0	-1.626072	3.173412	2.797001
31	1	0	-0.857006	2.982159	3.549161
32	1	0	-2.521656	3.585854	3.258547
33	1	0	-1.825325	2.255287	2.242169
34	1	0	-1.180767	6.380999	0.937513
35	1	0	0.506946	7.827740	0.017254
36	1	0	1.154314	7.707401	-2.417719
37	45	0	-0.558386	-2.558330	0.180098
38	45	0	-0.071328	-0.148905	-0.080601
39	8	0	-1.928019	-2.359433	-1.356259
40	6	0	-2.089607	-1.236842	-1.899599
41	8	0	-1.482873	-0.159763	-1.597858
42	8	0	0.914831	-2.914618	-1.240553
43	6	0	1.507499	-1.935027	-1.765104
44	8	0	1.304289	-0.710105	-1.500278
45	8	0	0.843111	-2.542246	1.717917
46	6	0	1.434376	-1.469500	2.019932
47	8	0	1.263642	-0.339189	1.470906
48	8	0	-2.007895	-2.023863	1.530889
49	6	0	-2.226434	-0.817748	1.803915
50	8	0	-1.583750	0.186574	1.348656
51	6	0	-3.086434	-1.125404	-3.059103
52	6	0	-3.360306	-0.538671	2.804896
53	6	0	-3.835505	-2.444445	-3.258990
54	1	0	-4.552383	-2.341268	-4.082816
55	1	0	-3.139678	-3.251527	-3.502885
56	6	0	-4.123689	-1.830009	3.119554
57	1	0	-3.461346	-2.573300	3.569847
58	1	0	-4.935028	-1.611931	3.825107
59	6	0	-4.330145	0.528057	2.227938
60	1	0	-5.096340	0.716932	2.990786
61	1	0	-3.786541	1.466181	2.084912
62	6	0	-2.725632	-0.009628	4.103232
63	1	0	-2.157581	0.908270	3.935184
64	1	0	-3.505074	0.196146	4.845931
65	1	0	-2.041698	-0.753666	4.526294
66	6	0	-2.278340	-0.783225	-4.323956
67	1	0	-2.951049	-0.689296	-5.184428
68	1	0	-1.736074	0.158603	-4.197591
69	1	0	-1.552029	-1.573143	-4.546580
70	6	0	-4.072245	0.041337	-2.774856
71	1	0	-3.497319	0.972870	-2.744328
72	1	0	-4.755442	0.108363	-3.631009
73	6	0	2.574622	-2.243549	-2.820810
74	6	0	2.459651	-1.536672	3.157617
75	6	0	3.622077	-3.203766	-2.191672
76	1	0	4.382004	-3.406685	-2.956800

77	6	0	3.520640	-2.615331	2.802559
78	1	0	4.249509	-2.640024	3.622365
79	1	0	3.020683	-3.588785	2.781182
80	6	0	4.232812	-2.392708	1.488352
81	6	0	5.436002	-1.686938	1.416191
82	6	0	3.682945	-2.893535	0.306392
83	6	0	6.061482	-1.485394	0.188575
84	1	0	5.890009	-1.303302	2.326719
85	6	0	4.282184	-2.679735	-0.936934
86	1	0	2.757783	-3.459660	0.355531
87	6	0	5.483996	-1.969121	-0.982435
88	1	0	7.007835	-0.952471	0.144270
89	1	0	5.976063	-1.806651	-1.938385
90	6	0	1.880176	-2.966401	-3.987610
91	1	0	1.139790	-2.312223	-4.462222
92	1	0	2.618951	-3.248560	-4.746512
93	1	0	1.369959	-3.868374	-3.638992
94	6	0	3.242763	-0.961582	-3.324434
95	1	0	3.998622	-1.215165	-4.077576
96	1	0	2.508968	-0.292507	-3.782761
97	1	0	3.730298	-0.412908	-2.514206
98	6	0	1.718803	-1.977238	4.431430
99	1	0	2.427194	-2.073990	5.262481
100	1	0	0.962263	-1.236768	4.715762
101	1	0	1.219668	-2.938162	4.279816
102	6	0	3.120627	-0.174141	3.381624
103	1	0	2.377446	0.576395	3.665680
104	1	0	3.860701	-0.252032	4.187588
105	1	0	3.621955	0.186215	2.479817
106	1	0	3.122606	-4.151953	-1.969210
107	1	0	-4.379799	-2.735720	-2.357289
108	1	0	-4.554398	-2.271080	2.218005
109	6	0	-4.990236	0.130737	0.927746
110	6	0	-4.324554	0.324568	-0.283915
111	6	0	-6.249040	-0.473155	0.908877
112	6	0	-4.864632	-0.106686	-1.497195
113	1	0	-3.346885	0.797165	-0.280459
114	6	0	-6.815286	-0.884231	-0.293758
115	1	0	-6.785087	-0.625484	1.842634
116	6	0	-6.125009	-0.708255	-1.489088
117	1	0	-7.797107	-1.348975	-0.299005
118	1	0	-6.566799	-1.042025	-2.424902

Zero-point correction= 0.997848 (Hartree/Particle)
Thermal correction to Energy= 1.054917
Thermal correction to Enthalpy= 1.055861
Thermal correction to Gibbs Free Energy= 0.912294
Sum of electronic and zero-point Energies= -2835.905514
Sum of electronic and thermal Energies= -2835.848446
Sum of electronic and thermal Enthalpies= -2835.847502
Sum of electronic and thermal Free Energies= -2835.991068
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -2837.61269904

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.967658	-1.402235	0.241078
2	6	0	1.984099	-0.423509	0.194457
3	6	0	0.686363	-0.733076	-0.237898
4	6	0	0.383730	-2.024465	-0.666700
5	6	0	1.373641	-3.000993	-0.628205
6	6	0	2.655157	-2.696732	-0.168569
7	1	0	3.972310	-1.163593	0.579626
8	1	0	-0.603003	-2.267122	-1.043867

9	1	0	1.148634	-4.007479	-0.968539
10	1	0	3.417601	-3.469798	-0.144860
11	6	0	2.098340	1.044505	0.549331
12	6	0	-0.123102	0.503658	-0.214949
13	6	0	-1.447138	0.722284	-0.146466
14	6	0	0.883737	1.644127	-0.195946
15	6	0	-2.037170	2.119270	-0.148066
16	6	0	0.297442	2.938462	0.346181
17	6	0	-1.010322	3.226734	-0.393070
18	1	0	1.007218	3.764239	0.222212
19	1	0	-0.799334	3.302487	-1.467659
20	1	0	1.204614	1.814599	-1.237016
21	6	0	3.430100	1.697364	0.193994
22	1	0	4.255206	1.266571	0.770809
23	1	0	3.654318	1.562797	-0.870156
24	1	0	3.404311	2.771577	0.406170
25	6	0	-2.484052	-0.342172	-0.049034
26	8	0	-3.579614	-0.263610	-0.561723
27	8	0	-2.115152	-1.377418	0.723052
28	6	0	-3.066309	-2.433011	0.824170
29	1	0	-4.007389	-2.065225	1.240278
30	1	0	-3.262824	-2.872354	-0.157916
31	1	0	-2.614942	-3.170668	1.487275
32	1	0	-1.431037	4.189606	-0.084980
33	1	0	0.103057	2.833383	1.422433
34	1	0	-2.835358	2.157249	-0.896656
35	1	0	-2.532928	2.281314	0.820122
36	1	0	1.924643	1.159381	1.630247

Zero-point correction= 0.310412 (Hartree/Particle)
Thermal correction to Energy= 0.326190
Thermal correction to Enthalpy= 0.327135
Thermal correction to Gibbs Free Energy= 0.267217
Sum of electronic and zero-point Energies= -770.462250
Sum of electronic and thermal Energies= -770.446471
Sum of electronic and thermal Enthalpies= -770.445527
Sum of electronic and thermal Free Energies= -770.505445
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -770.97765100

4'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.942329	-1.558340	0.332477
2	6	0	-2.016371	-0.533711	0.195520
3	6	0	-0.669359	-0.810234	-0.090681
4	6	0	-0.258910	-2.134585	-0.251304
5	6	0	-1.191316	-3.159218	-0.115014
6	6	0	-2.524397	-2.877962	0.176883
7	1	0	-3.983080	-1.337169	0.553327
8	1	0	0.767151	-2.362164	-0.504810
9	1	0	-0.875000	-4.189584	-0.249407
10	1	0	-3.241246	-3.688040	0.275338
11	6	0	-2.254223	0.952028	0.341569
12	6	0	0.067998	0.474242	-0.175398
13	6	0	1.365504	0.789107	-0.019130
14	6	0	-1.001685	1.550870	-0.329993
15	6	0	1.851310	2.227771	0.039175
16	6	0	-0.558881	2.918261	0.170665
17	6	0	0.810444	3.247175	-0.419850
18	1	0	2.156408	2.433381	1.073450
19	1	0	-0.493347	2.904609	1.267299
20	1	0	1.131372	4.253741	-0.131034
21	6	0	2.464889	-0.171513	0.281135
22	8	0	3.240756	-0.028094	1.199403

23	8	0	2.578945	-1.169834	-0.613681
24	6	0	3.638283	-2.092570	-0.357623
25	1	0	4.604052	-1.582478	-0.381431
26	1	0	3.510735	-2.565153	0.619450
27	1	0	3.578212	-2.834799	-1.153388
28	1	0	2.763978	2.326988	-0.561495
29	1	0	0.739610	3.236922	-1.515412
30	1	0	-1.297161	3.681154	-0.101426
31	6	0	-3.572103	1.460984	-0.234313
32	1	0	-4.432127	1.028938	0.287954
33	1	0	-3.642646	2.549829	-0.138313
34	1	0	-3.657473	1.203516	-1.295992
35	1	0	-1.219941	1.628292	-1.407975
36	1	0	-2.220234	1.201625	1.413387

Zero-point correction= 0.310573 (Hartree/Particle)
Thermal correction to Energy= 0.326300
Thermal correction to Enthalpy= 0.327245
Thermal correction to Gibbs Free Energy= 0.267298
Sum of electronic and zero-point Energies= -770.460371
Sum of electronic and thermal Energies= -770.444643
Sum of electronic and thermal Enthalpies= -770.443699
Sum of electronic and thermal Free Energies= -770.503646
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -770.97634947

CuI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	-1.544632
2	53	0	0.000000	0.000000	0.845176

Zero-point correction= 0.000652 (Hartree/Particle)
Thermal correction to Energy= 0.003450
Thermal correction to Enthalpy= 0.004394
Thermal correction to Gibbs Free Energy= -0.024585
Sum of electronic and zero-point Energies= -208.809249
Sum of electronic and thermal Energies= -208.806451
Sum of electronic and thermal Enthalpies= -208.805506
Sum of electronic and thermal Free Energies= -208.834486
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -208.83032175

INT1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.814289	-0.595623	-0.753264
2	6	0	1.432632	-0.358172	-0.762560
3	6	0	0.610302	-1.107731	0.106674
4	6	0	1.187831	-2.109653	0.888641
5	6	0	2.556552	-2.344430	0.878036
6	6	0	3.374264	-1.569510	0.061801
7	1	0	3.456706	-0.015761	-1.409158
8	1	0	0.549914	-2.683345	1.555738
9	1	0	2.981991	-3.114658	1.513857
10	1	0	4.447761	-1.733000	0.045391
11	6	0	0.918834	0.685988	-1.667767
12	7	0	-0.242033	0.531693	-2.220544
13	7	0	-1.267497	0.405340	-2.709768
14	6	0	-0.850301	-0.838961	0.258138
15	6	0	-1.327689	0.334282	0.706149
16	6	0	-1.774696	-1.952530	-0.184211
17	6	0	-2.797276	0.686993	0.723458
18	6	0	-3.233255	-1.725667	0.211136

19	1	0	-1.689081	-2.053934	-1.276370
20	6	0	-3.642685	-0.286472	-0.094330
21	1	0	-3.148327	0.710504	1.765574
22	1	0	-3.356995	-1.918990	1.284990
23	1	0	-4.705078	-0.128670	0.119404
24	1	0	-1.406819	-2.901825	0.225488
25	6	0	1.711984	1.904573	-2.064897
26	1	0	2.185946	2.342624	-1.180955
27	1	0	2.497076	1.675321	-2.796731
28	1	0	1.056504	2.663657	-2.498955
29	6	0	-0.419552	1.451593	1.106892
30	8	0	-0.563657	2.600498	0.748418
31	8	0	0.562137	1.056690	1.930710
32	6	0	1.539215	2.044634	2.238332
33	1	0	2.070341	2.347723	1.331291
34	1	0	1.076144	2.924744	2.690700
35	1	0	2.228606	1.568647	2.935025
36	1	0	-2.902385	1.708029	0.342195
37	1	0	-3.491312	-0.086648	-1.162059
38	1	0	-3.874823	-2.437030	-0.319631

Zero-point correction= 0.317729 (Hartree/Particle)
Thermal correction to Energy= 0.336676
Thermal correction to Enthalpy= 0.337621
Thermal correction to Gibbs Free Energy= 0.270152
Sum of electronic and zero-point Energies= -879.848850
Sum of electronic and thermal Energies= -879.829902
Sum of electronic and thermal Enthalpies= -879.828958
Sum of electronic and thermal Free Energies= -879.896427
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -880.39896074

INT2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.126992	-2.171223	1.427028
2	6	0	-0.646366	-1.443008	0.508000
3	6	0	-1.828824	-0.832928	0.956562
4	6	0	-2.180417	-0.958811	2.306204
5	6	0	-1.405275	-1.676115	3.205582
6	6	0	-0.245930	-2.299248	2.755926
7	1	0	1.060185	-2.627120	1.102571
8	1	0	-3.094741	-0.477700	2.642865
9	1	0	-1.703561	-1.748413	4.246547
10	1	0	0.379764	-2.866864	3.436827
11	6	0	-0.104683	-1.314092	-0.904494
12	7	0	0.271588	-2.530751	-1.387511
13	7	0	0.614215	-3.520090	-1.792022
14	6	0	-2.823582	-0.136756	0.083554
15	6	0	-2.869744	1.191205	-0.108674
16	6	0	-3.880014	-1.068793	-0.478622
17	6	0	-3.940687	1.865713	-0.938555
18	6	0	-5.104131	-0.347202	-1.041752
19	1	0	-3.414492	-1.695569	-1.254934
20	6	0	-4.679412	0.881214	-1.841685
21	1	0	-4.643180	2.371729	-0.264081
22	1	0	-5.750610	-0.028806	-0.213784
23	1	0	-5.547999	1.369979	-2.294748
24	1	0	-4.176606	-1.768834	0.312102
25	6	0	-0.710165	-0.466401	-2.029394
26	1	0	-1.715619	-0.793371	-2.313926
27	1	0	-0.760429	0.571187	-1.703509
28	1	0	-0.065271	-0.513644	-2.911851
29	6	0	-1.916998	2.150829	0.526993
30	8	0	-2.244535	3.268815	0.856111

31	8	0	-0.670989	1.676412	0.667006
32	6	0	0.249995	2.547121	1.336815
33	1	0	0.345084	3.488891	0.792660
34	1	0	-0.099476	2.748870	2.351965
35	1	0	1.200634	2.016041	1.349331
36	1	0	-3.481154	2.663869	-1.532307
37	1	0	-4.021825	0.571468	-2.665795
38	1	0	-5.691285	-1.036473	-1.657647
39	29	0	1.676530	-0.407189	-0.527647
40	53	0	3.800759	0.694873	-0.162823

Zero-point correction= 0.319928 (Hartree/Particle)
Thermal correction to Energy= 0.342703
Thermal correction to Enthalpy= 0.343647
Thermal correction to Gibbs Free Energy= 0.264021
Sum of electronic and zero-point Energies= -1088.690306
Sum of electronic and thermal Energies= -1088.667530
Sum of electronic and thermal Enthalpies= -1088.666586
Sum of electronic and thermal Free Energies= -1088.746213
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -1089.25884219

TS1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.307499	0.573237	2.073304
2	6	0	-0.499041	-0.006308	1.079700
3	6	0	-1.897956	0.165711	1.172702
4	6	0	-2.421240	0.909447	2.233831
5	6	0	-1.601159	1.478355	3.201343
6	6	0	-0.224679	1.304166	3.125884
7	1	0	1.386342	0.456995	2.000087
8	1	0	-3.498077	1.039632	2.294023
9	1	0	-2.040251	2.054253	4.010384
10	1	0	0.433578	1.739587	3.870370
11	6	0	0.233985	-0.699781	-0.035525
12	7	0	0.318104	-2.326753	0.550752
13	7	0	0.624454	-3.276086	1.028641
14	6	0	-2.904644	-0.466063	0.266401
15	6	0	-3.567996	0.197081	-0.695394
16	6	0	-3.218893	-1.910209	0.607906
17	6	0	-4.662633	-0.432934	-1.529088
18	6	0	-4.540189	-2.400328	0.017185
19	1	0	-2.393453	-2.544223	0.247226
20	6	0	-4.663381	-1.957474	-1.437925
21	1	0	-5.628030	-0.026921	-1.200523
22	1	0	-5.373397	-1.979673	0.594557
23	1	0	-5.576730	-2.356419	-1.890727
24	1	0	-3.218629	-2.019785	1.698982
25	6	0	-0.405829	-0.876745	-1.398424
26	1	0	-1.379772	-1.368451	-1.416536
27	1	0	-0.552833	0.142487	-1.772641
28	1	0	0.272688	-1.392226	-2.083001
29	6	0	-3.333842	1.638299	-1.008962
30	8	0	-4.204339	2.371307	-1.422027
31	8	0	-2.064558	2.031946	-0.828620
32	6	0	-1.805117	3.416135	-1.065166
33	1	0	-2.022756	3.672340	-2.104780
34	1	0	-2.418436	4.036876	-0.407843
35	1	0	-0.746838	3.555120	-0.847771
36	1	0	-4.549670	-0.110483	-2.570041
37	1	0	-3.820083	-2.363148	-2.013866
38	1	0	-4.605795	-3.489618	0.107246
39	29	0	2.143876	-0.351728	-0.201677
40	53	0	4.497051	0.180228	-0.478561

Zero-point correction=	0.316948 (Hartree/Particle)
Thermal correction to Energy=	0.340038
Thermal correction to Enthalpy=	0.340982
Thermal correction to Gibbs Free Energy=	0.260305
Sum of electronic and zero-point Energies=	-1088.677572
Sum of electronic and thermal Energies=	-1088.654481
Sum of electronic and thermal Enthalpies=	-1088.653537
Sum of electronic and thermal Free Energies=	-1088.734215

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -1089.24469892

INT3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.457950	1.826928	0.115194
2	6	0	-2.283218	1.110400	0.447049
3	6	0	-2.274663	-0.301432	0.260717
4	6	0	-3.415956	-0.931521	-0.229801
5	6	0	-4.541651	-0.195135	-0.582757
6	6	0	-4.564542	1.190101	-0.416143
7	1	0	-3.476656	2.905716	0.224998
8	1	0	-3.410651	-2.010478	-0.350582
9	1	0	-5.409750	-0.705084	-0.990097
10	1	0	-5.443162	1.761633	-0.696825
11	6	0	-1.073244	1.790573	0.828834
12	6	0	-1.139947	-1.151879	0.719330
13	6	0	-0.270963	-1.760339	-0.107748
14	6	0	-1.109209	-1.367599	2.222492
15	6	0	0.805937	-2.702638	0.375970
16	6	0	-0.267970	-2.572621	2.639777
17	6	0	1.053437	-2.583168	1.876704
18	1	0	0.515060	-3.726889	0.107018
19	1	0	-0.822009	-3.496399	2.426033
20	1	0	1.690709	-3.407549	2.212566
21	6	0	-0.290356	-1.584231	-1.591346
22	8	0	0.090284	-2.432963	-2.363786
23	8	0	-0.734735	-0.378342	-1.980050
24	6	0	-0.673908	-0.126013	-3.382545
25	1	0	0.362925	-0.164708	-3.724534
26	1	0	-1.264948	-0.861894	-3.933139
27	1	0	-1.083352	0.874716	-3.515951
28	1	0	1.727011	-2.492023	-0.176434
29	1	0	1.600808	-1.652334	2.074827
30	1	0	-0.099323	-2.542777	3.721505
31	6	0	-1.165769	3.153444	1.421675
32	1	0	-2.167161	3.544835	1.631769
33	1	0	-0.591504	3.141616	2.357901
34	1	0	-0.617198	3.856610	0.780039
35	1	0	-0.711696	-0.451104	2.685160
36	1	0	-2.138484	-1.467488	2.589444
37	29	0	0.631911	1.116455	0.428049
38	53	0	2.946969	0.645993	-0.239073

Zero-point correction=	0.308469 (Hartree/Particle)
Thermal correction to Energy=	0.329733
Thermal correction to Enthalpy=	0.330677
Thermal correction to Gibbs Free Energy=	0.254317
Sum of electronic and zero-point Energies=	-979.240618
Sum of electronic and thermal Energies=	-979.219354
Sum of electronic and thermal Enthalpies=	-979.218410
Sum of electronic and thermal Free Energies=	-979.294770

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.76854420

TS2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.143795	3.104050	-0.694611
2	6	0	-1.062906	1.963960	0.108390
3	6	0	-2.080924	0.994427	0.035863
4	6	0	-3.167335	1.179875	-0.814570
5	6	0	-3.238923	2.316479	-1.611066
6	6	0	-2.224478	3.271066	-1.553388
7	1	0	-0.357261	3.852086	-0.661904
8	1	0	-3.965581	0.444221	-0.836952
9	1	0	-4.089289	2.464107	-2.269033
10	1	0	-2.279526	4.159099	-2.175534
11	6	0	0.089592	1.743619	1.020453
12	6	0	-1.854950	-0.131094	0.960301
13	6	0	-2.024817	-1.451466	0.762728
14	6	0	-1.159012	0.370886	2.173964
15	6	0	-1.620346	-2.469335	1.806232
16	6	0	-0.645982	-0.625215	3.197977
17	6	0	-0.385400	-1.993221	2.572632
18	1	0	-2.455429	-2.652569	2.496310
19	1	0	-1.421311	-0.706368	3.972387
20	1	0	-0.121820	-2.712057	3.354185
21	6	0	-2.621974	-2.027310	-0.480095
22	8	0	-3.440406	-2.918848	-0.463387
23	8	0	-2.114084	-1.493814	-1.592752
24	6	0	-2.646383	-1.991974	-2.819735
25	1	0	-2.474349	-3.067528	-2.902616
26	1	0	-3.720463	-1.795869	-2.877929
27	1	0	-2.114981	-1.456149	-3.604612
28	1	0	-1.419297	-3.425919	1.316568
29	1	0	0.467976	-1.933919	1.884681
30	1	0	0.246419	-0.228607	3.696315
31	6	0	0.420947	2.856942	1.985551
32	1	0	-0.465515	3.323491	2.435529
33	1	0	1.103162	2.518937	2.769904
34	1	0	0.952368	3.633455	1.423150
35	1	0	-0.008824	0.669423	1.616637
36	1	0	-1.620835	1.252644	2.617507
37	29	0	1.535972	0.729768	0.180928
38	53	0	3.317687	-0.620200	-0.772758

Zero-point correction= 0.307062 (Hartree/Particle)
Thermal correction to Energy= 0.327014
Thermal correction to Enthalpy= 0.327958
Thermal correction to Gibbs Free Energy= 0.254957
Sum of electronic and zero-point Energies= -979.209055
Sum of electronic and thermal Energies= -979.189102
Sum of electronic and thermal Enthalpies= -979.188158
Sum of electronic and thermal Free Energies= -979.261160
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.74371895

TS2c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.313771	2.940871	0.800801
2	6	0	-0.533176	1.565305	0.764241
3	6	0	-1.635422	1.050021	0.053646
4	6	0	-2.479641	1.917415	-0.640201
5	6	0	-2.248423	3.287710	-0.605588
6	6	0	-1.174177	3.796905	0.121292
7	1	0	0.538382	3.339908	1.343115
8	1	0	-3.297180	1.524495	-1.232537

9	1	0	-2.900609	3.957460	-1.156636
10	1	0	-0.995247	4.867470	0.147465
11	6	0	0.365988	0.572854	1.418220
12	6	0	-1.769244	-0.417013	0.179073
13	6	0	-2.845265	-1.207104	0.041188
14	6	0	-0.482101	-1.028747	0.656047
15	6	0	-2.833794	-2.692778	0.335638
16	6	0	-0.601251	-2.310932	1.453783
17	6	0	-1.433930	-3.259296	0.581552
18	1	0	-3.476842	-2.861376	1.210372
19	1	0	-1.114036	-2.140279	2.408681
20	1	0	-1.506058	-4.237502	1.065725
21	6	0	-4.213349	-0.689878	-0.282099
22	8	0	-5.073005	-0.527526	0.549870
23	8	0	-4.397784	-0.510754	-1.597004
24	6	0	-5.704310	-0.062981	-1.973090
25	1	0	-6.459944	-0.786414	-1.659002
26	1	0	-5.921404	0.903693	-1.511596
27	1	0	-5.680335	0.025631	-3.058225
28	1	0	-3.308245	-3.227339	-0.496576
29	1	0	-0.919331	-3.412763	-0.374626
30	1	0	0.390113	-2.722166	1.660669
31	6	0	0.837757	0.789158	2.878264
32	1	0	0.019548	1.087716	3.546480
33	1	0	1.312661	-0.113792	3.272872
34	1	0	1.596509	1.575880	2.893262
35	29	0	2.009558	0.227860	0.374643
36	53	0	3.995549	-0.381892	-0.884198
37	1	0	0.247268	-1.133043	-0.144919
38	1	0	-0.415537	-0.218026	1.763769

Zero-point correction= 0.307779 (Hartree/Particle)
Thermal correction to Energy= 0.327959
Thermal correction to Enthalpy= 0.328903
Thermal correction to Gibbs Free Energy= 0.255407
Sum of electronic and zero-point Energies= -979.175871
Sum of electronic and thermal Energies= -979.155691
Sum of electronic and thermal Enthalpies= -979.154746
Sum of electronic and thermal Free Energies= -979.228243
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.71407310

TS3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.308044	-2.485457	-0.373183
2	6	0	-1.598460	-1.283150	-0.152016
3	6	0	-1.609372	-0.708295	1.147045
4	6	0	-2.162673	-1.412710	2.233324
5	6	0	-2.786534	-2.618618	2.005988
6	6	0	-2.865324	-3.147331	0.699639
7	1	0	-2.348540	-2.919341	-1.367316
8	1	0	-2.138297	-0.980356	3.228836
9	1	0	-3.241734	-3.158714	2.829900
10	1	0	-3.364452	-4.098728	0.542261
11	6	0	-0.770486	-0.663037	-1.151808
12	6	0	-1.025911	0.591010	1.191628
13	6	0	-1.018152	1.319127	-0.003512
14	6	0	-0.342196	1.081896	2.441883
15	6	0	-0.036087	2.468811	-0.182576
16	6	0	0.723223	2.152632	2.187343
17	6	0	0.247601	3.166590	1.150767
18	1	0	0.907131	2.079165	-0.583152
19	1	0	1.638539	1.669603	1.826376
20	1	0	1.010400	3.936625	0.997309

21	6	0	-2.266487	1.486297	-0.836882
22	8	0	-2.282203	2.111360	-1.873819
23	8	0	-3.372070	0.972353	-0.280431
24	6	0	-4.561110	1.108047	-1.056400
25	1	0	-4.789541	2.162552	-1.226979
26	1	0	-4.449751	0.607979	-2.022074
27	1	0	-5.346132	0.633153	-0.469065
28	1	0	-0.428944	3.167189	-0.923213
29	1	0	-0.658739	3.676182	1.505950
30	1	0	0.968136	2.645207	3.133825
31	6	0	-1.249662	-0.667651	-2.572630
32	1	0	-2.335175	-0.771300	-2.696799
33	1	0	-0.914860	0.236634	-3.087757
34	1	0	-0.751862	-1.506958	-3.078233
35	1	0	0.088627	0.233925	2.983480
36	29	0	1.098251	-0.547377	-0.770152
37	53	0	3.442520	-0.381774	-0.103417
38	1	0	-1.135442	1.496458	3.084481

Zero-point correction= 0.308594 (Hartree/Particle)
Thermal correction to Energy= 0.328646
Thermal correction to Enthalpy= 0.329590
Thermal correction to Gibbs Free Energy= 0.257689
Sum of electronic and zero-point Energies= -979.225902
Sum of electronic and thermal Energies= -979.205851
Sum of electronic and thermal Enthalpies= -979.204906
Sum of electronic and thermal Free Energies= -979.276807
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.75349050

INT4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.963475	-1.152676	-0.361618
2	6	0	1.615240	-0.632394	-0.341125
3	6	0	1.373588	0.688243	0.267620
4	6	0	2.485540	1.425838	0.820161
5	6	0	3.724620	0.886193	0.770275
6	6	0	3.964453	-0.417382	0.173537
7	1	0	3.162431	-2.123851	-0.805705
8	1	0	2.315425	2.398633	1.273052
9	1	0	4.572179	1.425052	1.183913
10	1	0	4.981763	-0.798444	0.164778
11	6	0	0.453999	-1.142070	-0.827777
12	6	0	0.055805	0.988329	0.177636
13	6	0	-0.642642	-0.129849	-0.543743
14	6	0	-0.722277	2.200988	0.580751
15	6	0	-1.311667	0.425778	-1.829459
16	6	0	-2.067104	2.236805	-0.167754
17	1	0	-0.901162	2.203410	1.664204
18	6	0	-1.882999	1.852356	-1.639693
19	1	0	-0.557716	0.433079	-2.621994
20	1	0	-2.510182	3.235138	-0.089991
21	1	0	-1.198486	2.578218	-2.096085
22	1	0	-0.146011	3.108098	0.354485
23	6	0	0.210149	-2.415837	-1.565825
24	1	0	-0.617449	-2.983257	-1.125544
25	1	0	-0.067784	-2.219745	-2.610295
26	1	0	1.100212	-3.051570	-1.571305
27	6	0	-1.675383	-0.854259	0.322063
28	8	0	-2.566923	-1.544571	-0.116333
29	8	0	-1.456363	-0.684390	1.633373
30	6	0	-2.320859	-1.423058	2.494677
31	1	0	-3.364683	-1.152165	2.318503
32	1	0	-2.199748	-2.496533	2.329279

33	1	0	-2.020983	-1.157822	3.508060
34	1	0	-2.091768	-0.280898	-2.127217
35	1	0	-2.835735	1.943643	-2.171119
36	1	0	-2.777636	1.548676	0.308299

Zero-point correction= 0.309175 (Hartree/Particle)
Thermal correction to Energy= 0.325373
Thermal correction to Enthalpy= 0.326317
Thermal correction to Gibbs Free Energy= 0.265787
Sum of electronic and zero-point Energies= -770.423226
Sum of electronic and thermal Energies= -770.407028
Sum of electronic and thermal Enthalpies= -770.406084
Sum of electronic and thermal Free Energies= -770.466614
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -770.93735837

TS4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.030775	2.548017	0.471145
2	6	0	-0.724618	1.461698	0.006111
3	6	0	-2.114475	1.428203	0.275982
4	6	0	-2.678171	2.486536	0.997063
5	6	0	-1.915608	3.567269	1.427275
6	6	0	-0.554900	3.607548	1.151574
7	1	0	1.101338	2.547693	0.286465
8	1	0	-3.734931	2.461199	1.244082
9	1	0	-2.388066	4.369255	1.986210
10	1	0	0.054389	4.440637	1.486537
11	6	0	0.009121	0.424547	-0.749382
12	6	0	-3.051505	0.343733	-0.148235
13	6	0	-2.913885	-0.970777	0.126119
14	6	0	-4.268288	0.843760	-0.907978
15	6	0	-3.969534	-2.013381	-0.190932
16	6	0	-5.034682	-0.264252	-1.623530
17	1	0	-4.943404	1.365004	-0.215895
18	6	0	-5.293766	-1.411076	-0.652919
19	1	0	-3.574933	-2.685253	-0.966983
20	1	0	-4.447682	-0.628874	-2.477039
21	1	0	-5.911580	-2.188967	-1.112496
22	1	0	-3.928668	1.605292	-1.619907
23	6	0	-0.586766	-0.049039	-2.037891
24	1	0	-1.672613	0.035824	-2.144320
25	1	0	-0.124731	0.606703	-2.791369
26	1	0	-0.259795	-1.063746	-2.279857
27	6	0	-1.679083	-1.499539	0.744364
28	8	0	-0.538566	-1.091164	0.537716
29	8	0	-1.887004	-2.535439	1.543609
30	6	0	-0.719925	-3.133496	2.127814
31	1	0	-0.205624	-2.412473	2.765853
32	1	0	-1.092587	-3.972751	2.712393
33	1	0	-0.036813	-3.473664	1.347025
34	1	0	-4.121954	-2.637252	0.694730
35	1	0	-5.848808	-1.030459	0.214373
36	1	0	-5.971193	0.135654	-2.025487
37	29	0	1.866185	0.111328	-0.473716
38	53	0	4.248768	-0.300151	-0.115408

Zero-point correction= 0.308790 (Hartree/Particle)
Thermal correction to Energy= 0.328835
Thermal correction to Enthalpy= 0.329779
Thermal correction to Gibbs Free Energy= 0.256696
Sum of electronic and zero-point Energies= -979.229093
Sum of electronic and thermal Energies= -979.209048
Sum of electronic and thermal Enthalpies= -979.208104

Sum of electronic and thermal Free Energies= -979.281187
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.75571899

INT5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.023910	2.533368	-0.322775
2	6	0	0.785349	1.396320	-0.034922
3	6	0	2.181383	1.437387	-0.269579
4	6	0	2.737656	2.609348	-0.811488
5	6	0	1.959456	3.719133	-1.103529
6	6	0	0.594339	3.688309	-0.840454
7	1	0	-1.046330	2.490548	-0.141357
8	1	0	3.800095	2.655037	-1.024952
9	1	0	2.420026	4.602950	-1.533627
10	1	0	-0.028579	4.551393	-1.053294
11	6	0	0.086635	0.192977	0.537725
12	6	0	3.123259	0.336797	0.060810
13	6	0	2.903971	-0.994718	-0.113303
14	6	0	4.463408	0.791175	0.614031
15	6	0	3.936817	-2.077996	0.152501
16	6	0	5.240410	-0.306518	1.332868
17	1	0	5.076631	1.174629	-0.213005
18	6	0	5.333321	-1.531882	0.432980
19	1	0	3.594066	-2.673865	1.010462
20	1	0	4.732371	-0.569124	2.269961
21	1	0	5.947379	-2.315099	0.888176
22	1	0	4.284390	1.642631	1.278499
23	6	0	0.566556	-0.202358	1.928956
24	1	0	1.651579	-0.179796	2.095864
25	1	0	0.116034	0.518037	2.619851
26	1	0	0.182357	-1.188840	2.207995
27	6	0	1.632615	-1.481550	-0.619424
28	8	0	0.496630	-0.958735	-0.475142
29	8	0	1.678470	-2.601384	-1.295142
30	6	0	0.433416	-3.142048	-1.785063
31	1	0	-0.001464	-2.462334	-2.519262
32	1	0	0.704244	-4.091160	-2.242384
33	1	0	-0.266471	-3.283981	-0.960180
34	1	0	3.962764	-2.763892	-0.698829
35	1	0	5.818918	-1.251385	-0.510610
36	1	0	6.234639	0.066003	1.598902
37	29	0	-1.860570	0.073207	0.378394
38	53	0	-4.276263	-0.233402	0.097371

Zero-point correction= 0.310761 (Hartree/Particle)
Thermal correction to Energy= 0.330780
Thermal correction to Enthalpy= 0.331724
Thermal correction to Gibbs Free Energy= 0.259695
Sum of electronic and zero-point Energies= -979.230997
Sum of electronic and thermal Energies= -979.210979
Sum of electronic and thermal Enthalpies= -979.210035
Sum of electronic and thermal Free Energies= -979.282064
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.75862982

INT6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.443499	-0.795787	1.669645
2	6	0	-0.533473	-0.221049	0.738914
3	6	0	-1.339570	-1.167351	-0.050199
4	6	0	-0.688079	-2.444235	-0.315698

5	6	0	0.375121	-2.884796	0.396932
6	6	0	0.895634	-2.089211	1.491166
7	1	0	0.723781	-0.242886	2.562712
8	1	0	-1.070719	-3.075167	-1.109193
9	1	0	0.828186	-3.846563	0.183091
10	1	0	1.532519	-2.554730	2.239636
11	6	0	-0.629696	1.124606	0.582385
12	6	0	-2.653568	-0.927324	-0.406357
13	6	0	-3.356300	0.298645	-0.073530
14	6	0	-3.483093	-1.979585	-1.125519
15	6	0	-4.833491	0.263020	0.265480
16	6	0	-4.927213	-2.073039	-0.619530
17	1	0	-3.503273	-1.721976	-2.194777
18	6	0	-5.603721	-0.706892	-0.628693
19	1	0	-4.952315	-0.049806	1.312807
20	1	0	-4.928750	-2.474493	0.402812
21	1	0	-6.640476	-0.786568	-0.283287
22	1	0	-3.027824	-2.967663	-1.047804
23	6	0	0.055003	2.216584	1.331650
24	1	0	0.680483	1.852596	2.147619
25	1	0	0.691785	2.785574	0.643960
26	1	0	-0.693493	2.903126	1.746397
27	6	0	-2.695758	1.478943	-0.030784
28	8	0	-1.402359	1.582342	-0.479802
29	8	0	-3.253952	2.615692	0.414285
30	6	0	-2.910099	3.808731	-0.291478
31	1	0	-3.148046	3.710038	-1.355632
32	1	0	-3.517987	4.596138	0.153552
33	1	0	-1.849391	4.044223	-0.178364
34	1	0	-5.248815	1.271358	0.194284
35	1	0	-5.633998	-0.318178	-1.655382
36	1	0	-5.479333	-2.784995	-1.242956
37	29	0	2.198705	-0.711365	0.535853
38	53	0	3.962916	0.439580	-0.663045

Zero-point correction= 0.310082 (Hartree/Particle)
Thermal correction to Energy= 0.330435
Thermal correction to Enthalpy= 0.331379
Thermal correction to Gibbs Free Energy= 0.256932
Sum of electronic and zero-point Energies= -979.230281
Sum of electronic and thermal Energies= -979.209928
Sum of electronic and thermal Enthalpies= -979.208984
Sum of electronic and thermal Free Energies= -979.283431
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.75775994

TS5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.455519	0.778903	1.749087
2	6	0	0.533433	0.239634	0.830895
3	6	0	1.274190	1.180017	0.006077
4	6	0	0.632548	2.458921	-0.216359
5	6	0	-0.430385	2.884920	0.515752
6	6	0	-0.942560	2.066164	1.583400
7	1	0	-0.766859	0.190680	2.608295
8	1	0	1.008821	3.106072	-0.999901
9	1	0	-0.884940	3.850543	0.323617
10	1	0	-1.620202	2.492952	2.318628
11	6	0	0.734872	-1.118962	0.734923
12	6	0	2.601908	0.949628	-0.388456
13	6	0	3.287585	-0.269897	-0.129097
14	6	0	3.401365	2.078331	-1.027675
15	6	0	4.795716	-0.313415	0.038975
16	6	0	4.890678	2.072959	-0.672485

17	1	0	3.295548	1.994691	-2.119356
18	6	0	5.500139	0.691011	-0.868763
19	1	0	5.046344	-0.088888	1.085470
20	1	0	5.015784	2.375768	0.375758
21	1	0	6.572924	0.703163	-0.646975
22	1	0	2.991741	3.050381	-0.747250
23	6	0	0.217650	-2.204040	1.618671
24	1	0	-0.177788	-1.824270	2.562105
25	1	0	-0.576747	-2.759372	1.104748
26	1	0	1.026412	-2.905435	1.854896
27	6	0	2.592992	-1.451413	0.002915
28	8	0	1.309618	-1.566937	-0.455798
29	8	0	3.185544	-2.583379	0.417229
30	6	0	2.851561	-3.770916	-0.306125
31	1	0	3.076875	-3.648312	-1.370421
32	1	0	3.477318	-4.555158	0.118882
33	1	0	1.795881	-4.024467	-0.186894
34	1	0	5.155503	-1.327759	-0.150589
35	1	0	5.389807	0.384108	-1.917350
36	1	0	5.407145	2.820864	-1.284080
37	29	0	-2.181986	0.675126	0.542169
38	53	0	-3.902534	-0.449863	-0.739138

Zero-point correction= 0.309589 (Hartree/Particle)
Thermal correction to Energy= 0.329226
Thermal correction to Enthalpy= 0.330171
Thermal correction to Gibbs Free Energy= 0.258469
Sum of electronic and zero-point Energies= -979.229949
Sum of electronic and thermal Energies= -979.210311
Sum of electronic and thermal Enthalpies= -979.209367
Sum of electronic and thermal Free Energies= -979.281069
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.75637318

INT7c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.249273	-2.779011	-0.280371
2	6	0	1.901827	-1.468742	0.049511
3	6	0	1.056968	-1.210555	1.150005
4	6	0	0.535790	-2.309800	1.846233
5	6	0	0.864704	-3.611418	1.493594
6	6	0	1.737382	-3.851813	0.437092
7	1	0	2.911192	-2.967603	-1.119278
8	1	0	-0.152052	-2.154506	2.668252
9	1	0	0.435197	-4.440901	2.046423
10	1	0	2.001791	-4.867570	0.161247
11	6	0	2.364939	-0.337458	-0.792543
12	6	0	0.738019	0.174551	1.566255
13	6	0	1.165838	1.240493	0.854533
14	6	0	-0.110441	0.354928	2.805526
15	6	0	0.849209	2.673036	1.216126
16	6	0	-0.141063	1.790483	3.327236
17	1	0	-1.131351	0.023957	2.565124
18	6	0	-0.331686	2.772124	2.177639
19	1	0	1.741405	3.142105	1.652653
20	1	0	0.802300	2.014548	3.843299
21	1	0	-0.424060	3.798206	2.548666
22	1	0	0.256160	-0.307261	3.597704
23	6	0	3.555789	-0.521811	-1.693038
24	1	0	4.381610	-0.964133	-1.128485
25	1	0	3.307500	-1.182175	-2.528954
26	1	0	3.885997	0.438744	-2.089515
27	6	0	1.963072	1.029566	-0.384343
28	8	0	1.257363	0.378086	-1.476569

29	8	0	2.740011	2.090579	-0.769600
30	6	0	2.274455	2.851867	-1.878147
31	1	0	2.428214	2.314617	-2.819177
32	1	0	1.211710	3.099470	-1.784226
33	1	0	2.863607	3.769379	-1.874475
34	1	0	0.629383	3.239815	0.305118
35	1	0	-1.259040	2.531639	1.641602
36	1	0	-0.942061	1.890016	4.066824
37	29	0	-0.672039	0.025033	-1.153333
38	53	0	-3.009091	-0.200608	-0.598276

Zero-point correction= 0.311963 (Hartree/Particle)
Thermal correction to Energy= 0.331591
Thermal correction to Enthalpy= 0.332535
Thermal correction to Gibbs Free Energy= 0.259886
Sum of electronic and zero-point Energies= -979.272748
Sum of electronic and thermal Energies= -979.253120
Sum of electronic and thermal Enthalpies= -979.252176
Sum of electronic and thermal Free Energies= -979.324825
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.79669951

TS6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.814036	-2.808078	0.136443
2	6	0	1.649816	-1.445519	0.374401
3	6	0	0.848918	-1.021624	1.449491
4	6	0	0.244813	-1.990344	2.262905
5	6	0	0.417113	-3.344880	2.018441
6	6	0	1.201938	-3.756540	0.947944
7	1	0	2.411450	-3.145476	-0.702793
8	1	0	-0.391078	-1.691838	3.086938
9	1	0	-0.071881	-4.074501	2.655661
10	1	0	1.335011	-4.813255	0.738411
11	6	0	2.253368	-0.439497	-0.590822
12	6	0	0.584335	0.411509	1.661748
13	6	0	1.115599	1.362362	0.842977
14	6	0	-0.386608	0.793143	2.750055
15	6	0	0.731151	2.825902	0.905484
16	6	0	-0.496793	2.294506	3.005359
17	1	0	-1.366755	0.393046	2.451856
18	6	0	-0.562755	3.046315	1.682269
19	1	0	1.548802	3.404467	1.356680
20	1	0	0.372724	2.639640	3.580988
21	1	0	-0.717295	4.117616	1.846139
22	1	0	-0.108146	0.280627	3.677844
23	6	0	2.060424	0.972489	-0.178195
24	8	0	1.375811	-0.112331	-1.659438
25	8	0	2.663222	2.011289	-0.710166
26	6	0	3.308332	2.060337	-1.986747
27	1	0	4.384387	1.919034	-1.866712
28	1	0	2.870096	1.319520	-2.653865
29	1	0	3.115629	3.067795	-2.356864
30	1	0	0.623687	3.199085	-0.117951
31	1	0	-1.410871	2.676510	1.092198
32	1	0	-1.383946	2.489242	3.616013
33	6	0	3.637240	-0.888445	-1.056500
34	1	0	4.202358	-0.103660	-1.551270
35	1	0	4.227573	-1.256255	-0.212377
36	1	0	3.513980	-1.697020	-1.781839
37	29	0	-0.517090	-0.213132	-1.400933
38	53	0	-2.849018	-0.116325	-0.728806

Zero-point correction= 0.310992 (Hartree/Particle)

Thermal correction to Energy= 0.330330
Thermal correction to Enthalpy= 0.331274
Thermal correction to Gibbs Free Energy= 0.260680
Sum of electronic and zero-point Energies= -979.255403
Sum of electronic and thermal Energies= -979.236065
Sum of electronic and thermal Enthalpies= -979.235121
Sum of electronic and thermal Free Energies= -979.305714
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.78037997

INT8c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.661802	1.630032	1.188636
2	6	0	-2.081355	0.652551	0.382848
3	6	0	-1.989284	-0.668680	0.843456
4	6	0	-2.524044	-0.984793	2.107336
5	6	0	-3.121821	-0.013083	2.889661
6	6	0	-3.182708	1.303936	2.431661
7	1	0	-2.670706	2.657111	0.839167
8	1	0	-2.455516	-1.994198	2.495280
9	1	0	-3.524895	-0.274107	3.862750
10	1	0	-3.628260	2.076061	3.051405
11	6	0	-1.553916	1.091924	-0.977104
12	6	0	-1.249369	-1.659887	0.064200
13	6	0	-0.608537	-1.336454	-1.110438
14	6	0	-1.116603	-3.049614	0.632757
15	6	0	0.329253	-2.278174	-1.836901
16	6	0	-0.485198	-4.070466	-0.310854
17	1	0	-0.506849	-2.962081	1.543739
18	6	0	0.743899	-3.466790	-0.976986
19	1	0	-0.148087	-2.626079	-2.763248
20	1	0	-1.212671	-4.368195	-1.077498
21	1	0	1.261083	-4.206459	-1.595970
22	1	0	-2.103766	-3.397088	0.957966
23	6	0	-0.777376	-0.032785	-1.648795
24	8	0	-0.689336	2.167563	-0.842373
25	8	0	-0.200929	0.129706	-2.799979
26	6	0	-0.055234	1.379575	-3.511986
27	1	0	-0.755935	1.360019	-4.348752
28	1	0	-0.222611	2.217578	-2.837814
29	1	0	0.969131	1.365338	-3.884143
30	1	0	1.214678	-1.711004	-2.139327
31	1	0	1.453146	-3.128134	-0.211181
32	1	0	-0.230813	-4.971727	0.255841
33	6	0	-2.784707	1.434008	-1.854702
34	1	0	-2.500343	1.703526	-2.873588
35	1	0	-3.494630	0.600287	-1.893849
36	1	0	-3.284174	2.296764	-1.407064
37	29	0	0.861933	1.550372	0.029734
38	53	0	2.692077	0.234634	0.951435

Zero-point correction= 0.311803 (Hartree/Particle)
Thermal correction to Energy= 0.331364
Thermal correction to Enthalpy= 0.332308
Thermal correction to Gibbs Free Energy= 0.261289
Sum of electronic and zero-point Energies= -979.260864
Sum of electronic and thermal Energies= -979.241302
Sum of electronic and thermal Enthalpies= -979.240358
Sum of electronic and thermal Free Energies= -979.311377
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.78757909

TS7c

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.357186	2.388600	-1.123104
2	6	0	-1.120392	1.293739	-0.708768
3	6	0	-2.245165	1.471907	0.117637
4	6	0	-2.561251	2.780350	0.528661
5	6	0	-1.795001	3.859169	0.124368
6	6	0	-0.691413	3.666588	-0.711280
7	1	0	0.503917	2.212196	-1.758332
8	1	0	-3.406936	2.955198	1.183848
9	1	0	-2.052843	4.858066	0.462275
10	1	0	-0.091167	4.513318	-1.028341
11	6	0	-0.689949	-0.061184	-1.137947
12	6	0	-3.035991	0.316165	0.537519
13	6	0	-2.661548	-0.946128	0.195561
14	6	0	-4.289198	0.560166	1.351230
15	6	0	-3.404052	-2.186943	0.640163
16	6	0	-5.215353	-0.652242	1.424341
17	1	0	-3.995101	0.867397	2.364798
18	6	0	-4.413860	-1.906049	1.749815
19	1	0	-3.912446	-2.625417	-0.230970
20	1	0	-5.723858	-0.784558	0.460106
21	1	0	-5.071037	-2.772369	1.875599
22	1	0	-4.833661	1.407949	0.921311
23	6	0	-1.477147	-1.159833	-0.638277
24	8	0	0.477480	-0.219922	-1.672759
25	8	0	-1.146046	-2.438588	-0.732292
26	6	0	0.040755	-2.931458	-1.375646
27	1	0	0.125975	-2.544730	-2.390756
28	1	0	0.929944	-2.663858	-0.804507
29	1	0	-0.094519	-4.013030	-1.381760
30	1	0	-2.680520	-2.937862	0.968150
31	1	0	-3.885386	-1.763122	2.701214
32	1	0	-5.992558	-0.473604	2.174373
33	6	0	-2.016468	-0.473376	-2.455908
34	1	0	-2.200519	-1.513593	-2.728842
35	1	0	-2.937659	0.076489	-2.276795
36	1	0	-1.378403	0.001761	-3.200335
37	29	0	2.023175	-0.110988	-0.572404
38	53	0	3.942878	-0.121327	0.894696

Zero-point correction= 0.310023 (Hartree/Particle)
Thermal correction to Energy= 0.329436
Thermal correction to Enthalpy= 0.330380
Thermal correction to Gibbs Free Energy= 0.259590
Sum of electronic and zero-point Energies= -979.241103
Sum of electronic and thermal Energies= -979.221690
Sum of electronic and thermal Enthalpies= -979.220746
Sum of electronic and thermal Free Energies= -979.291536

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -979.76694682

5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.876975	1.136439	-0.161835
2	6	0	1.572933	0.645104	-0.114059
3	6	0	1.313709	-0.733162	0.010678
4	6	0	2.419138	-1.591051	0.087771
5	6	0	3.717847	-1.095367	0.059291
6	6	0	3.956438	0.271437	-0.062967
7	1	0	3.017027	2.206427	-0.277307
8	1	0	2.275503	-2.662666	0.162701
9	1	0	4.551707	-1.788319	0.126586
10	1	0	4.971925	0.654209	-0.085365

11	6	0	0.449923	1.602401	-0.250041
12	6	0	-0.078029	-1.239515	-0.011508
13	6	0	-1.122428	-0.389786	-0.028686
14	6	0	-0.274206	-2.742431	-0.030739
15	6	0	-2.554001	-0.849230	-0.158528
16	6	0	-1.719846	-3.170190	0.216481
17	1	0	0.079119	-3.142395	-0.992353
18	6	0	-2.673069	-2.305233	-0.597729
19	1	0	-3.066529	-0.706524	0.805382
20	1	0	-1.955078	-3.056542	1.283184
21	1	0	-3.708150	-2.644992	-0.484232
22	1	0	0.362183	-3.198437	0.737093
23	6	0	-1.002355	1.359363	1.719788
24	1	0	-0.237357	0.766752	2.228297
25	1	0	-0.832318	2.414846	1.951545
26	1	0	-1.983999	1.063586	2.102228
27	6	0	-0.933490	1.107294	0.193109
28	8	0	0.619974	2.747608	-0.621673
29	8	0	-1.950546	1.768557	-0.526123
30	6	0	-2.316241	3.078429	-0.142510
31	1	0	-2.823823	3.091827	0.831751
32	1	0	-1.459111	3.755480	-0.124518
33	1	0	-3.023483	3.416888	-0.902884
34	1	0	-3.062134	-0.185173	-0.862044
35	1	0	-2.422382	-2.389502	-1.663309
36	1	0	-1.838311	-4.231798	-0.025486

Zero-point correction= 0.310147 (Hartree/Particle)
Thermal correction to Energy= 0.325594
Thermal correction to Enthalpy= 0.326538
Thermal correction to Gibbs Free Energy= 0.268205
Sum of electronic and zero-point Energies= -770.437693
Sum of electronic and thermal Energies= -770.422247
Sum of electronic and thermal Enthalpies= -770.421302
Sum of electronic and thermal Free Energies= -770.479635
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -770.95151650

INT9c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.039001	3.043343	0.845706
2	6	0	-1.603271	1.767526	0.718958
3	6	0	-0.873327	0.657003	1.196543
4	6	0	0.350693	0.867019	1.837653
5	6	0	0.896787	2.140391	1.957254
6	6	0	0.200696	3.229544	1.445771
7	1	0	-1.585299	3.906351	0.477546
8	1	0	0.914071	0.012108	2.199989
9	1	0	1.870575	2.267077	2.417331
10	1	0	0.616684	4.229319	1.522329
11	6	0	-2.920763	1.650703	0.066064
12	7	0	-3.745232	0.727299	0.454408
13	7	0	-4.466181	-0.100409	0.773708
14	6	0	-1.331220	-0.750733	1.012366
15	6	0	-1.494901	-1.315042	-0.198414
16	6	0	-1.627202	-1.512551	2.285550
17	6	0	-2.017111	-2.722396	-0.405072
18	6	0	-2.411806	-2.805885	2.064217
19	1	0	-0.666798	-1.727753	2.775941
20	6	0	-1.865588	-3.566171	0.858748
21	1	0	-3.073208	-2.666927	-0.700159
22	1	0	-3.467400	-2.563429	1.888704
23	1	0	-2.388938	-4.519011	0.729428
24	1	0	-2.165864	-0.845988	2.969277

25	6	0	-3.433200	2.644837	-0.945575
26	1	0	-2.632585	2.902323	-1.646825
27	1	0	-4.265519	2.222289	-1.515659
28	1	0	-3.784141	3.575261	-0.481189
29	6	0	-1.239035	-0.540040	-1.434829
30	8	0	-0.231278	0.119783	-1.702308
31	8	0	-2.220192	-0.645968	-2.313615
32	6	0	-2.043025	0.026333	-3.566688
33	1	0	-1.154877	-0.352120	-4.076706
34	1	0	-2.942625	-0.194118	-4.138608
35	1	0	-1.939507	1.101116	-3.405204
36	1	0	-1.486272	-3.192416	-1.241208
37	1	0	-0.804523	-3.798105	1.018084
38	1	0	-2.368730	-3.421741	2.968418
39	29	0	1.512655	0.037715	-0.843831
40	53	0	3.759571	-0.284717	-0.003572

Zero-point correction= 0.319893 (Hartree/Particle)
Thermal correction to Energy= 0.343021
Thermal correction to Enthalpy= 0.343965
Thermal correction to Gibbs Free Energy= 0.263426
Sum of electronic and zero-point Energies= -1088.706986
Sum of electronic and thermal Energies= -1088.683859
Sum of electronic and thermal Enthalpies= -1088.682914
Sum of electronic and thermal Free Energies= -1088.763453
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -1089.27204742

TS8c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.288872	3.158328	-0.033167
2	6	0	-1.432089	1.806143	0.266411
3	6	0	-0.571545	1.176872	1.184679
4	6	0	0.419449	1.957036	1.788688
5	6	0	0.565281	3.305193	1.483609
6	6	0	-0.286644	3.911225	0.569049
7	1	0	-1.953086	3.633618	-0.747069
8	1	0	1.119611	1.498990	2.476448
9	1	0	1.360593	3.875541	1.952392
10	1	0	-0.172867	4.961351	0.320582
11	6	0	-2.488852	0.978513	-0.413232
12	7	0	-3.483221	0.632718	0.480715
13	7	0	-4.180797	0.137571	1.199129
14	6	0	-0.648633	-0.280502	1.463181
15	6	0	-1.186075	-1.139586	0.578964
16	6	0	0.019881	-0.776441	2.726797
17	6	0	-1.159967	-2.641411	0.742638
18	6	0	-0.316494	-2.228890	3.057626
19	1	0	1.107206	-0.684088	2.591604
20	6	0	-0.166674	-3.093133	1.809296
21	1	0	-2.173951	-2.989860	0.982361
22	1	0	-1.346974	-2.298743	3.432012
23	1	0	-0.325003	-4.151830	2.040209
24	1	0	-0.248716	-0.120475	3.564189
25	6	0	-3.077947	1.461059	-1.724970
26	1	0	-2.255771	1.497753	-2.443675
27	1	0	-3.830167	0.754294	-2.082514
28	1	0	-3.536480	2.450232	-1.643967
29	6	0	-1.716300	-0.695064	-0.775179
30	8	0	-0.867394	-0.471890	-1.709346
31	8	0	-2.831590	-1.440316	-1.117847
32	6	0	-2.881038	-1.926451	-2.453952
33	1	0	-2.011060	-2.552045	-2.671443
34	1	0	-3.793908	-2.521326	-2.507433

35	1	0	-2.920070	-1.116827	-3.187651
36	1	0	-0.909090	-3.094594	-0.224347
37	1	0	0.854127	-2.990995	1.418901
38	1	0	0.341180	-2.581426	3.858785
39	29	0	0.983457	-0.254881	-1.243529
40	53	0	3.258741	-0.115278	-0.411906

Zero-point correction= 0.319020 (Hartree/Particle)
Thermal correction to Energy= 0.340733
Thermal correction to Enthalpy= 0.341677
Thermal correction to Gibbs Free Energy= 0.266176
Sum of electronic and zero-point Energies= -1088.681919
Sum of electronic and thermal Energies= -1088.660206
Sum of electronic and thermal Enthalpies= -1088.659262
Sum of electronic and thermal Free Energies= -1088.734764
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -1089.24526228

INT10c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.544830	3.071964	-0.328162
2	6	0	-1.535927	1.742206	0.085619
3	6	0	-0.652812	1.299131	1.087608
4	6	0	0.220548	2.239396	1.644048
5	6	0	0.219722	3.563313	1.221689
6	6	0	-0.662469	3.986714	0.234195
7	1	0	-2.225742	3.402611	-1.104772
8	1	0	0.939766	1.928398	2.391700
9	1	0	0.924643	4.263462	1.658591
10	1	0	-0.660757	5.017580	-0.104237
11	6	0	-2.457680	0.722553	-0.540745
12	7	0	-3.518492	0.478933	0.413327
13	7	0	-4.224292	0.139665	1.196347
14	6	0	-0.592722	-0.125382	1.492280
15	6	0	-1.075352	-1.089398	0.686892
16	6	0	0.161888	-0.459615	2.758952
17	6	0	-0.898477	-2.563760	0.950177
18	6	0	-0.024530	-1.910017	3.199745
19	1	0	1.230542	-0.275478	2.575872
20	6	0	0.165572	-2.844330	2.008356
21	1	0	-1.866397	-2.990405	1.246950
22	1	0	-1.031139	-2.047535	3.618628
23	1	0	0.114529	-3.893359	2.318972
24	1	0	-0.143058	0.223858	3.561560
25	6	0	-3.097946	1.063080	-1.877949
26	1	0	-2.275542	1.139983	-2.591930
27	1	0	-3.760901	0.253552	-2.188208
28	1	0	-3.657880	2.000190	-1.851652
29	6	0	-1.702999	-0.767020	-0.667633
30	8	0	-0.858290	-0.676482	-1.662850
31	8	0	-2.792465	-1.650108	-0.887926
32	6	0	-2.723431	-2.443125	-2.062408
33	1	0	-1.813435	-3.049568	-2.084517
34	1	0	-3.598907	-3.094389	-2.021913
35	1	0	-2.754521	-1.836028	-2.972556
36	1	0	-0.630791	-3.054443	0.006616
37	1	0	1.159659	-2.678168	1.573561
38	1	0	0.689229	-2.143326	3.996501
39	29	0	0.980453	-0.379264	-1.243089
40	53	0	3.236637	-0.015094	-0.418813

Zero-point correction= 0.319493 (Hartree/Particle)
Thermal correction to Energy= 0.340784
Thermal correction to Enthalpy= 0.341728

Thermal correction to Gibbs Free Energy= 0.268413
Sum of electronic and zero-point Energies= -1088.682252
Sum of electronic and thermal Energies= -1088.660961
Sum of electronic and thermal Enthalpies= -1088.660017
Sum of electronic and thermal Free Energies= -1088.733332
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -1089.24801367

TS9c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.745140	2.994525	-0.486629
2	6	0	-1.629388	1.682131	-0.026766
3	6	0	-0.736443	1.353891	1.013930
4	6	0	0.038915	2.386860	1.552020
5	6	0	-0.069161	3.689224	1.081027
6	6	0	-0.963363	4.001729	0.061538
7	1	0	-2.431285	3.235882	-1.291053
8	1	0	0.764241	2.167702	2.325887
9	1	0	0.561269	4.463532	1.506798
10	1	0	-1.044107	5.016929	-0.312329
11	6	0	-2.425684	0.573038	-0.637086
12	7	0	-3.588231	0.314919	0.403788
13	7	0	-4.216793	0.021836	1.261504
14	6	0	-0.577782	-0.039737	1.483613
15	6	0	-1.004491	-1.067650	0.725370
16	6	0	0.205227	-0.267862	2.756631
17	6	0	-0.736665	-2.513285	1.055206
18	6	0	0.107524	-1.704621	3.266290
19	1	0	1.259958	-0.030188	2.554101
20	6	0	0.344864	-2.682723	2.119239
21	1	0	-1.676819	-2.982788	1.375605
22	1	0	-0.886701	-1.879821	3.700470
23	1	0	0.354379	-3.716553	2.480694
24	1	0	-0.134158	0.431320	3.531440
25	6	0	-3.122034	0.816549	-1.958298
26	1	0	-2.328207	0.943176	-2.697058
27	1	0	-3.717442	-0.056423	-2.230040
28	1	0	-3.757971	1.703882	-1.945571
29	6	0	-1.663603	-0.836977	-0.633021
30	8	0	-0.813566	-0.784952	-1.646855
31	8	0	-2.713916	-1.794915	-0.789314
32	6	0	-2.587061	-2.686114	-1.884464
33	1	0	-1.636603	-3.226124	-1.861041
34	1	0	-3.412469	-3.393448	-1.778305
35	1	0	-2.664485	-2.170133	-2.847029
36	1	0	-0.441612	-3.028743	0.133431
37	1	0	1.326535	-2.482554	1.671089
38	1	0	0.839070	-1.856917	4.066601
39	29	0	1.010643	-0.425483	-1.236209
40	53	0	3.244500	0.062039	-0.408169

Zero-point correction= 0.318307 (Hartree/Particle)
Thermal correction to Energy= 0.340410
Thermal correction to Enthalpy= 0.341354
Thermal correction to Gibbs Free Energy= 0.263555
Sum of electronic and zero-point Energies= -1088.682808
Sum of electronic and thermal Energies= -1088.660704
Sum of electronic and thermal Enthalpies= -1088.659760
Sum of electronic and thermal Free Energies= -1088.737559
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-SDD energy= -1089.24807507