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Supporting Information

Mechanistic Insights into the Rh(I)-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Alkenes, Alkynes, and Nitriles: Does the Intermediacy of α-Thiavinyl Rh-Carbenoid Play an Important Role?

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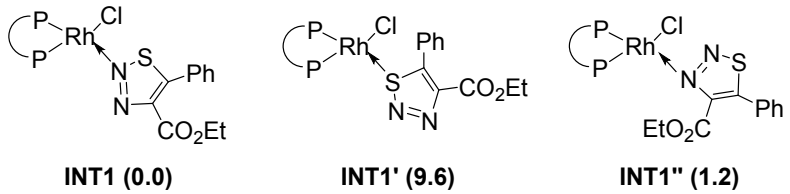

Figure S1. Possible structural conformers of the initial complex for the binding of **1a** with Rh(I). The relative Gibbs energies (in kcal/mol) are given in parentheses.

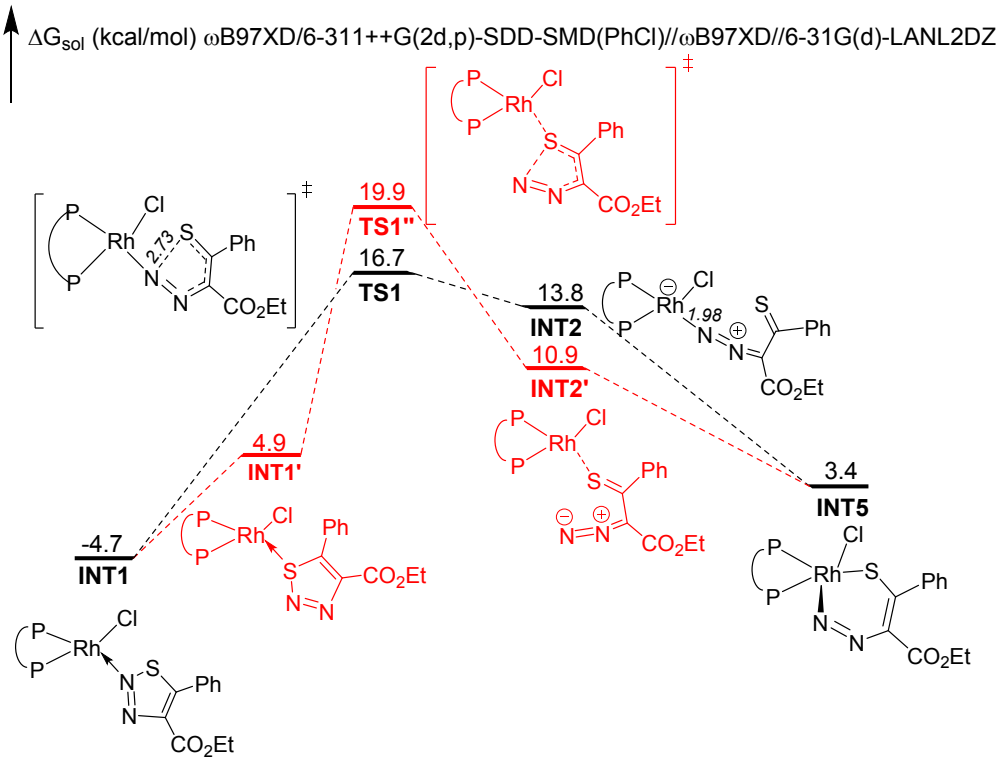

Figure S2. Energy profiles for the tautomerization of **1a** based on **INT1** and **INT1'**, respectively

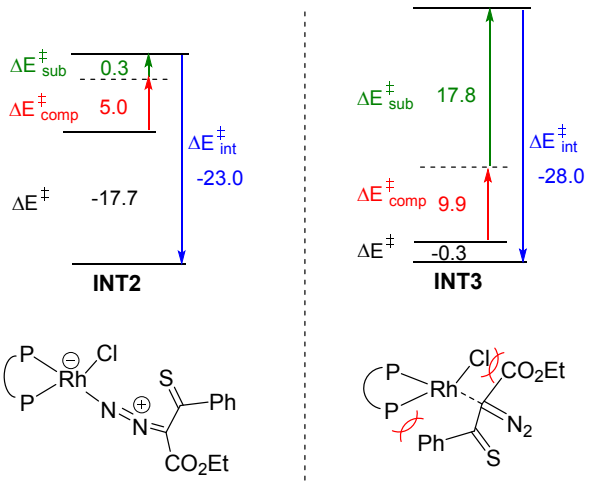

Figure S3. Distortion, interaction and activation energies for **INT2** and **INT3** (green arrow: distortion energy of substrate **1a**; red arrow: distortion energy of the organometallic moiety; blue arrow: interaction energy; black: activation energy, in kcal/mol).

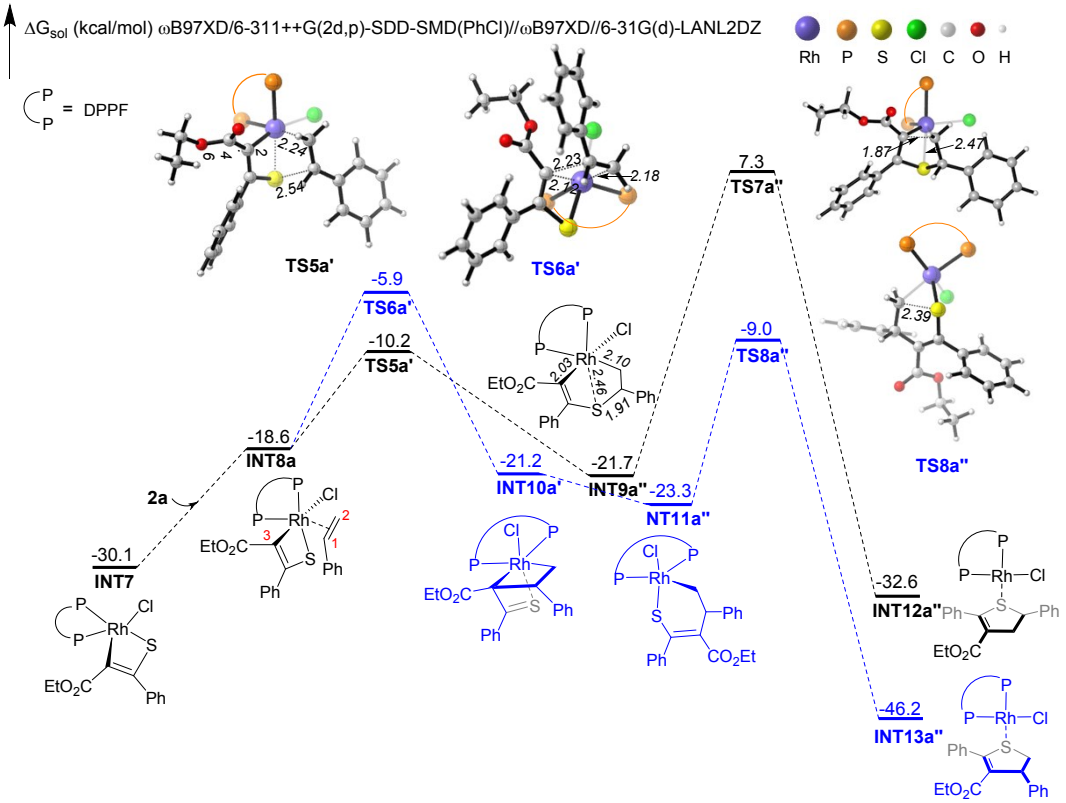

Figure S4. Energy profiles for the migratory insertion of C^1 of **2a** with S/C^3 atom from the *Si* face of styrene.

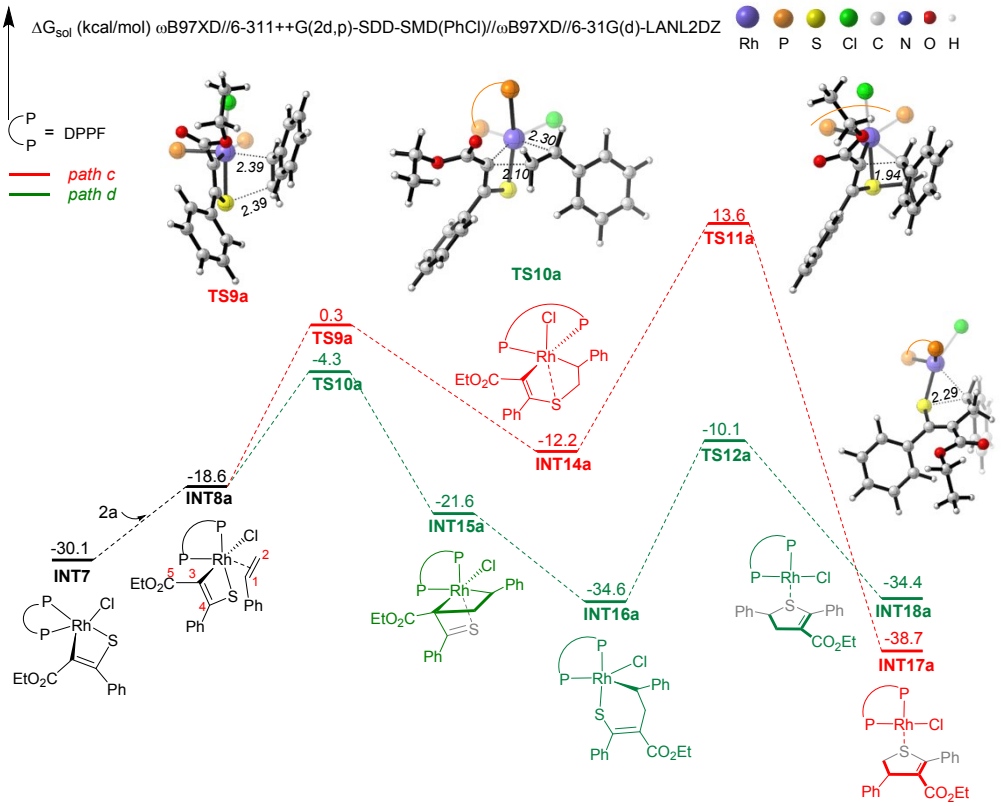

Figure S5. Energy profiles for the migratory insertion of C^2 of **2a** with **INT7** and the subsequent

reductive eliminations (*paths c* and *d*).

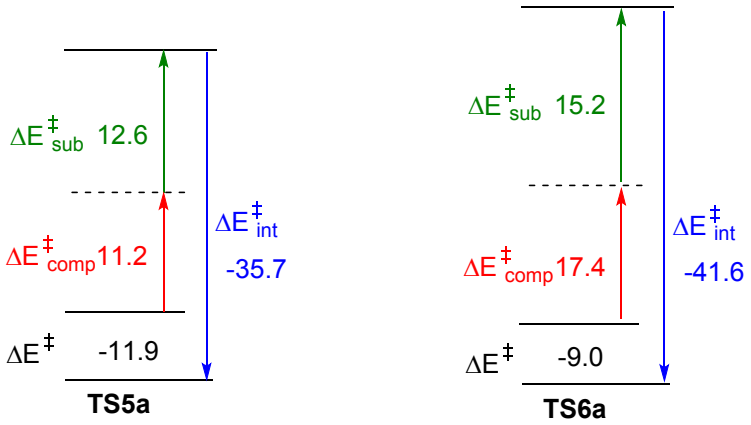

Figure S6. Distortion, interaction and activation energies for **TS5a** and **TS6a** (green arrow: distortion energy of substrate **2a**; red arrow: distortion energy of the organometallic moiety; blue arrow: interaction energy; black: activation energy, in kcal/mol).

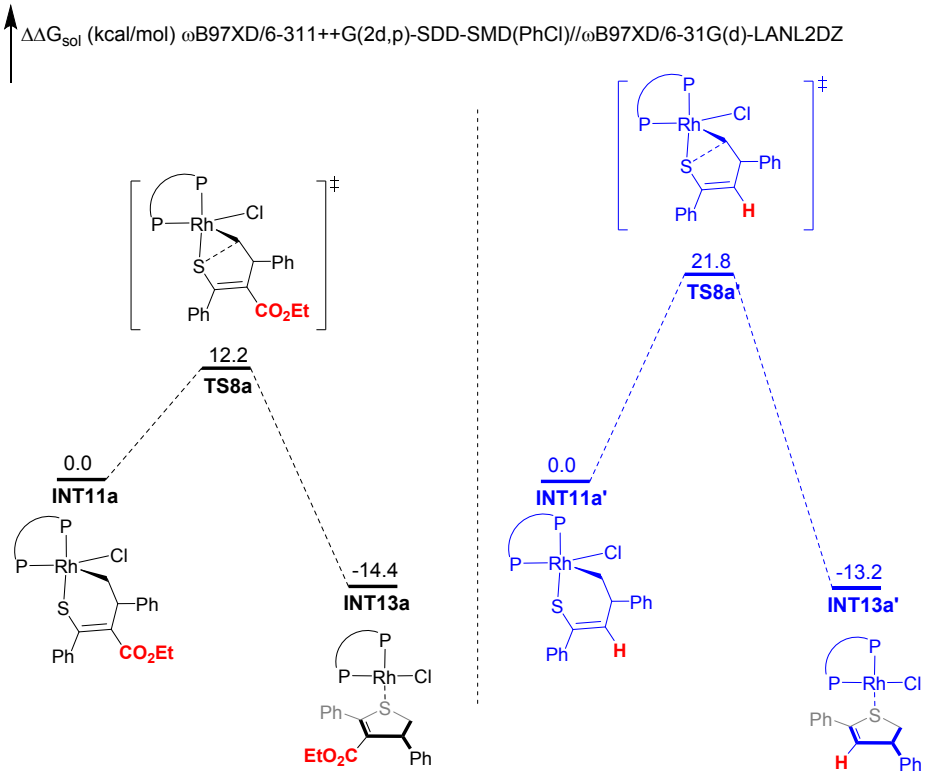

Figure S7. Comparisons for the reductive elimination step between **INT11a** and **INT11a′** (the ester group is replaced by H).

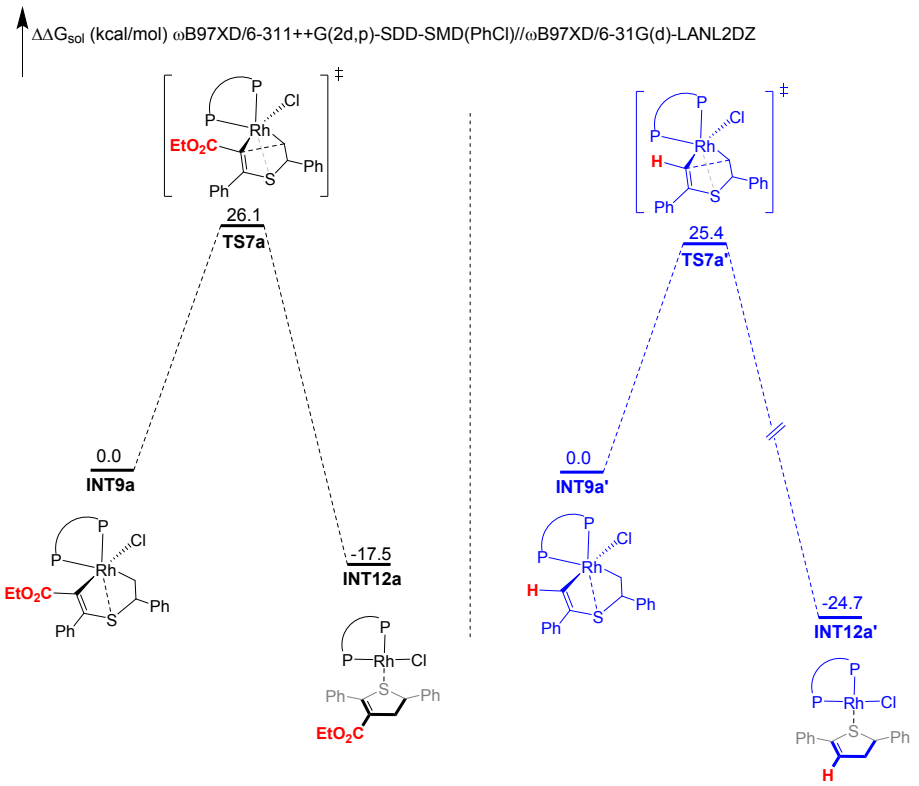

Figure S8. Comparisons for the reductive elimination step between **INT9a** and **INT9a'** (the ester group is replaced by H).

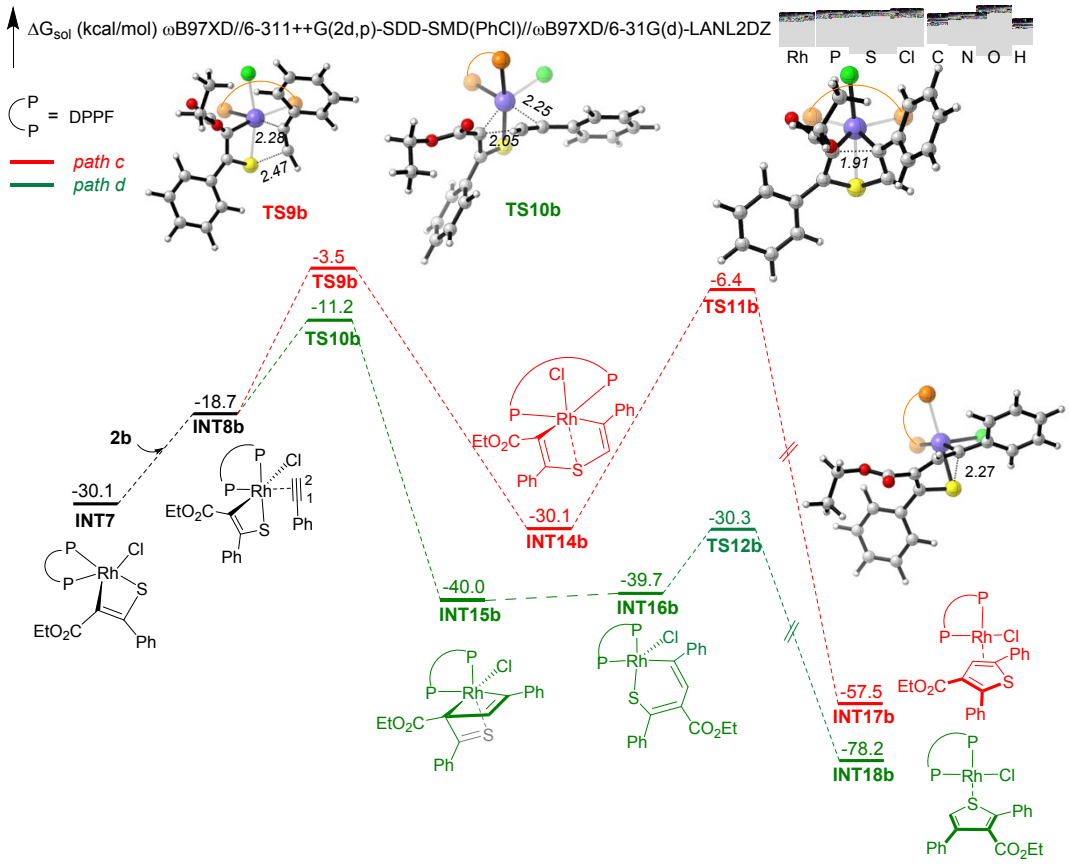

Figure S9. Energy profiles for the migratory insertion of C^2 of **2b** with **INT7** and the subsequent reductive elimination (*paths c* and *d*).

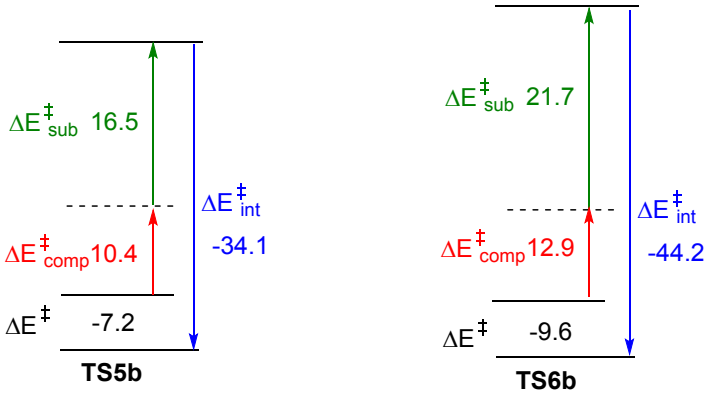

Figure S10. Distortion, interaction and activation energies for **TS5b** and **TS6b** (green arrow: distortion energy of substrate **2b**; red arrow: distortion energy of the organometallic moiety; blue arrow: interaction energy; black: activation energy, in kcal/mol).

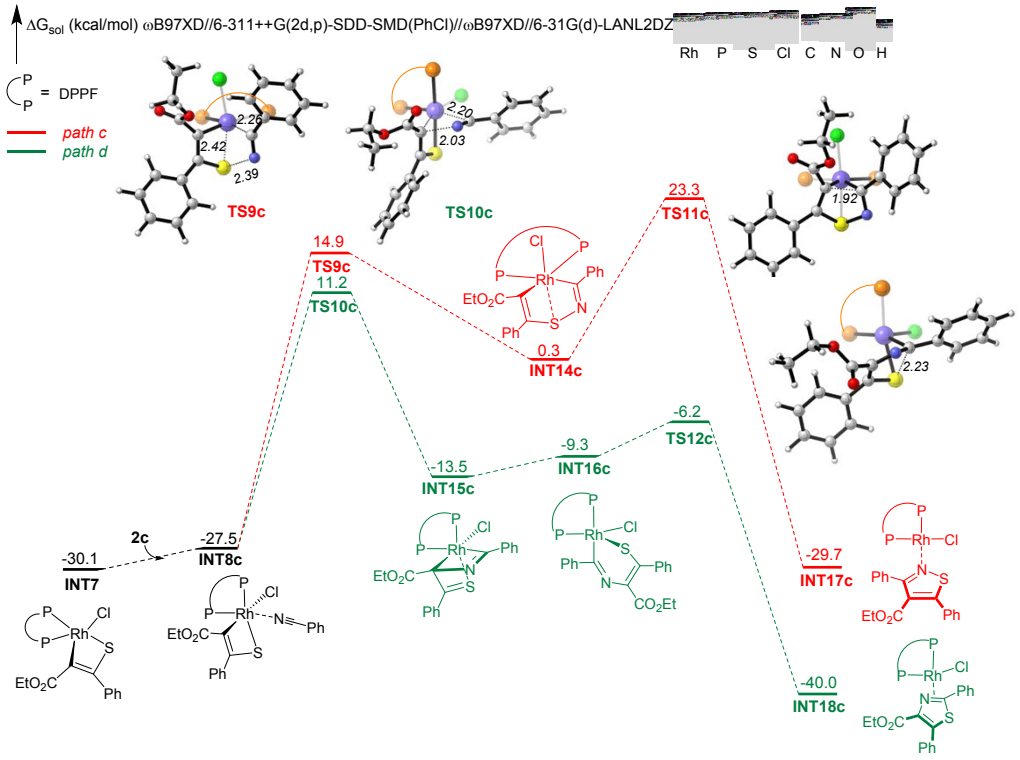

Figure S11. Energy profiles for the migratory insertion of N of **2c** with **INT7** and the subsequent reductive elimination (*paths c* and *d*).

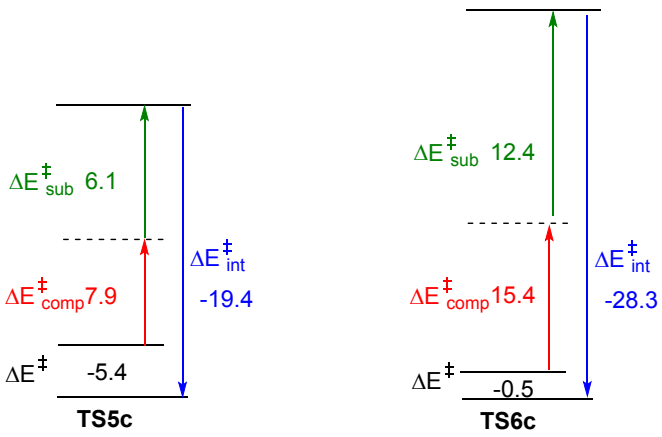

Figure S12. Distortion, interaction and activation energies for **TS5c** and **TS6c** (green arrow: distortion energy of substrate **2c**; red arrow: distortion energy of the organometallic moiety; blue arrow: interaction energy; black: activation energy, in kcal/mol).

Cartesian Coordinates and Energies

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.408222	1.105251	-0.008051
2	6	0	0.963851	1.107556	-0.152086
3	16	0	-0.891585	2.732255	0.176859
4	7	0	0.717830	3.309431	0.073069
5	7	0	1.533313	2.354441	-0.105032
6	6	0	-1.379691	-0.002547	-0.051795
7	6	0	-1.347080	-0.924127	-1.103530
8	6	0	-2.360399	-0.124448	0.936286
9	6	0	-2.273954	-1.956326	-1.156886
10	1	0	-0.598861	-0.822243	-1.883135
11	6	0	-3.285485	-1.161654	0.880923
12	1	0	-2.385996	0.583941	1.759467
13	6	0	-3.243801	-2.079107	-0.164049
14	1	0	-2.242762	-2.665509	-1.978190
15	1	0	-4.038642	-1.251241	1.657433
16	1	0	-3.968558	-2.886207	-0.207580
17	6	0	1.883885	-0.053411	-0.325899
18	8	0	2.959726	0.016628	-0.865299
19	8	0	1.356607	-1.167055	0.196503
20	6	0	2.115855	-2.376888	0.036213
21	6	0	3.165641	-2.516890	1.122840
22	1	0	2.572894	-2.379986	-0.956447
23	1	0	1.366743	-3.168958	0.094744
24	1	0	3.668543	-3.484490	1.026832
25	1	0	3.915634	-1.727137	1.034474
26	1	0	2.704088	-2.462384	2.112958

Zero-point correction= 0.198696 (Hartree/Particle)
Thermal correction to Energy= 0.212655
Thermal correction to Enthalpy= 0.213599
Thermal correction to Gibbs Free Energy= 0.156163
Sum of electronic and zero-point Energies= -1082.860902
Sum of electronic and thermal Energies= -1082.846943
Sum of electronic and thermal Enthalpies= -1082.845999
Sum of electronic and thermal Free Energies= -1082.903435
ωB97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1083.2976248

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.958145	0.335062	0.103383
2	6	0	-1.954896	-0.524855	-0.077366
3	1	0	-3.990624	0.003844	0.058143
4	1	0	-2.797597	1.389871	0.308716
5	1	0	-2.197173	-1.572132	-0.255462
6	6	0	-0.511710	-0.221465	-0.045740
7	6	0	0.403540	-1.279141	0.002445
8	6	0	-0.010064	1.086700	-0.065308
9	6	0	1.773530	-1.043358	0.047119
10	1	0	0.032573	-2.301385	0.010844
11	6	0	1.357226	1.325049	-0.020998
12	1	0	-0.695293	1.926913	-0.128060
13	6	0	2.255952	0.261381	0.037675
14	1	0	2.464907	-1.879996	0.087188
15	1	0	1.725771	2.346676	-0.039142
16	1	0	3.324839	0.449968	0.070515

Zero-point correction= 0.135255 (Hartree/Particle)
Thermal correction to Energy= 0.141920
Thermal correction to Enthalpy= 0.142864
Thermal correction to Gibbs Free Energy= 0.104136
Sum of electronic and zero-point Energies= -309.401233
Sum of electronic and thermal Energies= -309.394568
Sum of electronic and thermal Enthalpies= -309.393624
Sum of electronic and thermal Free Energies= -309.432352
ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -309.631216

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.661592	-1.017497	-0.480841
2	6	0	0.197842	-0.070045	-0.909878
3	16	0	-0.011514	-2.657616	-0.567631
4	6	0	-1.997874	-0.860916	0.132783
5	6	0	-3.102863	-1.553292	-0.365767
6	6	0	-2.150547	-0.047146	1.259861
7	6	0	-4.349702	-1.408683	0.235431
8	1	0	-2.986225	-2.194931	-1.234212

9	6	0	-3.393083	0.087875	1.864323
10	1	0	-1.286092	0.476938	1.656561
11	6	0	-4.497448	-0.588772	1.349662
12	1	0	-5.206250	-1.939947	-0.168146
13	1	0	-3.499892	0.719146	2.741532
14	1	0	-5.469537	-0.480932	1.821412
15	6	0	-0.050039	1.379655	-1.036227
16	8	0	0.842821	2.187490	-1.188464
17	8	0	-1.353199	1.700587	-1.016029
18	6	0	-1.672713	3.097214	-1.019884
19	6	0	-1.621401	3.662540	0.388543
20	1	0	-2.682450	3.145472	-1.432290
21	1	0	-0.983276	3.622911	-1.684422
22	1	0	-1.931298	4.712612	0.384147
23	1	0	-2.292710	3.103021	1.047057
24	1	0	-0.603771	3.606249	0.785231
25	6	0	1.447857	-2.079540	-1.512141
26	6	0	1.592068	-0.563397	-1.243322
27	1	0	2.328758	-2.640011	-1.194393
28	1	0	1.264723	-2.270392	-2.572823
29	1	0	1.945792	-0.079875	-2.159191
30	6	0	2.595515	-0.246640	-0.143097
31	6	0	2.316523	-0.512345	1.199960
32	6	0	3.837266	0.295177	-0.474112
33	6	0	3.263680	-0.251520	2.184779
34	1	0	1.351998	-0.927063	1.479202
35	6	0	4.785454	0.561028	0.508961
36	1	0	4.059129	0.523260	-1.513575
37	6	0	4.501710	0.286287	1.843051
38	1	0	3.032076	-0.465198	3.224301
39	1	0	5.743556	0.991281	0.232274
40	1	0	5.238792	0.494790	2.612867

Zero-point correction= 0.328767 (Hartree/Particle)
Thermal correction to Energy= 0.348224
Thermal correction to Enthalpy= 0.349168
Thermal correction to Gibbs Free Energy= 0.277942
Sum of electronic and zero-point Energies= -1282.879074
Sum of electronic and thermal Energies= -1282.859617
Sum of electronic and thermal Enthalpies= -1282.858673
Sum of electronic and thermal Free Energies= -1282.929900

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1283.4995892

COD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.185621	1.245584	-0.501056
2	6	0	-0.040590	1.693928	-0.224375
3	6	0	-1.095441	1.085551	0.669446
4	6	0	-1.915647	-0.020086	-0.016410
5	6	0	-1.185624	-1.245540	-0.501157
6	6	0	0.040592	-1.693906	-0.224529
7	6	0	1.095443	-1.085605	0.669342
8	6	0	1.915646	0.020078	-0.016444
9	1	0	1.778508	1.853202	-1.185382
10	1	0	-0.344226	2.611636	-0.727405
11	1	0	-1.794923	1.875969	0.965010
12	1	0	-0.664974	0.712772	1.601029
13	1	0	-2.718396	-0.338862	0.665018
14	1	0	-2.429271	0.420059	-0.882334
15	1	0	-1.778513	-1.853092	-1.185539
16	1	0	0.344234	-2.611560	-0.727653
17	1	0	1.794922	-1.876049	0.964847
18	1	0	0.664980	-0.712888	1.600950
19	1	0	2.718423	0.338788	0.664982
20	1	0	2.429235	-0.419999	-0.882424

Zero-point correction= 0.183377 (Hartree/Particle)
Thermal correction to Energy= 0.190717
Thermal correction to Enthalpy= 0.191661
Thermal correction to Gibbs Free Energy= 0.151932
Sum of electronic and zero-point Energies= -311.749877
Sum of electronic and thermal Energies= -311.742536
Sum of electronic and thermal Enthalpies= -311.741592
Sum of electronic and thermal Free Energies= -311.781321

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -312.0308671

Rh(DPPF)(COD)Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.776333	-1.549066	1.603639
2	15	0	-2.210020	-0.477471	0.098394
3	15	0	2.931766	0.318652	-0.408999
4	6	0	-3.993172	-0.788382	-2.025896
5	6	0	-3.206316	-0.135794	1.601341
6	6	0	-3.302927	0.554612	3.924342
7	6	0	-3.381082	-1.419891	-0.941237
8	6	0	-4.694143	0.581112	3.866876

9	6	0	-4.603508	-0.106008	1.553175
10	6	0	-2.565973	0.205542	2.797589
11	6	0	-5.340633	0.252335	2.679120
12	6	0	-3.708619	-2.744806	-0.639016
13	6	0	-4.641240	-3.427964	-1.411449
14	6	0	2.304773	-0.243125	1.209641
15	6	0	2.758497	-1.319128	2.038851
16	6	0	3.426282	-1.268970	-1.196290
17	6	0	0.042362	-3.460797	1.744550
18	6	0	1.257662	0.422047	1.923260
19	6	0	2.001654	-1.314038	3.239149
20	6	0	-4.933367	-1.471531	-2.792437
21	6	0	1.072883	-0.237511	3.169960
22	6	0	2.651530	-1.708415	-2.273771
23	6	0	-1.030121	-1.740186	0.640911
24	6	0	4.493087	-2.063646	-0.758094
25	6	0	0.688209	-3.272757	0.488183
26	6	0	-1.020235	-2.521778	1.842476
27	6	0	0.029171	-2.218014	-0.190775
28	6	0	4.565748	1.004674	0.104202
29	6	0	4.798510	1.492048	1.394024
30	6	0	4.748285	-3.293466	-1.356328
31	6	0	2.903496	-2.943016	-2.869044
32	6	0	3.945993	-3.740168	-2.406458
33	6	0	-5.256578	-2.790493	-2.487068
34	6	0	6.784231	1.752808	-0.535835
35	6	0	5.573100	1.150808	-0.858518
36	6	0	7.005903	2.233614	0.753169
37	6	0	6.009116	2.102678	1.714823
38	1	0	0.275429	-1.807371	-1.158132
39	1	0	1.567432	-3.791884	0.130013
40	1	0	0.339107	-4.159166	2.515495
41	1	0	-1.685040	-2.396072	2.686035
42	1	0	0.676410	1.247506	1.535409
43	1	0	0.345761	0.011740	3.930666
44	1	0	2.075903	-2.037459	4.040031
45	1	0	3.509723	-2.046881	1.767598
46	1	0	-1.482929	0.181101	2.844996
47	1	0	-2.789519	0.808496	4.847266
48	1	0	-5.271168	0.857000	4.744466
49	1	0	-6.425144	0.269594	2.625534
50	1	0	-5.120548	-0.367270	0.635026
51	1	0	-3.228407	-3.244484	0.197665
52	1	0	-4.883484	-4.460490	-1.178023
53	1	0	-5.981440	-3.326649	-3.092759
54	1	0	-5.399226	-0.977701	-3.639803
55	1	0	-3.710594	0.229252	-2.280799
56	1	0	5.135483	-1.711358	0.044873
57	1	0	5.576756	-3.903189	-1.006599
58	1	0	4.144418	-4.701910	-2.870949
59	1	0	2.284320	-3.275028	-3.697041
60	1	0	1.837899	-1.086333	-2.640782
61	1	0	5.413233	0.776827	-1.866988
62	1	0	7.556542	1.848036	-1.293769
63	1	0	7.950421	2.707180	1.004482
64	1	0	6.172685	2.473441	2.722872
65	1	0	4.033986	1.389324	2.158998
66	17	0	-0.646978	-0.046119	-2.805583
67	6	0	0.242296	2.888677	-1.631181
68	6	0	-0.928636	3.185312	-2.296091
69	6	0	-1.866432	4.313858	-1.919081
70	6	0	-3.005294	3.832256	-1.003494
71	6	0	-2.583315	2.766273	-0.014717
72	6	0	-1.378455	2.727617	0.712510
73	6	0	-0.309831	3.815420	0.685408
74	6	0	0.762262	3.588779	-0.397833
75	1	0	0.951511	2.229842	-2.128247
76	1	0	-1.076863	2.727665	-3.271334
77	1	0	-2.296038	4.740446	-2.831329
78	1	0	-1.303723	5.121700	-1.441646
79	1	0	-3.455277	4.683437	-0.470941
80	1	0	-3.799820	3.402194	-1.624510
81	1	0	-3.426633	2.228822	0.418943
82	1	0	-1.410721	2.153826	1.636149
83	1	0	0.181514	3.851773	1.663842
84	1	0	-0.788273	4.792602	0.558718
85	1	0	1.232227	4.542942	-0.676189
86	1	0	1.562334	2.962919	0.010544
87	45	0	-1.270922	1.392313	-0.963647

Zero-point correction=	0.714847 (Hartree/Particle)
Thermal correction to Energy=	0.757079
Thermal correction to Enthalpy=	0.758023
Thermal correction to Gibbs Free Energy=	0.637809
Sum of electronic and zero-point Energies=	-2999.192837
Sum of electronic and thermal Energies=	-2999.150605
Sum of electronic and thermal Enthalpies=	-2999.149661
Sum of electronic and thermal Free Energies=	-2999.269875

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3002.0619535

INT1

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	17	0	-0.139002	-3.276595	-0.079521
2	6	0	4.105777	-1.065599	0.221572
3	6	0	3.739787	-0.351052	-0.903347
4	16	0	2.676903	-1.611364	0.968925
5	7	0	1.716027	-0.849702	-0.193314
6	7	0	2.393519	-0.254288	-1.090889
7	6	0	5.430953	-1.321577	0.818106
8	6	0	5.872850	-2.627089	1.040614
9	6	0	6.233874	-0.242302	1.201158
10	6	0	7.117032	-2.850585	1.624138
11	1	0	5.251017	-3.465559	0.739736
12	6	0	7.470930	-0.470509	1.788798
13	1	0	5.876390	0.768897	1.033265
14	6	0	7.916851	-1.775194	1.997818
15	1	0	7.459209	-3.867987	1.785651
16	1	0	8.088914	0.370891	2.087874
17	1	0	8.885269	-1.951069	2.456088
18	6	0	4.611994	0.306561	-1.915905
19	8	0	4.215804	1.060605	-2.769903
20	8	0	5.888691	-0.050796	-1.753248
21	6	0	6.843067	0.575302	-2.620441
22	6	0	8.209722	0.071816	-2.205702
23	1	0	6.753535	1.661215	-2.515257
24	1	0	6.604867	0.319923	-3.657369
25	1	0	8.982448	0.541169	-2.822331
26	1	0	8.405081	0.307609	-1.155501
27	1	0	8.276522	-1.012735	-2.329868
28	26	0	-3.180946	2.061743	-1.307451
29	15	0	-0.364495	1.370883	0.334514
30	15	0	-2.653958	-1.109835	-0.099297
31	6	0	2.087034	1.933803	1.554881
32	6	0	-1.054791	1.955752	1.935002
33	6	0	-2.226439	1.466794	3.999200
34	6	0	1.308663	2.132449	0.408173
35	6	0	-2.162360	2.808723	4.361148
36	6	0	-0.958976	3.296461	2.327571
37	6	0	-1.667090	1.042337	2.795248
38	6	0	-1.516846	3.722076	3.527769
39	6	0	1.868044	2.793017	-0.685786
40	6	0	3.181247	3.255533	-0.633937
41	6	0	-3.771208	0.287060	-0.497518
42	6	0	-4.426371	0.496415	-1.752722
43	6	0	-3.129834	-2.241315	-1.463393
44	6	0	-2.539009	3.861613	-2.082471
45	6	0	-4.137947	1.379329	0.356239
46	6	0	-5.171980	1.703095	-1.675976
47	6	0	3.399451	2.390765	1.605350
48	6	0	-4.998524	2.244689	-0.371800
49	6	0	-2.328665	-2.267323	-2.607717
50	6	0	-1.219850	2.360432	-0.921560
51	6	0	-4.306292	-2.992284	-1.433537
52	6	0	-2.200829	2.800104	-2.968778
53	6	0	-1.933377	3.599475	-0.824220
54	6	0	-1.386483	1.878343	-2.261571
55	6	0	-3.456543	-1.799127	1.404625
56	6	0	-4.793227	-1.539766	1.728159
57	6	0	-4.680245	-3.753248	-2.537261
58	6	0	-2.710001	-3.018666	-3.714669
59	6	0	-3.886720	-3.762442	-3.681584
60	6	0	3.949464	3.054220	0.508565
61	6	0	-3.254210	-3.123238	3.420311
62	6	0	-2.690646	-2.599025	2.260541
63	6	0	-4.583392	-2.856638	3.738400
64	6	0	-5.353135	-2.066725	2.888773
65	1	0	-0.997800	0.937497	-2.628678
66	1	0	-2.548426	2.686484	-3.986488
67	1	0	-3.192011	4.693962	-2.308140
68	1	0	-2.060775	4.191405	0.070488
69	1	0	-3.796217	1.533915	1.369918
70	1	0	-5.405750	3.178727	-0.008935
71	1	0	-5.734270	2.151388	-2.483746
72	1	0	-4.329822	-0.138931	-2.622074
73	1	0	-1.706527	-0.006801	2.520053
74	1	0	-2.708983	0.742528	4.648670
75	1	0	-2.599427	3.143216	5.297490
76	1	0	-1.440233	4.765848	3.818250
77	1	0	-0.426709	4.006400	1.700313
78	1	0	1.288723	2.929293	-1.593413
79	1	0	3.607770	3.751408	-1.499569
80	1	0	4.973065	3.417616	0.548279
81	1	0	3.990317	2.232711	2.503395
82	1	0	1.662815	1.421670	2.414903
83	1	0	-4.932015	-2.991400	-0.545931
84	1	0	-5.593259	-4.340552	-2.501630
85	1	0	-4.180339	-4.356268	-4.542507
86	1	0	-2.077361	-3.035293	-4.597208
87	1	0	-1.392673	-1.715746	-2.616316
88	1	0	-1.657081	-2.815495	2.004638
89	1	0	-2.649503	-3.744072	4.074702
90	1	0	-5.019995	-3.265461	4.645267
91	1	0	-6.391964	-1.857871	3.127495

92	1	0	-5.401415	-0.918923	1.077417
93	45	0	-0.372505	-0.862489	-0.011852

Zero-point correction= 0.728168 (Hartree/Particle)
Thermal correction to Energy= 0.777200
Thermal correction to Enthalpy= 0.778144
Thermal correction to Gibbs Free Energy= 0.641726
Sum of electronic and zero-point Energies= -3770.300313
Sum of electronic and thermal Energies= -3770.251281
Sum of electronic and thermal Enthalpies= -3770.250337
Sum of electronic and thermal Free Energies= -3770.386755

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent =-3773.3358134

INT1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.172487	2.613924	-0.728733
2	6	0	-3.461098	-0.028709	-0.842561
3	6	0	-4.250935	0.847821	-1.532438
4	16	0	-2.098178	-0.378291	-1.833384
5	7	0	-2.651734	0.696288	-3.085966
6	7	0	-3.758256	1.199827	-2.778785
7	6	0	-3.618238	-0.674548	0.474748
8	6	0	-2.735177	-0.373670	1.514515
9	6	0	-4.602245	-1.648350	0.661294
10	6	0	-2.826519	-1.054843	2.724605
11	1	0	-1.976020	0.388719	1.360981
12	6	0	-4.687796	-2.328080	1.870976
13	1	0	-5.286501	-1.879652	-0.149084
14	6	0	-3.795986	-2.038085	2.902732
15	1	0	-2.126391	-0.823430	3.521249
16	1	0	-5.449818	-3.089877	2.006838
17	1	0	-3.860271	-2.575098	3.844317
18	6	0	-5.520420	1.488817	-1.095170
19	8	0	-6.233572	2.137892	-1.819142
20	8	0	-5.756914	1.249180	0.201043
21	6	0	-6.929656	1.859342	0.760483
22	6	0	-6.652390	3.295386	1.167407
23	1	0	-7.171566	1.235644	1.623494
24	1	0	-7.741222	1.804124	0.030773
25	1	0	-7.537777	3.721966	1.650377
26	1	0	-5.815379	3.340769	1.870275
27	1	0	-6.411509	3.901086	0.290097
28	26	0	3.869390	-1.006129	-0.730761
29	15	0	0.630081	-1.689091	-0.341346
30	15	0	1.713792	1.485560	0.228724
31	6	0	-1.589936	-3.389496	-0.192354
32	6	0	0.869469	-2.223645	1.398958
33	6	0	0.904815	-1.659497	3.756513
34	6	0	-0.475467	-3.020937	-0.954150
35	6	0	1.269392	-2.965160	4.068979
36	6	0	1.198237	-3.544535	1.726357
37	6	0	0.694716	-1.297844	2.427762
38	6	0	1.403969	-3.910434	3.052136
39	6	0	-0.291817	-3.589594	-2.216193
40	6	0	-1.208716	-4.514315	-2.709475
41	6	0	3.354769	0.675118	0.294337
42	6	0	4.446035	0.955173	-0.589807
43	6	0	2.168597	2.966265	-0.749444
44	6	0	4.326815	-2.735559	-1.754826
45	6	0	3.795404	-0.351607	1.194749
46	6	0	5.532962	0.108531	-0.245018
47	6	0	-2.506375	-4.309623	-0.689959
48	6	0	5.133569	-0.692911	0.860183
49	6	0	1.906150	2.970179	-2.121266
50	6	0	2.200256	-2.043538	-1.174098
51	6	0	2.855880	4.037381	-0.175869
52	6	0	3.935573	-1.715163	-2.667290
53	6	0	3.260899	-2.946747	-0.839145
54	6	0	2.627525	-1.290295	-2.318094
55	6	0	1.526438	2.074641	1.964474
56	6	0	2.610312	2.158760	2.845277
57	6	0	3.280099	5.099647	-0.968511
58	6	0	2.341919	4.027170	-2.913576
59	6	0	3.029143	5.093000	-2.338201
60	6	0	-2.318429	-4.873696	-1.949419
61	6	0	0.057779	2.786584	3.754572
62	6	0	0.247885	2.405412	2.430228
63	6	0	1.139269	2.848109	4.630311
64	6	0	2.416602	2.542790	4.169791
65	1	0	2.060318	-0.489407	-2.774464
66	1	0	4.547948	-1.298450	-3.455143
67	1	0	5.290195	-3.226254	-1.725017
68	1	0	3.283770	-3.615751	0.008939
69	1	0	3.205536	-0.804542	1.978803
70	1	0	5.722597	-1.466950	1.333277
71	1	0	6.480937	0.053969	-0.762507
72	1	0	4.423597	1.663252	-1.406317
73	1	0	0.396602	-0.284038	2.186996
74	1	0	0.783621	-0.914693	4.537778
75	1	0	1.435577	-3.252523	5.103041

76	1	0	1.661443	-4.937433	3.293722
77	1	0	1.271260	-4.295224	0.944302
78	1	0	0.567441	-3.309571	-2.819203
79	1	0	-1.055662	-4.952576	-3.691149
80	1	0	-3.035331	-5.591114	-2.337678
81	1	0	-3.370139	-4.578947	-0.089437
82	1	0	-1.749600	-2.955659	0.791360
83	1	0	3.055009	4.050783	0.891647
84	1	0	3.803114	5.935625	-0.513586
85	1	0	3.359266	5.923555	-2.955337
86	1	0	2.126737	4.025969	-3.977766
87	1	0	1.334067	2.157186	-2.558854
88	1	0	-0.591711	2.377915	1.741788
89	1	0	-0.940830	3.037563	4.099853
90	1	0	0.988039	3.138452	5.665989
91	1	0	3.267416	2.597675	4.842669
92	1	0	3.611742	1.916425	2.504849
93	45	0	-0.142255	0.431421	-0.626339

Zero-point correction= 0.728229 (Hartree/Particle)
Thermal correction to Energy= 0.777228
Thermal correction to Enthalpy= 0.778173
Thermal correction to Gibbs Free Energy= 0.642789
Sum of electronic and zero-point Energies= -3770.286389
Sum of electronic and thermal Energies= -3770.237389
Sum of electronic and thermal Enthalpies= -3770.236445
Sum of electronic and thermal Free Energies= -3770.371829

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.2521454

INT1''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.432768	-2.519476	1.737934
2	6	0	4.224469	-0.075913	1.044563
3	6	0	3.005497	-0.416278	0.513920
4	16	0	3.915369	0.819921	2.464220
5	7	0	2.251463	0.716524	2.293366
6	7	0	1.944907	0.065426	1.234933
7	6	0	5.568465	-0.328829	0.507001
8	6	0	6.606925	-0.767257	1.333081
9	6	0	5.811959	-0.108220	-0.853064
10	6	0	7.872114	-0.991790	0.800990
11	1	0	6.418020	-0.955735	2.386201
12	6	0	7.077106	-0.335734	-1.379488
13	1	0	5.010552	0.262155	-1.485771
14	6	0	8.108989	-0.778100	-0.554279
15	1	0	8.671902	-1.340034	1.446999
16	1	0	7.259155	-0.161690	-2.435459
17	1	0	9.097195	-0.954307	-0.967958
18	6	0	2.752020	-1.305490	-0.665092
19	8	0	1.955216	-1.071457	-1.543571
20	8	0	3.539692	-2.372508	-0.598774
21	6	0	3.322758	-3.408789	-1.575889
22	6	0	2.344146	-4.430238	-1.027497
23	1	0	4.312786	-3.837578	-1.743767
24	1	0	2.961284	-2.952483	-2.499920
25	1	0	2.171941	-5.213930	-1.773498
26	1	0	2.737157	-4.890673	-0.117407
27	1	0	1.389324	-3.961071	-0.775721
28	26	0	-2.903311	1.011782	-2.177818
29	15	0	-0.265479	1.676701	-0.209530
30	15	0	-2.212856	-1.082811	0.421867
31	6	0	2.043933	3.195928	0.386470
32	6	0	-1.108433	3.009858	0.727843
33	6	0	-2.492861	3.637824	2.613453
34	6	0	1.378649	2.427769	-0.573985
35	6	0	-2.471614	4.964610	2.193525
36	6	0	-1.071241	4.350933	0.327687
37	6	0	-1.807737	2.665486	1.887593
38	6	0	-1.752660	5.321997	1.053491
39	6	0	2.042195	2.112944	-1.763951
40	6	0	3.343076	2.555628	-1.986208
41	6	0	-3.416141	-0.230689	-0.659820
42	6	0	-3.953697	-0.720042	-1.893178
43	6	0	-2.226863	-2.729858	-0.389993
44	6	0	-2.315556	2.259344	-3.707652
45	6	0	-3.970496	1.072973	-0.444904
46	6	0	-4.809604	0.276328	-2.435811
47	6	0	3.347806	3.631952	0.166211
48	6	0	-4.823256	1.381018	-1.538817
49	6	0	-1.225192	-2.998555	-1.327201
50	6	0	-1.050813	1.734906	-1.845795
51	6	0	-3.234998	-3.671011	-0.178771
52	6	0	-1.770614	0.958274	-3.900501
53	6	0	-1.868444	2.745070	-2.448903
54	6	0	-0.987879	0.634413	-2.761437
55	6	0	-3.220698	-1.264411	1.949039
56	6	0	-4.620722	-1.255259	1.910238
57	6	0	-3.248025	-4.860309	-0.903495
58	6	0	-1.248634	-4.179333	-2.061863
59	6	0	-2.260786	-5.112888	-1.852037

60	6	0	4.003589	3.309354	-1.018917
61	6	0	-3.319231	-1.510746	4.354249
62	6	0	-2.574896	-1.392171	3.183410
63	6	0	-4.710512	-1.501991	4.307210
64	6	0	-5.360785	-1.375899	3.082282
65	1	0	-0.470777	-0.295517	-2.567896
66	1	0	-1.965261	0.305609	-4.740622
67	1	0	-2.997586	2.769106	-4.374766
68	1	0	-2.163866	3.678474	-1.991515
69	1	0	-3.744865	1.727354	0.385760
70	1	0	-5.344442	2.317112	-1.687337
71	1	0	-5.321885	0.220080	-3.386622
72	1	0	-3.704067	-1.665535	-2.353875
73	1	0	-1.806183	1.628761	2.217580
74	1	0	-3.035970	3.355875	3.510489
75	1	0	-3.003530	5.723782	2.759684
76	1	0	-1.718243	6.359531	0.733831
77	1	0	-0.493438	4.637946	-0.547153
78	1	0	1.547974	1.506434	-2.514828
79	1	0	3.841022	2.310288	-2.920473
80	1	0	5.021870	3.646573	-1.189287
81	1	0	3.852273	4.222948	0.925313
82	1	0	1.546285	3.443421	1.319624
83	1	0	-4.009341	-3.482709	0.558868
84	1	0	-4.030724	-5.591650	-0.723745
85	1	0	-2.274138	-6.040446	-2.417331
86	1	0	-0.464742	-4.376860	-2.787578
87	1	0	-0.410364	-2.290768	-1.455726
88	1	0	-1.489756	-1.412874	3.218394
89	1	0	-2.806149	-1.611684	5.306024
90	1	0	-5.287228	-1.591556	5.223543
91	1	0	-6.446105	-1.366232	3.037143
92	1	0	-5.137097	-1.144453	0.961156
93	45	0	-0.088368	-0.341840	0.773598

Zero-point correction=	0.729207 (Hartree/Particle)
Thermal correction to Energy=	0.777850
Thermal correction to Enthalpy=	0.778795
Thermal correction to Gibbs Free Energy=	0.645381
Sum of electronic and zero-point Energies=	-3770.305873
Sum of electronic and thermal Energies=	-3770.257230
Sum of electronic and thermal Enthalpies=	-3770.256286
Sum of electronic and thermal Free Energies=	-3770.389699

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.3375587

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.549492	-3.037322	-1.476153
2	26	0	-3.279405	2.380958	-0.367452
3	15	0	-0.225736	1.247049	0.419840
4	15	0	-2.778889	-0.993162	-0.278301
5	6	0	2.410829	1.771093	1.279033
6	6	0	-0.555531	1.339276	2.217158
7	6	0	-1.305571	0.229230	4.235585
8	6	0	1.458121	1.963992	0.274391
9	6	0	-1.158936	1.415768	4.947066
10	6	0	-0.372938	2.518508	2.949731
11	6	0	-0.996279	0.190235	2.877871
12	6	0	-0.680385	2.557914	4.305000
13	6	0	1.837528	2.597252	-0.913281
14	6	0	3.144037	3.042495	-1.087755
15	6	0	-3.839350	0.464345	0.023764
16	6	0	-4.740807	1.049274	-0.923528
17	6	0	-3.601147	-1.645170	-1.776573
18	6	0	-2.658375	4.307276	-0.797237
19	6	0	-3.905713	1.257547	1.216960
20	6	0	-5.335924	2.192814	-0.327306
21	6	0	3.716671	2.219385	1.102501
22	6	0	-4.825756	2.316765	0.995189
23	6	0	-3.055004	-1.343561	-3.025921
24	6	0	-1.265105	2.520486	-0.344058
25	6	0	-4.810293	-2.338389	-1.701272
26	6	0	-2.591406	3.498898	-1.966792
27	6	0	-1.838691	3.715145	0.200732
28	6	0	-1.730385	2.404062	-1.696405
29	6	0	-3.260062	-2.097293	1.107465
30	6	0	-4.469455	-1.930237	1.792613
31	6	0	-5.469896	-2.719936	-2.865666
32	6	0	-3.722254	-1.714992	-4.188427
33	6	0	-4.930499	-2.403056	-4.109727
34	6	0	4.084754	2.857647	-0.077812
35	6	0	-2.712039	-3.939174	2.577414
36	6	0	-2.383709	-3.113734	1.505923
37	6	0	-3.913727	-3.763620	3.258231
38	6	0	-4.794390	-2.761078	2.860701
39	1	0	-1.506419	1.576997	-2.357571
40	1	0	-3.139834	3.661214	-2.884446
41	1	0	-3.270635	5.189539	-0.668506
42	1	0	-1.736573	4.066052	1.217077
43	1	0	-3.335115	1.093021	2.120012

44	1	0	-5.055601	3.107780	1.696012
45	1	0	-6.024447	2.871686	-0.811483
46	1	0	-4.898651	0.701513	-1.934813
47	1	0	-1.099486	-0.739265	2.326636
48	1	0	-1.657869	-0.671142	4.729324
49	1	0	-1.400163	1.449834	6.005368
50	1	0	-0.539403	3.478147	4.864072
51	1	0	0.034117	3.401229	2.464526
52	1	0	1.113391	2.737702	-1.710838
53	1	0	3.427509	3.524750	-2.017929
54	1	0	5.104749	3.201128	-0.214606
55	1	0	4.450735	2.060698	1.886687
56	1	0	2.139060	1.260716	2.197401
57	1	0	-5.236979	-2.589134	-0.734687
58	1	0	-6.404856	-3.268326	-2.799865
59	1	0	-5.446046	-2.702169	-5.017620
60	1	0	-3.287193	-1.483420	-5.155844
61	1	0	-2.091746	-0.845589	-3.083238
62	1	0	-1.452555	-3.263545	0.967285
63	1	0	-2.022624	-4.722519	2.877078
64	1	0	-4.165172	-4.407800	4.095853
65	1	0	-5.735558	-2.620461	3.384041
66	1	0	-5.159154	-1.144920	1.499101
67	45	0	-0.451684	-0.831219	-0.511620
68	6	0	4.050728	-1.272979	0.296566
69	6	0	3.812647	-0.657183	-0.969996
70	16	0	2.811214	-1.784901	1.277969
71	7	0	1.465407	-0.834246	-0.893076
72	7	0	2.506549	-0.586929	-1.305083
73	6	0	5.461192	-1.502437	0.722555
74	6	0	6.306629	-2.305648	-0.046760
75	6	0	5.931415	-0.955424	1.916671
76	6	0	7.608875	-2.550195	0.371443
77	1	0	5.936435	-2.743058	-0.969203
78	6	0	7.242287	-1.183840	2.322143
79	1	0	5.262883	-0.353422	2.524244
80	6	0	8.083402	-1.982312	1.552155
81	1	0	8.254878	-3.186512	-0.226099
82	1	0	7.603057	-0.745406	3.247850
83	1	0	9.103359	-2.169263	1.874831
84	6	0	4.694599	0.008709	-1.945853
85	8	0	4.310958	0.375764	-3.036471
86	8	0	5.938314	0.179343	-1.487854
87	6	0	6.895237	0.712457	-2.412319
88	6	0	6.892069	2.229816	-2.401507
89	1	0	6.676778	0.328906	-3.411786
90	1	0	7.851191	0.311481	-2.068628
91	1	0	7.657852	2.608016	-3.086796
92	1	0	5.919020	2.607641	-2.726515
93	1	0	7.110478	2.609003	-1.398560

Zero-point correction= 0.726682 (Hartree/Particle)
Thermal correction to Energy= 0.776420
Thermal correction to Enthalpy= 0.777364
Thermal correction to Gibbs Free Energy= 0.638850
Sum of electronic and zero-point Energies= -3770.262453
Sum of electronic and thermal Energies= -3770.212715
Sum of electronic and thermal Enthalpies= -3770.211771
Sum of electronic and thermal Free Energies= -3770.350284

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.2987584

TS1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.202766	1.351319	-0.063450
2	6	0	-1.135542	0.872848	0.187636
3	16	0	0.525483	2.947924	-0.371923
4	7	0	-2.197188	2.996511	0.118646
5	7	0	-2.017633	1.882815	0.225692
6	6	0	1.313177	0.363527	0.035607
7	6	0	1.464074	-0.396962	1.198602
8	6	0	2.238571	0.227701	-1.000312
9	6	0	2.524147	-1.285861	1.319709
10	1	0	0.755166	-0.281071	2.013184
11	6	0	3.285017	-0.680225	-0.885027
12	1	0	2.128713	0.830945	-1.895685
13	6	0	3.432047	-1.436441	0.274418
14	1	0	2.642091	-1.860598	2.233235
15	1	0	3.993759	-0.788505	-1.700244
16	1	0	4.255418	-2.138438	0.365538
17	6	0	-1.740356	-0.469688	0.305173
18	8	0	-2.871420	-0.637060	0.707361
19	8	0	-0.921469	-1.433745	-0.109307
20	6	0	-1.399572	-2.785404	0.005728
21	6	0	-2.262151	-3.167172	-1.182453
22	1	0	-1.948077	-2.888908	0.944999
23	1	0	-0.486340	-3.381733	0.049954
24	1	0	-2.534366	-4.225308	-1.113933
25	1	0	-3.180035	-2.574403	-1.195474
26	1	0	-1.720269	-3.009465	-2.119385

Zero-point correction= 0.196523 (Hartree/Particle)
Thermal correction to Energy= 0.210795
Thermal correction to Enthalpy= 0.211739
Thermal correction to Gibbs Free Energy= 0.153466
Sum of electronic and zero-point Energies= -1082.832715
Sum of electronic and thermal Energies= -1082.818443
Sum of electronic and thermal Enthalpies= -1082.817498
Sum of electronic and thermal Free Energies= -1082.875772

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent =-1083.2625193

B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.187028	1.351645	-0.154141
2	6	0	-1.121080	0.853119	0.220121
3	16	0	0.406529	2.895983	-0.700570
4	7	0	-2.868934	2.531829	0.596832
5	7	0	-2.071201	1.767255	0.414556
6	6	0	1.337556	0.432850	0.037981
7	6	0	1.463735	-0.297919	1.224940
8	6	0	2.337436	0.337886	-0.932794
9	6	0	2.572176	-1.106617	1.436779
10	1	0	0.700033	-0.214407	1.992901
11	6	0	3.433639	-0.491611	-0.729259
12	1	0	2.242370	0.912527	-1.848319
13	6	0	3.555606	-1.212257	0.455831
14	1	0	2.670252	-1.653275	2.369678
15	1	0	4.198105	-0.569309	-1.496096
16	1	0	4.418384	-1.851556	0.617471
17	6	0	-1.678776	-0.517459	0.298668
18	8	0	-2.786321	-0.745820	0.737051
19	8	0	-0.842345	-1.424998	-0.196731
20	6	0	-1.266699	-2.798858	-0.137849
21	6	0	-2.141126	-3.152777	-1.325734
22	1	0	-1.789474	-2.967757	0.806338
23	1	0	-0.331277	-3.361168	-0.142219
24	1	0	-2.374420	-4.222167	-1.304964
25	1	0	-3.079609	-2.593965	-1.291013
26	1	0	-1.625534	-2.929722	-2.264194

Zero-point correction= 0.197129 (Hartree/Particle)
Thermal correction to Energy= 0.212137
Thermal correction to Enthalpy= 0.213081
Thermal correction to Gibbs Free Energy= 0.153190
Sum of electronic and zero-point Energies= -1082.838309
Sum of electronic and thermal Energies= -1082.823302
Sum of electronic and thermal Enthalpies= -1082.822358
Sum of electronic and thermal Free Energies= -1082.882249

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1083.269368

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.315073	-3.158823	-0.943162
2	26	0	-3.482520	2.147055	-0.762662
3	15	0	-0.423915	1.352235	0.334938
4	15	0	-2.764984	-1.137553	-0.181563
5	6	0	2.177718	1.981290	1.177578
6	6	0	-0.846034	1.691722	2.082770
7	6	0	-1.659257	0.870793	4.210953
8	6	0	1.225778	2.136024	0.164371
9	6	0	-1.545021	2.147796	4.751425
10	6	0	-0.701993	2.966244	2.644084
11	6	0	-1.302765	0.642571	2.883967
12	6	0	-1.056677	3.193964	3.968946
13	6	0	1.590805	2.768605	-1.026617
14	6	0	2.885307	3.250499	-1.196091
15	6	0	-3.932633	0.267962	-0.146242
16	6	0	-4.805086	0.651228	-1.215415
17	6	0	-3.431581	-2.030984	-1.631579
18	6	0	-2.970675	4.040713	-1.402044
19	6	0	-4.131781	1.206214	0.919996
20	6	0	-5.514086	1.815862	-0.818348
21	6	0	3.472921	2.458047	1.001916
22	6	0	-5.103461	2.153568	0.501303
23	6	0	-2.800999	-1.867810	-2.866867
24	6	0	-1.491225	2.433955	-0.649494
25	6	0	-4.609163	-2.776602	-1.551943
26	6	0	-2.777563	3.099911	-2.452256
27	6	0	-2.177878	3.639652	-0.293481
28	6	0	-1.865079	2.113160	-1.996920
29	6	0	-3.277328	-2.087833	1.302772
30	6	0	-4.538537	-1.915153	1.885873
31	6	0	-5.154418	-3.345276	-2.698816
32	6	0	-3.354193	-2.427313	-4.013923
33	6	0	-4.531903	-3.165709	-3.931605
34	6	0	3.828492	3.095713	-0.183720
35	6	0	-2.733710	-3.704788	3.018454

36	6	0	-2.376598	-2.992374	1.877357
37	6	0	-3.987247	-3.524388	3.596403
38	6	0	-4.890655	-2.631517	3.025877
39	1	0	-1.544372	1.229713	-2.533505
40	1	0	-3.278933	3.104478	-3.410276
41	1	0	-3.649947	4.882229	-1.419950
42	1	0	-2.159087	4.120126	0.673950
43	1	0	-3.611883	1.209831	1.867470
44	1	0	-5.430738	3.013144	1.070244
45	1	0	-6.209598	2.372073	-1.431813
46	1	0	-4.871221	0.160666	-2.176372
47	1	0	-1.378321	-0.357396	2.467347
48	1	0	-2.018748	0.045406	4.817664
49	1	0	-1.817643	2.327366	5.787120
50	1	0	-0.941818	4.185550	4.396469
51	1	0	-0.288692	3.777134	2.050408
52	1	0	0.866026	2.882808	-1.827214
53	1	0	3.156857	3.742889	-2.124839
54	1	0	4.840365	3.463679	-0.321694
55	1	0	4.206773	2.313736	1.788775
56	1	0	1.920042	1.465573	2.097773
57	1	0	-5.100667	-2.920881	-0.594383
58	1	0	-6.066308	-3.930685	-2.628129
59	1	0	-4.958823	-3.610626	-4.825625
60	1	0	-2.853856	-2.301255	-4.969161
61	1	0	-1.858677	-1.330565	-2.920863
62	1	0	-1.403561	-3.145440	1.420429
63	1	0	-2.025335	-4.403187	3.453386
64	1	0	-4.260854	-4.078219	4.489882
65	1	0	-5.871081	-2.487251	3.470178
66	1	0	-5.247904	-1.214273	1.456893
67	45	0	-0.451634	-0.843563	-0.292530
68	6	0	4.641698	-1.021628	0.845585
69	6	0	3.977493	-0.681372	-0.386931
70	16	0	3.825106	-1.162775	2.281541
71	7	0	1.524575	-0.825381	-0.392061
72	7	0	2.645531	-0.759562	-0.389498
73	6	0	6.097814	-1.311690	0.776169
74	6	0	6.594915	-2.178434	-0.203414
75	6	0	6.974223	-0.775362	1.721850
76	6	0	7.945445	-2.501373	-0.235085
77	1	0	5.913887	-2.614143	-0.928912
78	6	0	8.329750	-1.080238	1.673594
79	1	0	6.583747	-0.115442	2.489905
80	6	0	8.818242	-1.945875	0.698275
81	1	0	8.316580	-3.190324	-0.987774
82	1	0	9.005375	-0.647593	2.405261
83	1	0	9.875828	-2.190919	0.667929
84	6	0	4.479787	-0.091394	-1.646112
85	8	0	3.783267	0.055266	-2.628618
86	8	0	5.758001	0.280867	-1.556768
87	6	0	6.374488	0.752958	-2.763457
88	6	0	6.129076	2.236117	-2.967983
89	1	0	5.992883	0.173612	-3.607669
90	1	0	7.435102	0.535867	-2.621897
91	1	0	6.662135	2.581032	-3.860112
92	1	0	5.061536	2.424645	-3.104851
93	1	0	6.488688	2.808487	-2.107581

Zero-point correction=	0.727496 (Hartree/Particle)
Thermal correction to Energy=	0.777219
Thermal correction to Enthalpy=	0.778163
Thermal correction to Gibbs Free Energy=	0.637497
Sum of electronic and zero-point Energies=	-3770.264882
Sum of electronic and thermal Energies=	-3770.215159
Sum of electronic and thermal Enthalpies=	-3770.214215
Sum of electronic and thermal Free Energies=	-3770.354881

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.3021099

TS2''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.951555	-1.137754	1.402335
2	6	0	3.332563	1.204915	-0.077586
3	6	0	3.278203	0.432301	-1.232006
4	16	0	1.934459	2.080764	0.378876
5	7	0	1.115206	1.103564	-1.594165
6	7	0	2.126023	0.589833	-1.951162
7	6	0	4.581595	1.419100	0.687938
8	6	0	4.611896	1.201849	2.067984
9	6	0	5.729508	1.876619	0.033879
10	6	0	5.787562	1.420999	2.777582
11	1	0	3.720840	0.827894	2.561481
12	6	0	6.896890	2.108762	0.750154
13	1	0	5.698360	2.055583	-1.036785
14	6	0	6.929385	1.877015	2.123607
15	1	0	5.810201	1.235419	3.847283
16	1	0	7.781996	2.471543	0.236126
17	1	0	7.843813	2.054188	2.682387
18	6	0	4.179741	-0.624575	-1.746732
19	8	0	3.973966	-1.206403	-2.790400

20	8	0	5.173832	-0.898010	-0.905251
21	6	0	5.930694	-2.088044	-1.171182
22	6	0	5.212747	-3.301589	-0.607083
23	1	0	6.886259	-1.915964	-0.672251
24	1	0	6.092165	-2.178776	-2.247890
25	1	0	5.828642	-4.196939	-0.744468
26	1	0	5.016172	-3.165439	0.459785
27	1	0	4.256057	-3.455052	-1.114240
28	26	0	-3.321987	-0.498158	-1.856086
29	15	0	-1.478960	1.703764	-0.091662
30	15	0	-0.983138	-1.680191	0.374640
31	6	0	-0.645214	4.250308	0.690142
32	6	0	-2.758388	1.910204	1.204520
33	6	0	-3.765244	1.163211	3.277756
34	6	0	-0.969729	3.435161	-0.400250
35	6	0	-4.735363	2.154562	3.169841
36	6	0	-3.719441	2.925390	1.120962
37	6	0	-2.777427	1.048299	2.302137
38	6	0	-4.705520	3.041739	2.094175
39	6	0	-0.804104	3.927421	-1.695839
40	6	0	-0.326310	5.220004	-1.896826
41	6	0	-2.569226	-1.830920	-0.519294
42	6	0	-2.774978	-2.474002	-1.780051
43	6	0	0.013982	-2.956829	-0.485116
44	6	0	-4.104625	0.925666	-3.126793
45	6	0	-3.841815	-1.338130	-0.079287
46	6	0	-4.151115	-2.364208	-2.117368
47	6	0	-0.169150	5.539788	0.486566
48	6	0	-4.810069	-1.670449	-1.064101
49	6	0	0.702571	-2.577957	-1.641383
50	6	0	-2.421836	1.287836	-1.584068
51	6	0	0.123022	-4.268717	-0.024869
52	6	0	-2.897387	0.397822	-3.664459
53	6	0	-3.816793	1.479517	-1.851086
54	6	0	-1.859547	0.621197	-2.723099
55	6	0	-1.464751	-2.414926	1.989555
56	6	0	-2.453259	-3.404307	2.064892
57	6	0	0.910972	-5.186897	-0.714679
58	6	0	1.488780	-3.493967	-2.330402
59	6	0	1.594500	-4.803210	-1.864599
60	6	0	-0.008307	6.026903	-0.808852
61	6	0	-1.257995	-2.482803	4.400382
62	6	0	-0.866511	-1.962558	3.169373
63	6	0	-2.241753	-3.465006	4.466349
64	6	0	-2.835351	-3.929401	3.294864
65	1	0	-0.829217	0.310924	-2.817617
66	1	0	-2.794861	-0.128033	-4.603734
67	1	0	-5.083755	0.863278	-3.581854
68	1	0	-4.541261	1.899176	-1.167988
69	1	0	-4.025914	-0.787694	0.833119
70	1	0	-5.855401	-1.393903	-1.039390
71	1	0	-4.606382	-2.710917	-3.035008
72	1	0	-2.001006	-2.923797	-2.386410
73	1	0	-2.015253	0.282470	2.397725
74	1	0	-3.766754	0.476410	4.118852
75	1	0	-5.506414	2.247284	3.928973
76	1	0	-5.448701	3.829855	2.018165
77	1	0	-3.686064	3.636646	0.300188
78	1	0	-1.044452	3.303182	-2.550653
79	1	0	-0.199887	5.594994	-2.908094
80	1	0	0.369028	7.032573	-0.968612
81	1	0	0.082446	6.162396	1.339794
82	1	0	-0.761413	3.872587	1.702900
83	1	0	-0.383058	-4.574579	0.884859
84	1	0	1.001332	-6.202366	-0.340109
85	1	0	2.218311	-5.518807	-2.392421
86	1	0	2.043228	-3.169627	-3.204980
87	1	0	0.646972	-1.552791	-1.991405
88	1	0	-0.081968	-1.214021	3.117223
89	1	0	-0.786131	-2.119561	5.308362
90	1	0	-2.544989	-3.870676	5.427227
91	1	0	-3.601475	-4.697794	3.337318
92	1	0	-2.931285	-3.765337	1.159020
93	45	0	0.248529	0.299261	0.440969

Zero-point correction= 0.726719 (Hartree/Particle)
Thermal correction to Energy= 0.776430
Thermal correction to Enthalpy= 0.777374
Thermal correction to Gibbs Free Energy= 0.640482
Sum of electronic and zero-point Energies= -3770.267003
Sum of electronic and thermal Energies= -3770.217293
Sum of electronic and thermal Enthalpies= -3770.216348
Sum of electronic and thermal Free Energies= -3770.353240

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.2954041

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.305253	-1.659786	1.930648
2	15	0	0.248823	-1.623077	-0.266064
3	15	0	-1.877330	1.028168	-0.094579

4	6	0	2.218741	-3.255260	-1.491150
5	6	0	-0.784584	-2.440986	-1.549972
6	6	0	-2.211314	-2.200335	-3.497391
7	6	0	1.731305	-2.722665	-0.293035
8	6	0	-2.480314	-3.564560	-3.476324
9	6	0	-1.020607	-3.821496	-1.570093
10	6	0	-1.358646	-1.647053	-2.544408
11	6	0	-1.870029	-4.377101	-2.519882
12	6	0	2.386362	-3.041112	0.900370
13	6	0	3.513729	-3.855301	0.893421
14	6	0	-2.983808	-0.149708	0.770763
15	6	0	-3.491837	-0.002802	2.103923
16	6	0	-2.127356	2.466100	1.017854
17	6	0	-1.532195	-3.185162	3.084235
18	6	0	-3.463829	-1.407265	0.276170
19	6	0	-4.245138	-1.161441	2.428425
20	6	0	3.351103	-4.063428	-1.498918
21	6	0	-4.230308	-2.026041	1.298972
22	6	0	-1.314538	2.548511	2.150700
23	6	0	-0.451221	-2.129579	1.332969
24	6	0	-3.133176	3.411322	0.828203
25	6	0	-1.055837	-1.929874	3.556606
26	6	0	-1.152614	-3.318695	1.721884
27	6	0	-0.377356	-1.286524	2.490310
28	6	0	-2.873028	1.382232	-1.601010
29	6	0	-4.258689	1.185525	-1.622924
30	6	0	-3.323987	4.425507	1.764904
31	6	0	-1.515598	3.549241	3.092640
32	6	0	-2.522451	4.493728	2.899954
33	6	0	4.004293	-4.362755	-0.306319
34	6	0	-2.960884	2.040080	-3.929617
35	6	0	-2.231492	1.819138	-2.765267
36	6	0	-4.338000	1.833311	-3.945367
37	6	0	-4.986388	1.411806	-2.787760
38	1	0	0.084822	-0.308830	2.511229
39	1	0	-1.219979	-1.515545	4.541824
40	1	0	-2.130148	-3.890630	3.645271
41	1	0	-1.426034	-4.140778	1.077677
42	1	0	-3.252231	-1.829756	-0.695623
43	1	0	-4.681998	-3.007012	1.239633
44	1	0	-4.711901	-1.364445	3.382585
45	1	0	-3.290713	0.826715	2.766216
46	1	0	-1.144552	-0.583709	-2.561037
47	1	0	-2.663497	-1.556110	-4.245452
48	1	0	-3.149838	-4.000730	-4.211882
49	1	0	-2.051918	-5.447878	-2.519711
50	1	0	-0.518560	-4.468686	-0.857297
51	1	0	2.015401	-2.651107	1.842888
52	1	0	4.012137	-4.089662	1.829570
53	1	0	4.888181	-4.993454	-0.311764
54	1	0	3.719912	-4.463950	-2.438350
55	1	0	1.702260	-3.055954	-2.425741
56	1	0	-3.762988	3.368995	-0.054872
57	1	0	-4.101937	5.165868	1.603041
58	1	0	-2.676304	5.283178	3.629807
59	1	0	-0.881033	3.599910	3.973474
60	1	0	-0.514037	1.827717	2.281177
61	1	0	-1.159729	1.992315	-2.750487
62	1	0	-2.448234	2.377299	-4.825499
63	1	0	-4.904204	2.002792	-4.856774
64	1	0	-6.060729	1.252233	-2.789917
65	1	0	-4.774341	0.846989	-0.729545
66	45	0	0.370520	0.649708	-0.528318
67	17	0	0.342835	3.068034	-0.868303
68	6	0	3.522955	0.144471	0.032603
69	6	0	2.622635	0.744964	-1.037684
70	16	0	4.821466	-0.749651	-0.414387
71	7	0	2.527120	-0.598446	-3.125703
72	7	0	2.586147	-0.032677	-2.168306
73	6	0	3.182611	0.423792	1.447797
74	6	0	3.695108	-0.413111	2.451531
75	6	0	2.350002	1.490834	1.826106
76	6	0	3.370913	-0.209839	3.785730
77	1	0	4.338405	-1.238162	2.166844
78	6	0	2.061347	1.713336	3.168489
79	1	0	1.948357	2.172035	1.085966
80	6	0	2.555470	0.859332	4.150389
81	1	0	3.760969	-0.883831	4.542278
82	1	0	1.444894	2.564850	3.440842
83	1	0	2.314103	1.029655	5.195677
84	6	0	3.024609	2.128869	-1.544729
85	8	0	2.982541	2.440358	-2.708676
86	8	0	3.499347	2.864176	-0.550432
87	6	0	3.762041	4.248488	-0.852506
88	6	0	5.149115	4.426399	-1.439812
89	1	0	3.660210	4.750175	0.111098
90	1	0	2.980781	4.604352	-1.526777
91	1	0	5.348989	5.492439	-1.590974
92	1	0	5.910674	4.023441	-0.765170
93	1	0	5.223270	3.920535	-2.405533

Zero-point correction= 0.727161 (Hartree/Particle)
Thermal correction to Energy= 0.777482

Thermal correction to Enthalpy= 0.778426
Thermal correction to Gibbs Free Energy= 0.641933
Sum of electronic and zero-point Energies= -3770.251861
Sum of electronic and thermal Energies= -3770.201540
Sum of electronic and thermal Enthalpies= -3770.200596
Sum of electronic and thermal Free Energies= -3770.337089

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.2743528

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.171959	-1.028797	-2.300840
2	15	0	-0.429976	-1.698210	-0.278383
3	15	0	1.853538	0.836990	0.553305
4	6	0	-2.689540	-2.959752	0.694218
5	6	0	0.599141	-2.847481	0.712138
6	6	0	1.992458	-3.219059	2.659938
7	6	0	-1.957380	-2.678504	-0.464775
8	6	0	2.268042	-4.509491	2.220493
9	6	0	0.834996	-4.166445	0.307485
10	6	0	1.150178	-2.399115	1.913030
11	6	0	1.673354	-4.988045	1.052169
12	6	0	-2.403156	-3.154546	-1.697956
13	6	0	-3.568010	-3.917038	-1.769393
14	6	0	2.897679	0.003632	-0.698242
15	6	0	3.376809	0.586038	-1.914784
16	6	0	2.128772	2.572760	0.041312
17	6	0	1.422095	-2.074304	-3.912144
18	6	0	3.355421	-1.354301	-0.670158
19	6	0	4.103841	-0.403476	-2.629354
20	6	0	-3.845966	-3.722991	0.618217
21	6	0	4.097528	-1.598186	-1.856554
22	6	0	1.250420	3.120096	-0.897152
23	6	0	0.287659	-1.662929	-1.940008
24	6	0	3.229800	3.316763	0.467429
25	6	0	0.958717	-0.728888	-3.946062
26	6	0	1.007650	-2.655452	-2.683971
27	6	0	0.254155	-0.473976	-2.742056
28	6	0	2.851505	0.601320	2.076343
29	6	0	4.221692	0.320857	2.031624
30	6	0	3.454749	4.590077	-0.048794
31	6	0	1.487232	4.384682	-1.424732
32	6	0	2.590317	5.121915	-1.001755
33	6	0	-4.286757	-4.204079	-0.614100
34	6	0	2.923652	0.436459	4.489915
35	6	0	2.208478	0.663719	3.317725
36	6	0	4.285480	0.148672	4.436945
37	6	0	4.934148	0.096551	3.206186
38	1	0	-0.190930	0.465255	-2.439928
39	1	0	1.154148	-0.007748	-4.727815
40	1	0	2.035620	-2.555253	-4.661975
41	1	0	1.258276	-3.650634	-2.347987
42	1	0	3.151493	-2.076146	0.108336
43	1	0	4.532612	-2.545846	-2.143671
44	1	0	4.548776	-0.278252	-3.607034
45	1	0	3.177543	1.595066	-2.247587
46	1	0	0.917041	-1.401010	2.266298
47	1	0	2.430080	-2.837804	3.577638
48	1	0	2.926894	-5.152744	2.796254
49	1	0	1.856638	-6.007920	0.727138
50	1	0	0.343808	-4.560780	-0.577267
51	1	0	-1.851015	-2.927704	-2.605002
52	1	0	-3.915021	-4.279947	-2.732378
53	1	0	-5.196650	-4.794206	-0.673218
54	1	0	-4.412178	-3.929131	1.521096
55	1	0	-2.373290	-2.550411	1.649479
56	1	0	3.912526	2.907837	1.205957
57	1	0	4.309068	5.165887	0.294753
58	1	0	2.771405	6.112550	-1.408683
59	1	0	0.799617	4.794233	-2.158094
60	1	0	0.371122	2.560991	-1.205411
61	1	0	1.147852	0.896516	3.360073
62	1	0	2.412245	0.486212	5.446479
63	1	0	4.839778	-0.032509	5.353382
64	1	0	5.996817	-0.122217	3.156607
65	1	0	4.735325	0.266794	1.076702
66	45	0	-0.561927	0.390844	0.677714
67	17	0	-0.603452	2.377600	2.124819
68	6	0	-3.107904	0.834924	-0.612158
69	6	0	-2.438124	0.568244	0.647806
70	16	0	-4.261767	-0.268319	-1.016461
71	6	0	-2.688750	1.968310	-1.461731
72	6	0	-2.702546	1.856544	-2.857117
73	6	0	-2.321173	3.179709	-0.863595
74	6	0	-2.336839	2.940698	-3.644555
75	1	0	-2.991560	0.913559	-3.310711
76	6	0	-1.992381	4.271804	-1.659221
77	1	0	-2.283803	3.261687	0.218301
78	6	0	-1.991098	4.152848	-3.046984
79	1	0	-2.331231	2.843921	-4.726089
80	1	0	-1.718226	5.210293	-1.187841

81	1	0	-1.720543	5.004221	-3.665573
82	6	0	-3.266092	0.563935	1.904591
83	8	0	-3.314751	-0.362910	2.677973
84	8	0	-3.918173	1.718006	2.033874
85	6	0	-4.673244	1.897932	3.245221
86	6	0	-6.051228	1.274698	3.115362
87	1	0	-4.726932	2.980269	3.371199
88	1	0	-4.112013	1.464375	4.076168
89	1	0	-6.635295	1.475779	4.019625
90	1	0	-6.583008	1.693769	2.256104
91	1	0	-5.968961	0.192431	2.987478

Zero-point correction= 0.716558 (Hartree/Particle)
Thermal correction to Energy= 0.765384
Thermal correction to Enthalpy= 0.766328
Thermal correction to Gibbs Free Energy= 0.630863
Sum of electronic and zero-point Energies= -3660.804048
Sum of electronic and thermal Energies= -3660.755222
Sum of electronic and thermal Enthalpies= -3660.754278
Sum of electronic and thermal Free Energies= -3660.889743

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent =-3663.7889445

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.197195	2.690656	1.747616
2	6	0	-3.277717	0.428386	0.716124
3	6	0	-3.188708	1.063123	-0.528001
4	16	0	-1.994651	-0.049690	1.694562
5	7	0	-0.842552	1.225370	-1.047970
6	7	0	-2.013518	1.306252	-1.177260
7	6	0	-4.623782	0.047524	1.234348
8	6	0	-5.049566	0.464386	2.496471
9	6	0	-5.453477	-0.769377	0.461076
10	6	0	-6.300850	0.082361	2.969692
11	1	0	-4.403791	1.099076	3.095144
12	6	0	-6.697101	-1.159247	0.942635
13	1	0	-5.112170	-1.103383	-0.513902
14	6	0	-7.126369	-0.730289	2.196826
15	1	0	-6.631229	0.422095	3.946809
16	1	0	-7.332068	-1.798975	0.336440
17	1	0	-8.100230	-1.030791	2.572387
18	6	0	-4.349619	1.528672	-1.338019
19	8	0	-4.390362	1.471230	-2.547809
20	8	0	-5.319909	2.045839	-0.576356
21	6	0	-6.538325	2.403539	-1.240071
22	6	0	-6.453210	3.800883	-1.827723
23	1	0	-7.298832	2.339355	-0.459027
24	1	0	-6.752412	1.662755	-2.015154
25	1	0	-7.418496	4.082741	-2.261620
26	1	0	-6.194564	4.528481	-1.052794
27	1	0	-5.694993	3.834022	-2.613774
28	26	0	2.919463	-1.016886	-2.211302
29	15	0	0.173843	-1.574901	-0.287093
30	15	0	2.346328	1.148476	0.379535
31	6	0	-2.117206	-3.135997	0.230108
32	6	0	1.010948	-2.822275	0.753696
33	6	0	2.408910	-3.302241	2.673975
34	6	0	-1.438458	-2.342923	-0.701463
35	6	0	2.405913	-4.653666	2.342934
36	6	0	0.992328	-4.187560	0.442535
37	6	0	1.707358	-2.393312	1.885941
38	6	0	1.689637	-5.096030	1.231198
39	6	0	-2.040341	-2.072406	-1.933691
40	6	0	-3.287031	-2.610767	-2.240988
41	6	0	3.488701	0.235571	-0.713707
42	6	0	4.009173	0.702782	-1.960667
43	6	0	2.627897	2.853857	-0.215904
44	6	0	2.307838	-2.320422	-3.689842
45	6	0	4.011342	-1.082992	-0.500575
46	6	0	4.832401	-0.316152	-2.511187
47	6	0	-3.359779	-3.676090	-0.080585
48	6	0	4.840382	-1.414333	-1.606266
49	6	0	1.731389	3.379972	-1.148672
50	6	0	1.034748	-1.651690	-1.881113
51	6	0	3.746618	3.598043	0.164020
52	6	0	1.821434	-1.011109	-3.957975
53	6	0	1.821996	-2.722604	-2.417486
54	6	0	1.036594	-0.594044	-2.851494
55	6	0	3.228104	1.003990	1.989485
56	6	0	4.610811	0.786316	2.049765
57	6	0	3.969978	4.853873	-0.391901
58	6	0	1.963954	4.631560	-1.710176
59	6	0	3.082758	5.369475	-1.333476
60	6	0	-3.943036	-3.421812	-1.319660
61	6	0	3.143294	0.904088	4.408720
62	6	0	2.501705	1.070327	3.184408
63	6	0	4.515821	0.679075	4.458058
64	6	0	5.249620	0.628367	3.275603
65	1	0	0.561045	0.368355	-2.724067
66	1	0	2.055384	-0.411347	-4.826818

67	1	0	2.979285	-2.891173	-4.316704
68	1	0	2.066362	-3.645853	-1.912045
69	1	0	3.791660	-1.722187	0.343637
70	1	0	5.341766	-2.360759	-1.756826
71	1	0	5.328606	-0.277379	-3.471195
72	1	0	3.776314	1.654582	-2.417878
73	1	0	1.708229	-1.341403	2.155993
74	1	0	2.949856	-2.946977	3.545617
75	1	0	2.950607	-5.365516	2.955943
76	1	0	1.669395	-6.152798	0.982144
77	1	0	0.418920	-4.541809	-0.409589
78	1	0	-1.539221	-1.444193	-2.663462
79	1	0	-3.742646	-2.391131	-3.201426
80	1	0	-4.914213	-3.844862	-1.559540
81	1	0	-3.877461	-4.288888	0.650700
82	1	0	-1.675685	-3.332382	1.201942
83	1	0	4.440953	3.206158	0.900989
84	1	0	4.837142	5.431298	-0.085203
85	1	0	3.258314	6.350101	-1.766057
86	1	0	1.259166	5.035339	-2.430731
87	1	0	0.842427	2.819175	-1.418962
88	1	0	1.435439	1.274338	3.157250
89	1	0	2.564112	0.956167	5.325645
90	1	0	5.013524	0.547433	5.414421
91	1	0	6.322178	0.460215	3.304874
92	1	0	5.193620	0.730069	1.135728
93	45	0	0.041645	0.532189	0.681421

Zero-point correction= 0.728537 (Hartree/Particle)
Thermal correction to Energy= 0.778352
Thermal correction to Enthalpy= 0.779296
Thermal correction to Gibbs Free Energy= 0.642613
Sum of electronic and zero-point Energies= -3770.284999
Sum of electronic and thermal Energies= -3770.235184
Sum of electronic and thermal Enthalpies= -3770.234239
Sum of electronic and thermal Free Energies= -3770.370923

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.3237456

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.765240	1.538286	2.038335
2	6	0	2.449157	1.943257	-0.914612
3	6	0	2.346669	0.581657	-1.276363
4	16	0	1.022444	2.866728	-1.022261
5	7	0	0.347230	0.307204	-2.282827
6	7	0	1.536410	0.262097	-2.501268
7	6	0	3.694944	2.516832	-0.361103
8	6	0	3.668087	3.293622	0.799916
9	6	0	4.909256	2.293930	-1.021502
10	6	0	4.851129	3.820925	1.304944
11	1	0	2.723720	3.435764	1.315079
12	6	0	6.085866	2.838740	-0.520672
13	1	0	4.928413	1.703307	-1.933901
14	6	0	6.058923	3.598769	0.646956
15	1	0	4.828931	4.406369	2.219193
16	1	0	7.022967	2.672517	-1.043544
17	1	0	6.978918	4.019467	1.042555
18	6	0	3.471764	-0.369417	-1.040996
19	8	0	3.996769	-1.047974	-1.891632
20	8	0	3.841089	-0.339931	0.247711
21	6	0	5.121094	-0.897014	0.576314
22	6	0	5.048209	-2.388202	0.841298
23	1	0	5.426116	-0.343028	1.466536
24	1	0	5.818078	-0.674444	-0.236676
25	1	0	6.022546	-2.748914	1.188784
26	1	0	4.302719	-2.606538	1.612693
27	1	0	4.780668	-2.919462	-0.074197
28	26	0	-3.216088	-1.710099	-1.015687
29	15	0	-1.963212	1.248325	-0.058099
30	15	0	0.050167	-1.683244	0.144079
31	6	0	-1.761796	3.986350	0.333470
32	6	0	-2.738931	1.121218	1.595421
33	6	0	-2.814700	0.218450	3.836401
34	6	0	-2.281186	2.989814	-0.502453
35	6	0	-4.032084	0.855002	4.059325
36	6	0	-3.949678	1.782110	1.834984
37	6	0	-2.167727	0.354033	2.611384
38	6	0	-4.596729	1.642782	3.058529
39	6	0	-3.005098	3.343289	-1.641149
40	6	0	-3.216902	4.688040	-1.939932
41	6	0	-1.583407	-2.483008	-0.067728
42	6	0	-1.983917	-3.349648	-1.136111
43	6	0	1.082373	-2.747224	-0.945531
44	6	0	-4.889566	-0.902402	-1.905932
45	6	0	-2.697298	-2.390365	0.833021
46	6	0	-3.319946	-3.766409	-0.901246
47	6	0	-1.981568	5.324544	0.032070
48	6	0	-3.757156	-3.180550	0.317430
49	6	0	0.905939	-2.697717	-2.334876
50	6	0	-3.084524	0.302518	-1.117765

51	6	0	2.024743	-3.632747	-0.418003
52	6	0	-3.837642	-1.012687	-2.858321
53	6	0	-4.435520	-0.088561	-0.835599
54	6	0	-2.726387	-0.269986	-2.383874
55	6	0	0.555985	-2.211007	1.818876
56	6	0	-0.043255	-3.295134	2.470490
57	6	0	2.780983	-4.442564	-1.261355
58	6	0	1.662552	-3.506338	-3.172907
59	6	0	2.607118	-4.378119	-2.638575
60	6	0	-2.709981	5.676975	-1.103539
61	6	0	2.122499	-2.002351	3.647549
62	6	0	1.646657	-1.568047	2.413349
63	6	0	1.514668	-3.071978	4.298287
64	6	0	0.431487	-3.718544	3.707543
65	1	0	-1.757324	-0.176701	-2.854594
66	1	0	-3.860437	-1.602853	-3.764387
67	1	0	-5.849287	-1.398344	-1.957454
68	1	0	-4.983344	0.134556	0.068798
69	1	0	-2.738363	-1.801894	1.736854
70	1	0	-4.742272	-3.270918	0.754362
71	1	0	-3.911703	-4.386715	-1.560302
72	1	0	-1.382645	-3.623425	-1.989684
73	1	0	-1.198484	-0.107149	2.463583
74	1	0	-2.352349	-0.374614	4.619409
75	1	0	-4.532853	0.752272	5.017578
76	1	0	-5.536956	2.157453	3.232314
77	1	0	-4.384603	2.414339	1.065637
78	1	0	-3.405490	2.574666	-2.295398
79	1	0	-3.779087	4.959003	-2.828630
80	1	0	-2.877470	6.724335	-1.336797
81	1	0	-1.577648	6.094108	0.682586
82	1	0	-1.177154	3.707802	1.207705
83	1	0	2.175653	-3.698195	0.653498
84	1	0	3.511887	-5.122795	-0.833972
85	1	0	3.206506	-5.002273	-3.294231
86	1	0	1.521031	-3.442236	-4.247119
87	1	0	0.178890	-2.021222	-2.769505
88	1	0	2.119078	-0.727161	1.919541
89	1	0	2.963901	-1.489417	4.103135
90	1	0	1.884920	-3.403518	5.264189
91	1	0	-0.042262	-4.559199	4.205690
92	1	0	-0.874322	-3.819158	2.010831
93	45	0	0.290576	0.685181	-0.306489

Zero-point correction= 0.729159 (Hartree/Particle)
Thermal correction to Energy= 0.778266
Thermal correction to Enthalpy= 0.779210
Thermal correction to Gibbs Free Energy= 0.646485
Sum of electronic and zero-point Energies= -3770.269203
Sum of electronic and thermal Energies= -3770.220096
Sum of electronic and thermal Enthalpies= -3770.219152
Sum of electronic and thermal Free Energies= -3770.351877

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.3040982

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.055984	-1.206900	2.420418
2	15	0	0.483746	-1.655275	0.151257
3	15	0	-2.055700	0.920447	-0.270111
4	6	0	2.906326	-2.900007	-0.557338
5	6	0	-0.321484	-3.071102	-0.681189
6	6	0	-1.959072	-3.872651	-2.278815
7	6	0	2.201323	-2.224113	0.444007
8	6	0	-1.670290	-5.186441	-1.921956
9	6	0	-0.026750	-4.396025	-0.339700
10	6	0	-1.282623	-2.823011	-1.663770
11	6	0	-0.699886	-5.446090	-0.955458
12	6	0	2.843518	-1.935573	1.651471
13	6	0	4.168417	-2.311408	1.851718
14	6	0	-2.932412	-0.016544	1.028066
15	6	0	-3.314406	0.411172	2.336751
16	6	0	-2.406072	2.660948	0.158599
17	6	0	-1.136290	-2.408206	3.817876
18	6	0	-3.366219	-1.376776	0.880707
19	6	0	-3.961181	-0.674205	2.988875
20	6	0	4.230920	-3.272300	-0.354457
21	6	0	-3.999783	-1.774428	2.087625
22	6	0	-1.813195	3.204609	1.302551
23	6	0	-0.194264	-1.706433	1.830463
24	6	0	-3.224187	3.461911	-0.639750
25	6	0	-0.721662	-1.055891	3.979402
26	6	0	-0.805320	-2.817376	2.498925
27	6	0	-0.139205	-0.617807	2.761153
28	6	0	-3.173965	0.542936	-1.688511
29	6	0	-4.554345	0.414344	-1.480904
30	6	0	-3.462982	4.786865	-0.286206
31	6	0	-2.063299	4.526642	1.655781
32	6	0	-2.889316	5.320270	0.863471
33	6	0	4.866277	-2.974362	0.847146
34	6	0	-3.512392	-0.017990	-4.022771

35	6	0	-2.664932	0.337671	-2.974899
36	6	0	-4.878349	-0.153287	-3.802824
37	6	0	-5.399639	0.073938	-2.530060
38	1	0	0.227180	0.375594	2.530681
39	1	0	-0.879261	-0.444920	4.857771
40	1	0	-1.665907	-3.004418	4.548667
41	1	0	-1.037138	-3.774808	2.054049
42	1	0	-3.212874	-1.999144	0.009952
43	1	0	-4.393869	-2.759102	2.298580
44	1	0	-4.321602	-0.672261	4.008569
45	1	0	-3.110806	1.381173	2.767548
46	1	0	-1.516347	-1.803123	-1.955361
47	1	0	-2.705068	-3.656411	-3.037448
48	1	0	-2.191942	-6.009131	-2.401808
49	1	0	-0.463342	-6.470647	-0.684473
50	1	0	0.738682	-4.605290	0.402236
51	1	0	2.313048	-1.414958	2.442100
52	1	0	4.655636	-2.078613	2.793883
53	1	0	5.904168	-3.254765	0.999050
54	1	0	4.768679	-3.787573	-1.144286
55	1	0	2.424288	-3.129253	-1.501015
56	1	0	-3.665607	3.061679	-1.545810
57	1	0	-4.094243	5.404177	-0.918211
58	1	0	-3.075059	6.355428	1.134491
59	1	0	-1.597279	4.939831	2.545646
60	1	0	-1.125282	2.610702	1.893399
61	1	0	-1.608919	0.490539	-3.175905
62	1	0	-3.096519	-0.175995	-5.013093
63	1	0	-5.539069	-0.427642	-4.620019
64	1	0	-6.466769	-0.019596	-2.352339
65	1	0	-4.971343	0.577681	-0.491793
66	45	0	0.188524	0.318361	-1.060701
67	17	0	-0.018846	2.356024	-2.295004
68	6	0	2.864772	0.664408	-0.985914
69	6	0	1.857325	1.037911	-0.178928
70	16	0	2.121859	-0.224387	-2.306814
71	6	0	4.322492	0.835943	-0.874469
72	6	0	4.957743	0.763804	0.369059
73	6	0	5.094107	1.026222	-2.024278
74	6	0	6.337989	0.888333	0.461642
75	1	0	4.363719	0.588525	1.259242
76	6	0	6.475281	1.159117	-1.929054
77	1	0	4.601812	1.083091	-2.990809
78	6	0	7.101108	1.089128	-0.687067
79	1	0	6.821030	0.821259	1.432300
80	1	0	7.062882	1.317981	-2.828470
81	1	0	8.180293	1.188501	-0.613432
82	6	0	1.810112	2.019138	0.896996
83	8	0	0.959409	2.080134	1.772849
84	8	0	2.824695	2.891149	0.827481
85	6	0	2.852626	3.928663	1.814867
86	6	0	1.960126	5.087379	1.405193
87	1	0	3.902177	4.227090	1.862300
88	1	0	2.548699	3.516520	2.780567
89	1	0	2.028579	5.890601	2.147099
90	1	0	2.266469	5.481698	0.432283
91	1	0	0.918385	4.762697	1.334657

Zero-point correction=	0.718163 (Hartree/Particle)
Thermal correction to Energy=	0.766395
Thermal correction to Enthalpy=	0.767339
Thermal correction to Gibbs Free Energy=	0.633651
Sum of electronic and zero-point Energies=	-3660.843149
Sum of electronic and thermal Energies=	-3660.794917
Sum of electronic and thermal Enthalpies=	-3660.793972
Sum of electronic and thermal Free Energies=	-3660.927661

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3663.839878

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.104735	-1.650224	2.041839
2	15	0	0.375496	-1.610380	-0.268183
3	15	0	-1.938670	0.954515	-0.118162
4	6	0	2.328695	-3.216726	-1.536589
5	6	0	-0.710990	-2.483328	-1.469065
6	6	0	-2.254418	-2.326781	-3.335274
7	6	0	1.858398	-2.705248	-0.322668
8	6	0	-2.510328	-3.690719	-3.244634
9	6	0	-0.934391	-3.865072	-1.422961
10	6	0	-1.349174	-1.733009	-2.458258
11	6	0	-1.834373	-4.461983	-2.298010
12	6	0	2.528334	-3.047017	0.855538
13	6	0	3.657174	-3.859668	0.818062
14	6	0	-2.937157	-0.235990	0.853412
15	6	0	-3.378131	-0.055877	2.205216
16	6	0	-2.213550	2.431751	0.933137
17	6	0	-1.195585	-3.066206	3.232653
18	6	0	-3.362324	-1.542879	0.443295
19	6	0	-4.040293	-1.240231	2.623543
20	6	0	3.460429	-4.024128	-1.574876

21	6	0	-4.034712	-2.154959	1.534185
22	6	0	-1.333845	2.635478	1.998768
23	6	0	-0.250365	-2.052748	1.381008
24	6	0	-3.301157	3.287967	0.771522
25	6	0	-0.768674	-1.763667	3.616770
26	6	0	-0.869333	-3.253659	1.862905
27	6	0	-0.175608	-1.144576	2.487357
28	6	0	-3.012332	1.188203	-1.592673
29	6	0	-4.380545	0.896563	-1.557387
30	6	0	-3.506924	4.333504	1.669604
31	6	0	-1.548652	3.667553	2.903216
32	6	0	-2.637107	4.522193	2.738937
33	6	0	4.131401	-4.343884	-0.397152
34	6	0	-3.224980	1.757493	-3.936246
35	6	0	-2.442288	1.628331	-2.792684
36	6	0	-4.584192	1.456373	-3.894955
37	6	0	-5.161780	1.031676	-2.701571
38	1	0	0.230479	-0.143748	2.436400
39	1	0	-0.912985	-1.305146	4.585346
40	1	0	-1.729929	-3.770622	3.855886
41	1	0	-1.120637	-4.125473	1.277853
42	1	0	-3.177672	-1.997827	-0.519500
43	1	0	-4.429248	-3.162096	1.545232
44	1	0	-4.441326	-1.425094	3.610680
45	1	0	-3.190238	0.815979	2.815182
46	1	0	-1.141659	-0.670916	-2.533452
47	1	0	-2.758129	-1.714141	-4.076972
48	1	0	-3.219627	-4.159593	-3.920332
49	1	0	-2.006533	-5.533059	-2.245584
50	1	0	-0.384993	-4.481053	-0.717777
51	1	0	2.166231	-2.677863	1.809823
52	1	0	4.167334	-4.112374	1.743044
53	1	0	5.014778	-4.974681	-0.426453
54	1	0	3.814446	-4.410055	-2.526141
55	1	0	1.796836	-3.002874	-2.459277
56	1	0	-3.986853	3.148741	-0.058558
57	1	0	-4.350126	5.003465	1.529350
58	1	0	-2.802441	5.335403	3.439610
59	1	0	-0.860340	3.814495	3.731131
60	1	0	-0.471567	1.985841	2.107482
61	1	0	-1.385400	1.876371	-2.822315
62	1	0	-2.768085	2.098657	-4.860377
63	1	0	-5.192010	1.555303	-4.789814
64	1	0	-6.222286	0.801260	-2.658555
65	1	0	-4.840236	0.554279	-0.635423
66	45	0	0.387377	0.663613	-0.626404
67	17	0	0.194563	3.059308	-1.082779
68	6	0	3.381630	0.309770	0.041737
69	6	0	2.402511	0.875227	-0.952158
70	16	0	4.699056	-0.551571	-0.418114
71	7	0	2.557789	-0.592854	-3.362435
72	7	0	2.735010	-0.070899	-2.407181
73	6	0	3.071346	0.583176	1.473518
74	6	0	3.579850	-0.279504	2.454747
75	6	0	2.274016	1.666715	1.881304
76	6	0	3.283507	-0.087247	3.798447
77	1	0	4.201492	-1.113135	2.148396
78	6	0	2.012884	1.875458	3.230582
79	1	0	1.871240	2.361178	1.154029
80	6	0	2.501712	0.994714	4.192641
81	1	0	3.670521	-0.781583	4.537921
82	1	0	1.418480	2.734744	3.526845
83	1	0	2.280475	1.155169	5.243805
84	6	0	2.899478	2.198001	-1.554042
85	8	0	2.975125	2.428569	-2.734648
86	8	0	3.292060	3.006347	-0.576770
87	6	0	3.552390	4.375842	-0.940354
88	6	0	4.971702	4.548761	-1.446867
89	1	0	3.380898	4.928779	-0.015374
90	1	0	2.810169	4.679087	-1.681322
91	1	0	5.168565	5.610709	-1.628351
92	1	0	5.693533	4.184315	-0.709537
93	1	0	5.112567	4.004738	-2.383728

Zero-point correction= 0.725450 (Hartree/Particle)
Thermal correction to Energy= 0.775621
Thermal correction to Enthalpy= 0.776565
Thermal correction to Gibbs Free Energy= 0.640496
Sum of electronic and zero-point Energies= -3770.239771
Sum of electronic and thermal Energies= -3770.189600
Sum of electronic and thermal Enthalpies= -3770.188656
Sum of electronic and thermal Free Energies= -3770.324725

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.2614324

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.793565	1.126011	2.175533
2	6	0	2.771038	1.812713	-0.522361
3	6	0	2.455317	0.472957	-0.684888
4	16	0	1.355551	2.771516	-0.517462

5	7	0	0.535984	0.396273	-2.253438
6	7	0	1.675986	0.289603	-2.411033
7	6	0	4.121266	2.363996	-0.308338
8	6	0	4.334399	3.382616	0.625294
9	6	0	5.204855	1.861635	-1.039334
10	6	0	5.615113	3.881667	0.832526
11	1	0	3.493219	3.756821	1.200615
12	6	0	6.482229	2.370170	-0.834667
13	1	0	5.040780	1.082987	-1.779347
14	6	0	6.690670	3.378914	0.103366
15	1	0	5.774804	4.663561	1.568986
16	1	0	7.315326	1.981415	-1.412790
17	1	0	7.689599	3.773490	0.264966
18	6	0	3.444670	-0.622207	-0.571632
19	8	0	3.740291	-1.403654	-1.448362
20	8	0	4.009835	-0.624830	0.650486
21	6	0	5.156652	-1.468383	0.825231
22	6	0	4.783098	-2.917402	1.081323
23	1	0	5.675601	-1.031761	1.680884
24	1	0	5.792744	-1.381296	-0.060537
25	1	0	5.685320	-3.493307	1.315158
26	1	0	4.092360	-2.998954	1.926164
27	1	0	4.312175	-3.346824	0.194841
28	26	0	-3.359939	-1.358391	-1.195247
29	15	0	-1.891846	1.411302	-0.013842
30	15	0	-0.149998	-1.742990	0.077518
31	6	0	-1.437680	4.096736	0.515676
32	6	0	-2.795448	1.321867	1.577881
33	6	0	-3.105380	0.372233	3.780324
34	6	0	-1.994111	3.194727	-0.399810
35	6	0	-4.260388	1.128907	3.952542
36	6	0	-3.944106	2.099855	1.768386
37	6	0	-2.372365	0.470633	2.600243
38	6	0	-4.676736	1.998244	2.946133
39	6	0	-2.570480	3.672106	-1.577370
40	6	0	-2.597456	5.041142	-1.835183
41	6	0	-1.852684	-2.346990	-0.224644
42	6	0	-2.311321	-3.128273	-1.334883
43	6	0	0.798115	-2.825545	-1.065387
44	6	0	-4.897773	-0.351890	-2.138771
45	6	0	-2.979919	-2.157151	0.643398
46	6	0	-3.693183	-3.398239	-1.156650
47	6	0	-1.471298	5.461409	0.255001
48	6	0	-4.103940	-2.804929	0.068074
49	6	0	0.651601	-2.664108	-2.448415
50	6	0	-3.044226	0.644325	-1.184574
51	6	0	1.655227	-3.819755	-0.590174
52	6	0	-3.803343	-0.515947	-3.033608
53	6	0	-4.439135	0.368567	-1.004482
54	6	0	-2.662439	0.098399	-2.455683
55	6	0	0.242480	-2.445369	1.720044
56	6	0	-0.520368	-3.466826	2.297298
57	6	0	2.356607	-4.629001	-1.479946
58	6	0	1.348844	-3.475470	-3.334035
59	6	0	2.209067	-4.457871	-2.850986
60	6	0	-2.051316	5.935649	-0.920288
61	6	0	1.775343	-2.567273	3.586225
62	6	0	1.400023	-2.004394	2.370080
63	6	0	1.002700	-3.569571	4.165141
64	6	0	-0.143976	-4.020854	3.516852
65	1	0	-1.666872	0.125190	-2.874039
66	1	0	-3.823019	-1.057300	-3.969641
67	1	0	-5.893297	-0.753495	-2.270688
68	1	0	-5.018991	0.599666	-0.122175
69	1	0	-2.986206	-1.598223	1.566386
70	1	0	-5.107601	-2.796517	0.470633
71	1	0	-4.326817	-3.926787	-1.855618
72	1	0	-1.715618	-3.441109	-2.179005
73	1	0	-1.449563	-0.088575	2.492874
74	1	0	-2.758761	-0.288236	4.569246
75	1	0	-4.827884	1.054907	4.875651
76	1	0	-5.567025	2.605165	3.081469
77	1	0	-4.262601	2.793611	0.995018
78	1	0	-3.003259	2.979841	-2.293475
79	1	0	-3.048210	5.406345	-2.753215
80	1	0	-2.073203	7.002240	-1.123514
81	1	0	-1.036782	6.154942	0.968305
82	1	0	-0.972741	3.726216	1.426458
83	1	0	1.785179	-3.967194	0.476197
84	1	0	3.024303	-5.393308	-1.093290
85	1	0	2.763236	-5.085097	-3.542634
86	1	0	1.227905	-3.330950	-4.403196
87	1	0	-0.012922	-1.901813	-2.841205
88	1	0	2.008960	-1.220549	1.935444
89	1	0	2.669585	-2.205919	4.084913
90	1	0	1.293855	-4.000250	5.118827
91	1	0	-0.746507	-4.810111	3.956507
92	1	0	-1.405050	-3.842068	1.794566
93	45	0	0.372408	0.618998	-0.185520

Zero-point correction= 0.726286 (Hartree/Particle)
Thermal correction to Energy= 0.775589
Thermal correction to Enthalpy= 0.776534

Thermal correction to Gibbs Free Energy= 0.642956
Sum of electronic and zero-point Energies= -3770.263519
Sum of electronic and thermal Energies= -3770.214216
Sum of electronic and thermal Enthalpies= -3770.213272
Sum of electronic and thermal Free Energies= -3770.346850

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.2947832

INT8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.520181	0.221793	-3.073707
2	16	0	-1.717038	1.386262	-1.858015
3	6	0	-3.856619	1.146384	-0.018619
4	6	0	-4.351381	2.396670	-0.409514
5	6	0	-4.691862	0.302376	0.718906
6	6	0	-5.632979	2.800133	-0.049810
7	1	0	-3.723535	3.056087	-1.002830
8	6	0	-5.972295	0.703336	1.078514
9	1	0	-4.352180	-0.692346	0.978627
10	6	0	-6.447864	1.956870	0.701164
11	1	0	-5.997447	3.774830	-0.361900
12	1	0	-6.606102	0.025769	1.644151
13	1	0	-7.450554	2.269116	0.978829
14	6	0	-1.837825	-0.892284	1.395339
15	8	0	-1.737707	-2.107060	1.454504
16	8	0	-2.148912	-0.138211	2.464606
17	6	0	-2.428037	-0.827236	3.688644
18	6	0	-3.861372	-1.326653	3.739196
19	1	0	-2.243126	-0.077767	4.461870
20	1	0	-1.717516	-1.649071	3.805945
21	1	0	-4.064804	-1.768790	4.720380
22	1	0	-4.563394	-0.504518	3.571959
23	1	0	-4.024672	-2.094120	2.977021
24	26	0	4.165524	0.227830	0.144749
25	15	0	1.442795	-1.732511	-0.033946
26	15	0	0.967450	1.811986	-0.087122
27	6	0	1.909777	-3.881616	-1.775943
28	6	0	1.348900	-1.939169	1.786162
29	6	0	0.977784	-0.920819	3.953371
30	6	0	1.185610	-3.436276	-0.666103
31	6	0	1.412110	-2.082348	4.583986
32	6	0	1.780517	-3.105548	2.426838
33	6	0	0.942642	-0.859439	2.564128
34	6	0	1.806712	-3.176719	3.816142
35	6	0	0.218453	-4.275016	-0.098007
36	6	0	-0.004682	-5.542811	-0.626986
37	6	0	2.739154	1.694730	0.385019
38	6	0	3.759525	2.123608	-0.525997
39	6	0	1.064623	3.351178	-1.101759
40	6	0	5.486561	-1.344797	0.303377
41	6	0	3.398342	1.369422	1.622158
42	6	0	5.008184	2.101615	0.146174
43	6	0	1.676502	-5.147242	-2.305656
44	6	0	4.786236	1.643623	1.474164
45	6	0	1.459151	4.516165	-0.429999
46	6	0	3.241270	-1.524201	-0.216572
47	6	0	0.818204	3.403371	-2.471554
48	6	0	5.320796	-0.988114	-1.063464
49	6	0	4.214199	-1.688824	0.827503
50	6	0	3.947304	-1.101705	-1.391833
51	6	0	0.062308	2.480845	1.378391
52	6	0	0.504333	2.425405	2.701783
53	6	0	0.959597	4.607771	-3.158586
54	6	0	1.596244	5.714535	-1.117877
55	6	0	1.344444	5.762684	-2.487722
56	6	0	0.722302	-5.981463	-1.730715
57	6	0	-1.979893	3.536206	2.157018
58	6	0	-1.178950	3.076622	1.121115
59	6	0	-1.545111	3.438987	3.475811
60	6	0	-0.292750	2.899223	3.741768
61	1	0	3.484204	-0.828452	-2.328356
62	1	0	6.096092	-0.631637	-1.727931
63	1	0	6.410444	-1.310025	0.864948
64	1	0	4.009675	-1.956465	1.853508
65	1	0	2.955745	0.921516	2.498296
66	1	0	5.544156	1.466403	2.224986
67	1	0	5.966166	2.336540	-0.296653
68	1	0	3.591517	2.389355	-1.560413
69	1	0	0.560496	0.032705	2.086076
70	1	0	0.643709	-0.063890	4.531863
71	1	0	1.436523	-2.141478	5.668168
72	1	0	2.141768	-4.089106	4.300265
73	1	0	2.106209	-3.959539	1.840983
74	1	0	-0.370201	-3.926081	0.746061
75	1	0	-0.755235	-6.186134	-0.177353
76	1	0	0.542868	-6.969185	-2.144678
77	1	0	2.243891	-5.479715	-3.169540
78	1	0	2.656407	-3.240674	-2.233876
79	1	0	0.543880	2.504155	-3.007536
80	1	0	0.766901	4.633858	-4.226741
81	1	0	1.450810	6.699320	-3.027400

82	1	0	1.898310	6.610298	-0.583549
83	1	0	1.658249	4.489637	0.637486
84	1	0	-1.521874	3.176707	0.097753
85	1	0	-2.951251	3.962536	1.926841
86	1	0	-2.172472	3.796216	4.287083
87	1	0	0.079301	2.848974	4.761358
88	1	0	1.478099	2.028435	2.945306
89	45	0	0.001179	-0.080353	-1.079945
90	6	0	-2.484458	0.751884	-0.389294
91	6	0	-1.606914	-0.078399	0.197628
92	6	0	-0.877592	-1.716054	-2.739699
93	6	0	-1.778198	-2.182632	-1.837802
94	1	0	-1.158557	-1.070513	-3.564390
95	1	0	0.110482	-2.155293	-2.795934
96	1	0	-1.427019	-2.878350	-1.084418
97	6	0	-3.227563	-1.969625	-1.829314
98	6	0	-3.886631	-1.122119	-2.729687
99	6	0	-3.991029	-2.707405	-0.913510
100	6	0	-5.270375	-1.001237	-2.694178
101	1	0	-3.314487	-0.541582	-3.443840
102	6	0	-5.376362	-2.605034	-0.897517
103	1	0	-3.481811	-3.351526	-0.202168
104	6	0	-6.018652	-1.743713	-1.783866
105	1	0	-5.767254	-0.323827	-3.381680
106	1	0	-5.954648	-3.186069	-0.184870
107	1	0	-7.099954	-1.645514	-1.761594

Zero-point correction=	0.858265 (Hartree/Particle)
Thermal correction to Energy=	0.913404
Thermal correction to Enthalpy=	0.914348
Thermal correction to Gibbs Free Energy=	0.769212
Sum of electronic and zero-point Energies=	-3970.267839
Sum of electronic and thermal Energies=	-3970.212700
Sum of electronic and thermal Enthalpies=	-3970.211756
Sum of electronic and thermal Free Energies=	-3970.356892

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4841831

TS5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.148192	0.106214	-3.209204
2	6	0	2.548508	-0.451806	-0.140634
3	6	0	1.541278	0.261880	0.396739
4	16	0	2.009797	-1.025215	-1.727525
5	6	0	3.890723	-0.774562	0.380766
6	6	0	4.520822	-1.965671	0.002186
7	6	0	4.558877	0.073953	1.270774
8	6	0	5.765326	-2.311530	0.518962
9	1	0	4.026365	-2.628567	-0.702924
10	6	0	5.799668	-0.271722	1.791064
11	1	0	4.115682	1.027156	1.537493
12	6	0	6.408062	-1.469136	1.421985
13	1	0	6.234037	-3.242379	0.212716
14	1	0	6.298370	0.404650	2.479902
15	1	0	7.379399	-1.737384	1.826990
16	6	0	1.615625	0.963293	1.690939
17	8	0	1.611014	2.174804	1.825157
18	8	0	1.692741	0.109385	2.720424
19	6	0	1.804614	0.667576	4.035901
20	6	0	3.244387	1.009277	4.374181
21	1	0	1.421340	-0.119477	4.689306
22	1	0	1.157506	1.544804	4.109160
23	1	0	3.318158	1.301175	5.427253
24	1	0	3.894747	0.146850	4.201425
25	1	0	3.594867	1.844716	3.761852
26	26	0	-4.174390	-0.474380	-0.127818
27	15	0	-1.549255	1.683226	-0.027017
28	15	0	-0.917280	-1.839092	-0.150373
29	6	0	-2.146999	3.942787	-1.596897
30	6	0	-1.621060	1.831957	1.800423
31	6	0	-1.523231	0.722829	3.952151
32	6	0	-1.358389	3.419845	-0.570867
33	6	0	-2.001565	1.870740	4.575767
34	6	0	-2.095184	2.985366	2.434360
35	6	0	-1.328213	0.712906	2.574861
36	6	0	-2.278497	3.004319	3.813526
37	6	0	-0.348492	4.208767	-0.005000
38	6	0	-0.148185	5.509446	-0.453087
39	6	0	-2.720823	-1.900460	0.189584
40	6	0	-3.640172	-2.333163	-0.819793
41	6	0	-0.781894	-3.300941	-1.263738
42	6	0	-5.569815	1.036740	-0.043169
43	6	0	-3.494863	-1.647511	1.374998
44	6	0	-4.943838	-2.373134	-0.261210
45	6	0	-1.936399	5.244350	-2.046538
46	6	0	-4.854316	-1.958350	1.095676
47	6	0	-1.010725	-4.573095	-0.722238
48	6	0	-3.301743	1.335479	-0.367059
49	6	0	-0.516962	-3.174623	-2.626313
50	6	0	-5.272139	0.720120	-1.397819
51	6	0	-4.364306	1.426709	0.593864

52	6	0	-3.881692	0.903462	-1.606384
53	6	0	-0.073943	-2.519946	1.346147
54	6	0	-0.612589	-2.576747	2.633130
55	6	0	-0.479052	-4.308827	-3.436668
56	6	0	-0.969619	-5.700140	-1.532822
57	6	0	-0.701179	-5.569279	-2.894738
58	6	0	-0.941148	6.029854	-1.474318
59	6	0	2.021020	-3.362019	2.240366
60	6	0	1.244602	-2.958074	1.163072
61	6	0	1.485516	-3.370574	3.525395
62	6	0	0.160380	-2.997245	3.714037
63	1	0	-3.326305	0.687991	-2.507901
64	1	0	-5.972967	0.346110	-2.131873
65	1	0	-6.534644	0.944065	0.436934
66	1	0	-4.255233	1.683678	1.637575
67	1	0	-3.147079	-1.221796	2.303159
68	1	0	-5.679439	-1.835712	1.784059
69	1	0	-5.851033	-2.625218	-0.792915
70	1	0	-3.375576	-2.561307	-1.842993
71	1	0	-0.917036	-0.171322	2.107376
72	1	0	-1.279839	-0.164437	4.530405
73	1	0	-2.151679	1.888018	5.651273
74	1	0	-2.646069	3.906515	4.293095
75	1	0	-2.333066	3.868506	1.850157
76	1	0	0.287354	3.796189	0.775061
77	1	0	0.635075	6.115385	-0.007363
78	1	0	-0.779200	7.044532	-1.826096
79	1	0	-2.554711	5.641630	-2.845818
80	1	0	-2.924809	3.337460	-2.050560
81	1	0	-0.366321	-2.192475	-3.059237
82	1	0	-0.275170	-4.196137	-4.497162
83	1	0	-0.668219	-6.450382	-3.529427
84	1	0	-1.145593	-6.680618	-1.100337
85	1	0	-1.218736	-4.684645	0.337926
86	1	0	1.669039	-2.982128	0.166007
87	1	0	3.051248	-3.658883	2.069759
88	1	0	2.092441	-3.684828	4.369476
89	1	0	-0.286587	-3.039677	4.703531
90	1	0	-1.644911	-2.313749	2.813398
91	45	0	0.053362	0.209775	-0.979397
92	6	0	1.043753	1.982981	-1.900299
93	6	0	2.062565	1.358678	-2.636033
94	1	0	0.175964	2.281248	-2.481473
95	1	0	1.332597	2.665856	-1.109977
96	1	0	1.787899	0.943231	-3.602092
97	6	0	3.491579	1.545497	-2.385289
98	6	0	3.962041	2.222521	-1.252532
99	6	0	4.420173	1.037020	-3.306324
100	6	0	5.328399	2.374350	-1.044973
101	1	0	3.263946	2.605261	-0.515309
102	6	0	5.781355	1.196488	-3.101327
103	1	0	4.058046	0.497343	-4.177329
104	6	0	6.238782	1.862937	-1.963737
105	1	0	5.682923	2.885159	-0.155011
106	1	0	6.489427	0.796750	-3.820785
107	1	0	7.305046	1.981665	-1.795812

Zero-point correction= 0.857839 (Hartree/Particle)
Thermal correction to Energy= 0.911996
Thermal correction to Enthalpy= 0.912940
Thermal correction to Gibbs Free Energy= 0.770027
Sum of electronic and zero-point Energies= -3970.260908
Sum of electronic and thermal Energies= -3970.206751
Sum of electronic and thermal Enthalpies= -3970.205806
Sum of electronic and thermal Free Energies= -3970.348719

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4772485

TS5a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.621391	2.780873	1.131564
2	6	0	-2.685728	-0.535504	-0.219512
3	6	0	-1.498294	-0.676848	-0.832900
4	16	0	-2.546033	0.769109	0.971960
5	6	0	-3.973500	-1.207579	-0.477263
6	6	0	-4.833677	-1.522821	0.581536
7	6	0	-4.367901	-1.532633	-1.780437
8	6	0	-6.038279	-2.176256	0.347001
9	1	0	-4.550830	-1.252934	1.595758
10	6	0	-5.571753	-2.188854	-2.014623
11	1	0	-3.730624	-1.256215	-2.615429
12	6	0	-6.409145	-2.518015	-0.952017
13	1	0	-6.691018	-2.418799	1.180793
14	1	0	-5.858990	-2.433897	-3.033259
15	1	0	-7.351277	-3.026310	-1.134931
16	6	0	-1.264443	-1.626880	-1.935664
17	8	0	-1.005000	-1.313912	-3.083858
18	8	0	-1.377413	-2.898059	-1.525071
19	6	0	-1.230161	-3.924331	-2.513963
20	6	0	-2.542654	-4.185437	-3.230463
21	1	0	-0.907500	-4.798497	-1.943401

22	1	0	-0.442135	-3.636953	-3.214046
23	1	0	-2.439784	-5.051725	-3.892798
24	1	0	-3.341261	-4.383431	-2.509703
25	1	0	-2.825344	-3.320738	-3.837009
26	26	0	3.883843	0.090549	1.116123
27	15	0	1.631941	0.545371	-1.390468
28	15	0	0.487523	-0.671657	1.771856
29	6	0	2.256963	2.913142	-2.775552
30	6	0	1.986074	-1.086264	-2.150412
31	6	0	2.046921	-3.494012	-1.890524
32	6	0	1.598377	1.683013	-2.823547
33	6	0	2.743543	-3.613963	-3.089079
34	6	0	2.684176	-1.213376	-3.355270
35	6	0	1.667248	-2.236483	-1.434086
36	6	0	3.054263	-2.470635	-3.822905
37	6	0	0.822437	1.358230	-3.943527
38	6	0	0.727850	2.249679	-5.006603
39	6	0	2.293991	-0.829001	2.061138
40	6	0	2.963105	0.071065	2.952034
41	6	0	-0.037225	-0.179344	3.468584
42	6	0	5.483788	0.617718	-0.069753
43	6	0	3.278396	-1.776671	1.612525
44	6	0	4.317192	-0.333587	3.076702
45	6	0	2.151387	3.805090	-3.840027
46	6	0	4.512039	-1.479012	2.256540
47	6	0	0.173339	-1.095977	4.507915
48	6	0	3.258303	0.869664	-0.642076
49	6	0	-0.598881	1.063203	3.755422
50	6	0	4.980509	1.761921	0.608969
51	6	0	4.433651	0.069973	-0.849657
52	6	0	3.616490	1.925870	0.260640
53	6	0	-0.204920	-2.383404	1.736579
54	6	0	0.502380	-3.547619	1.431116
55	6	0	-0.950073	1.382121	5.066970
56	6	0	-0.176522	-0.774097	5.812272
57	6	0	-0.743584	0.468566	6.093500
58	6	0	1.390981	3.474121	-4.957289
59	6	0	-2.237361	-3.707206	1.844002
60	6	0	-1.582142	-2.490759	1.975165
61	6	0	-1.526340	-4.853449	1.499162
62	6	0	-0.152018	-4.772066	1.312075
63	1	0	2.929832	2.658717	0.657271
64	1	0	5.524574	2.370736	1.318352
65	1	0	6.475906	0.198992	0.032427
66	1	0	4.494637	-0.827793	-1.447209
67	1	0	3.153527	-2.542905	0.863172
68	1	0	5.447315	-1.996758	2.093140
69	1	0	5.077174	0.175082	3.653660
70	1	0	2.504226	0.929396	3.423031
71	1	0	1.086062	-2.157219	-0.525420
72	1	0	1.773760	-4.375028	-1.316007
73	1	0	3.036889	-4.592978	-3.456604
74	1	0	3.590436	-2.556918	-4.763198
75	1	0	2.948464	-0.329459	-3.926728
76	1	0	0.283326	0.414147	-3.972762
77	1	0	0.127426	1.988133	-5.872927
78	1	0	1.311046	4.171289	-5.786247
79	1	0	2.666364	4.759847	-3.792597
80	1	0	2.850876	3.181463	-1.908103
81	1	0	-0.737580	1.790580	2.965373
82	1	0	-1.387467	2.353392	5.276893
83	1	0	-1.019678	0.720761	7.113475
84	1	0	-0.009087	-1.493645	6.608267
85	1	0	0.613262	-2.066456	4.296021
86	1	0	-2.145225	-1.609637	2.262840
87	1	0	-3.310080	-3.754836	2.003979
88	1	0	-2.038378	-5.805348	1.394372
89	1	0	0.423233	-5.664139	1.079596
90	1	0	1.573802	-3.524372	1.294486
91	45	0	-0.297518	0.733663	-0.013706
92	6	0	-1.181782	2.147296	-1.511615
93	6	0	-2.447262	2.413604	-0.961157
94	1	0	-0.440030	2.939307	-1.501457
95	1	0	-1.197853	1.535229	-2.408057
96	1	0	-3.262204	1.786695	-1.311327
97	6	0	-2.879522	3.652901	-0.311950
98	6	0	-1.991431	4.681434	0.027340
99	6	0	-4.249387	3.827518	-0.064667
100	6	0	-2.468437	5.852637	0.603548
101	1	0	-0.927686	4.550458	-0.130455
102	6	0	-4.724948	5.002425	0.499188
103	1	0	-4.939041	3.023853	-0.310729
104	6	0	-3.831546	6.018536	0.836808
105	1	0	-1.769683	6.638619	0.873034
106	1	0	-5.788151	5.126620	0.680783
107	1	0	-4.199495	6.938169	1.282734

Zero-point correction= 0.856199 (Hartree/Particle)
Thermal correction to Energy= 0.910893
Thermal correction to Enthalpy= 0.911837
Thermal correction to Gibbs Free Energy= 0.764696
Sum of electronic and zero-point Energies= -3970.256134
Sum of electronic and thermal Energies= -3970.201439

Sum of electronic and thermal Enthalpies= -3970.200495
Sum of electronic and thermal Free Energies= -3970.347636
ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4711592

TS6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.417573	0.136890	-3.190443
2	16	0	1.711832	-1.183633	-1.998677
3	6	0	3.815679	-1.196764	-0.145128
4	6	0	4.248333	-2.451504	-0.594065
5	6	0	4.681068	-0.439475	0.650006
6	6	0	5.497185	-2.943483	-0.233755
7	1	0	3.596845	-3.044846	-1.229370
8	6	0	5.933985	-0.925390	1.002064
9	1	0	4.388317	0.552750	0.969887
10	6	0	6.345037	-2.182927	0.569001
11	1	0	5.812022	-3.920986	-0.587535
12	1	0	6.592507	-0.313115	1.611508
13	1	0	7.323338	-2.565253	0.845466
14	6	0	1.896507	0.812452	1.428247
15	8	0	1.845327	1.990138	1.744269
16	8	0	2.105521	-0.165293	2.325650
17	6	0	2.363529	0.226187	3.678967
18	6	0	3.832966	0.541300	3.893325
19	1	0	2.053778	-0.640913	4.266712
20	1	0	1.733512	1.082043	3.931185
21	1	0	4.017661	0.743161	4.953839
22	1	0	4.457379	-0.300963	3.581632
23	1	0	4.122099	1.427807	3.320760
24	26	0	-4.203347	-0.270271	0.167489
25	15	0	-1.490666	1.735840	-0.011503
26	15	0	-1.025599	-1.795676	-0.138191
27	6	0	-1.965072	3.947027	-1.667130
28	6	0	-1.388992	1.870901	1.815163
29	6	0	-0.992041	0.783795	3.943575
30	6	0	-1.252959	3.465588	-0.564635
31	6	0	-1.461353	1.906910	4.616724
32	6	0	-1.852272	3.000682	2.499609
33	6	0	-0.947851	0.776658	2.552836
34	6	0	-1.882645	3.019290	3.890206
35	6	0	-0.273676	4.272957	0.026554
36	6	0	-0.021203	5.546314	-0.474774
37	6	0	-2.783822	-1.751851	0.398145
38	6	0	-3.833100	-2.188303	-0.473524
39	6	0	-1.115282	-3.272667	-1.239500
40	6	0	-5.532806	1.299326	0.285182
41	6	0	-3.404651	-1.394955	1.645481
42	6	0	-5.063934	-2.134796	0.230335
43	6	0	-1.706395	5.220204	-2.165924
44	6	0	-4.799903	-1.655148	1.542061
45	6	0	-1.399586	-4.517410	-0.661328
46	6	0	-3.281857	1.487229	-0.207034
47	6	0	-0.958179	-3.181314	-2.621208
48	6	0	-5.345002	0.921634	-1.073320
49	6	0	-4.269794	1.657396	0.822134
50	6	0	-3.967699	1.039169	-1.384692
51	6	0	-0.082398	-2.529128	1.269938
52	6	0	-0.490186	-2.536726	2.606554
53	6	0	-1.073530	-4.323502	-3.413314
54	6	0	-1.509123	-5.652983	-1.453153
55	6	0	-1.343399	-5.557738	-2.834472
56	6	0	-0.735862	6.021914	-1.571076
57	6	0	2.008932	-3.557153	1.954659
58	6	0	1.168268	-3.076348	0.959327
59	6	0	1.605566	-3.526512	3.285893
60	6	0	0.345759	-3.031025	3.605054
61	1	0	-3.486990	0.767857	-2.313260
62	1	0	-6.109238	0.551756	-1.743294
63	1	0	-6.463937	1.265500	0.834776
64	1	0	-4.079687	1.938701	1.847378
65	1	0	-2.930198	-0.939653	2.501304
66	1	0	-5.534779	-1.455035	2.309922
67	1	0	-6.036124	-2.368286	-0.181343
68	1	0	-3.699586	-2.484509	-1.504578
69	1	0	-0.542385	-0.087304	2.042494
70	1	0	-0.642671	-0.087432	4.490764
71	1	0	-1.492885	1.921900	5.702241
72	1	0	-2.243084	3.903548	4.407166
73	1	0	-2.199951	3.867078	1.945254
74	1	0	0.293161	3.905224	0.878294
75	1	0	0.739034	6.165456	-0.007913
76	1	0	-0.534863	7.014072	-1.964004
77	1	0	-2.263331	5.583362	-3.024177
78	1	0	-2.713052	3.323252	-2.146319
79	1	0	-0.774663	-2.218494	-3.084147
80	1	0	-0.949024	-4.236942	-4.488396
81	1	0	-1.427353	-6.445736	-3.454568
82	1	0	-1.722160	-6.612678	-0.991664
83	1	0	-1.532525	-4.600916	0.413410
84	1	0	1.484203	-3.132546	-0.075717

85	1	0	2.984749	-3.947661	1.682947
86	1	0	2.262033	-3.900980	4.065943
87	1	0	-0.000090	-3.035142	4.635342
88	1	0	-1.469768	-2.176619	2.886981
89	45	0	-0.021996	0.203290	-1.117920
90	6	0	2.491792	-0.677222	-0.535324
91	6	0	1.700967	0.266401	0.072618
92	6	0	1.002794	1.801271	-2.228568
93	6	0	1.962450	2.059332	-1.231386
94	1	0	1.319538	1.409096	-3.188852
95	1	0	0.168953	2.491063	-2.293860
96	1	0	1.641157	2.675409	-0.399305
97	6	0	3.420103	2.040156	-1.421227
98	6	0	4.038487	1.418159	-2.513866
99	6	0	4.218074	2.710550	-0.482326
100	6	0	5.422414	1.441704	-2.641670
101	1	0	3.438700	0.904895	-3.256683
102	6	0	5.599187	2.752521	-0.626810
103	1	0	3.740934	3.181409	0.372861
104	6	0	6.205805	2.109232	-1.703368
105	1	0	5.890650	0.943361	-3.484977
106	1	0	6.203581	3.281189	0.104602
107	1	0	7.285790	2.133298	-1.815110

Zero-point correction=	0.857735 (Hartree/Particle)
Thermal correction to Energy=	0.911616
Thermal correction to Enthalpy=	0.912560
Thermal correction to Gibbs Free Energy=	0.771661
Sum of electronic and zero-point Energies=	-3970.257883
Sum of electronic and thermal Energies=	-3970.204002
Sum of electronic and thermal Enthalpies=	-3970.203058
Sum of electronic and thermal Free Energies=	-3970.343957

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4717104

TS6a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.257021	1.999535	1.930819
2	16	0	0.749231	-0.352841	-2.179431
3	6	0	3.478554	-0.958041	-2.035808
4	6	0	3.282311	-2.220449	-2.609701
5	6	0	4.755506	-0.385661	-2.085582
6	6	0	4.339751	-2.907350	-3.191306
7	1	0	2.297591	-2.673205	-2.571442
8	6	0	5.808268	-1.068967	-2.684440
9	1	0	4.922148	0.582167	-1.632046
10	6	0	5.607401	-2.331901	-3.234340
11	1	0	4.172687	-3.894136	-3.613203
12	1	0	6.792074	-0.610123	-2.717345
13	1	0	6.434631	-2.864545	-3.694875
14	6	0	3.215531	0.734556	0.714978
15	8	0	4.422369	0.716242	0.566153
16	8	0	2.640911	0.959489	1.906563
17	6	0	3.495678	1.295771	2.999737
18	6	0	4.008896	0.047960	3.697479
19	1	0	2.859690	1.891539	3.658515
20	1	0	4.318111	1.915036	2.632429
21	1	0	4.590820	0.323803	4.583493
22	1	0	3.175573	-0.587703	4.015991
23	1	0	4.655313	-0.523827	3.025641
24	26	0	-2.969969	-1.966794	-1.560137
25	15	0	-2.330915	1.114468	-0.401528
26	15	0	-0.139673	-1.608218	0.608588
27	6	0	-3.059664	3.057462	-2.331902
28	6	0	-3.464637	0.967596	1.033578
29	6	0	-3.996166	-0.006025	3.184996
30	6	0	-2.722715	2.803935	-1.001105
31	6	0	-5.267038	0.558546	3.134953
32	6	0	-4.738609	1.546565	0.997208
33	6	0	-3.100032	0.206349	2.141283
34	6	0	-5.634313	1.341528	2.041674
35	6	0	-2.609074	3.876559	-0.107364
36	6	0	-2.836425	5.177107	-0.542119
37	6	0	-1.459002	-2.545426	-0.251607
38	6	0	-1.330676	-3.163491	-1.539752
39	6	0	1.337814	-2.706977	0.443995
40	6	0	-4.674517	-1.415012	-2.570431
41	6	0	-2.751302	-2.902611	0.254331
42	6	0	-2.497874	-3.937506	-1.787573
43	6	0	-3.282111	4.363682	-2.764715
44	6	0	-3.378881	-3.768907	-0.683074
45	6	0	2.496145	-2.271331	1.095978
46	6	0	-3.182742	0.051951	-1.595412
47	6	0	1.362677	-3.947975	-0.196088
48	6	0	-3.543216	-1.307003	-3.427179
49	6	0	-4.462110	-0.573762	-1.447150
50	6	0	-2.622989	-0.405268	-2.831808
51	6	0	-0.431035	-1.947270	2.396800
52	6	0	-0.980532	-3.152066	2.850415
53	6	0	2.536192	-4.698190	-0.235821
54	6	0	3.671278	-3.008795	1.040190

55	6	0	3.699056	-4.221878	0.358769
56	6	0	-3.171823	5.424593	-1.872087
57	6	0	-0.045786	-1.288085	4.692104
58	6	0	0.058209	-1.026693	3.327611
59	6	0	-0.627755	-2.470021	5.138190
60	6	0	-1.088634	-3.405281	4.213113
61	1	0	-1.651760	-0.139985	-3.224913
62	1	0	-3.382636	-1.858753	-4.343488
63	1	0	-5.524436	-2.067265	-2.719613
64	1	0	-5.120322	-0.471469	-0.596703
65	1	0	-3.182295	-2.552373	1.182283
66	1	0	-4.376037	-4.177899	-0.593849
67	1	0	-2.706955	-4.492643	-2.691846
68	1	0	-0.498903	-3.029025	-2.216407
69	1	0	-2.101320	-0.198894	2.208445
70	1	0	-3.685424	-0.600455	4.039273
71	1	0	-5.968402	0.400627	3.949259
72	1	0	-6.619467	1.796903	2.002096
73	1	0	-5.034624	2.155609	0.147820
74	1	0	-2.329984	3.687307	0.925480
75	1	0	-2.747923	5.999816	0.161187
76	1	0	-3.346200	6.441822	-2.210221
77	1	0	-3.543911	4.547790	-3.802530
78	1	0	-3.157286	2.237815	-3.037408
79	1	0	0.470118	-4.352506	-0.655923
80	1	0	2.536471	-5.659142	-0.742232
81	1	0	4.618618	-4.796267	0.301940
82	1	0	4.564565	-2.627543	1.524641
83	1	0	2.470711	-1.351612	1.667216
84	1	0	0.493697	-0.093655	2.985253
85	1	0	0.323259	-0.555643	5.403889
86	1	0	-0.716307	-2.668396	6.202449
87	1	0	-1.525097	-4.339829	4.553324
88	1	0	-1.315171	-3.902191	2.141303
89	45	0	0.084745	0.713336	-0.169297
90	6	0	2.331241	-0.234746	-1.452634
91	6	0	2.188815	0.535263	-0.327143
92	6	0	0.387765	2.672636	-1.078383
93	6	0	1.787961	2.549867	-1.182770
94	1	0	-0.154986	2.610698	-2.017830
95	1	0	-0.014399	3.376923	-0.358769
96	1	0	2.156270	2.173372	-2.132056
97	6	0	2.776396	3.329879	-0.424114
98	6	0	4.056525	3.479224	-0.971497
99	6	0	2.487600	3.922279	0.812345
100	6	0	5.028491	4.220182	-0.311974
101	1	0	4.288585	3.002627	-1.920643
102	6	0	3.466911	4.650145	1.476560
103	1	0	1.513679	3.770458	1.266921
104	6	0	4.734730	4.805666	0.916377
105	1	0	6.015273	4.331383	-0.750413
106	1	0	3.239668	5.098826	2.439012
107	1	0	5.493911	5.379127	1.440457

Zero-point correction=	0.857217 (Hartree/Particle)
Thermal correction to Energy=	0.911659
Thermal correction to Enthalpy=	0.912604
Thermal correction to Gibbs Free Energy=	0.768851
Sum of electronic and zero-point Energies=	-3970.250024
Sum of electronic and thermal Energies=	-3970.195582
Sum of electronic and thermal Enthalpies=	-3970.194638
Sum of electronic and thermal Free Energies=	-3970.338391

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.463556

INT9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.881932	0.595662	-3.188943
2	6	0	2.539847	-0.509554	0.000104
3	6	0	1.488987	0.090045	0.580241
4	16	0	2.130016	-0.706408	-1.743085
5	6	0	3.829275	-0.984966	0.532109
6	6	0	4.406817	-2.157506	0.031111
7	6	0	4.489450	-0.300894	1.559304
8	6	0	5.594782	-2.648422	0.561687
9	1	0	3.919854	-2.690808	-0.781104
10	6	0	5.673697	-0.795103	2.093508
11	1	0	4.081238	0.634137	1.929049
12	6	0	6.229838	-1.972938	1.600639
13	1	0	6.025911	-3.560798	0.160043
14	1	0	6.168893	-0.250253	2.892317
15	1	0	7.157164	-2.356078	2.015953
16	6	0	1.527903	0.530774	1.992366
17	8	0	1.645173	1.690786	2.338506
18	8	0	1.439336	-0.498661	2.838853
19	6	0	1.516474	-0.214171	4.242562
20	6	0	2.958220	-0.132334	4.709019
21	1	0	0.996256	-1.054058	4.708138
22	1	0	0.974387	0.711044	4.450776
23	1	0	2.989776	-0.056087	5.801159
24	1	0	3.513331	-1.022812	4.400004

25	1	0	3.447835	0.750731	4.290166
26	26	0	-4.230391	-0.120273	-0.318783
27	15	0	-1.403346	1.775702	0.106268
28	15	0	-1.168452	-1.795675	-0.370460
29	6	0	-1.704493	4.238269	-1.218644
30	6	0	-1.572212	1.724038	1.931514
31	6	0	-1.728055	0.377368	3.938773
32	6	0	-1.012695	3.522513	-0.240834
33	6	0	-2.110080	1.497624	4.670739
34	6	0	-1.948539	2.847677	2.674033
35	6	0	-1.453396	0.497525	2.580873
36	6	0	-2.210447	2.734026	4.036213
37	6	0	0.066050	4.119091	0.424505
38	6	0	0.428590	5.426997	0.123815
39	6	0	-2.977791	-1.748290	-0.076147
40	6	0	-3.913307	-1.987765	-1.131910
41	6	0	-1.083404	-3.112868	-1.652500
42	6	0	-5.455928	1.531912	-0.207814
43	6	0	-3.746818	-1.481149	1.108559
44	6	0	-5.228344	-1.894538	-0.604574
45	6	0	-1.331204	5.545804	-1.520021
46	6	0	-5.126686	-1.592155	0.780470
47	6	0	-1.468042	-4.421585	-1.328932
48	6	0	-3.151138	1.603508	-0.365871
49	6	0	-0.646912	-2.826712	-2.945480
50	6	0	-5.097668	1.274649	-1.560695
51	6	0	-4.263553	1.739180	0.531517
52	6	0	-3.684125	1.318967	-1.666788
53	6	0	-0.432655	-2.718308	1.047900
54	6	0	-1.042266	-2.952979	2.281336
55	6	0	-0.593062	-3.839227	-3.904004
56	6	0	-1.412695	-5.425984	-2.285459
57	6	0	-0.971816	-5.135623	-3.577332
58	6	0	-0.268533	6.142155	-0.848561
59	6	0	1.603389	-3.724682	1.909711
60	6	0	0.892074	-3.140060	0.871803
61	6	0	0.995722	-3.918157	3.148225
62	6	0	-0.331978	-3.546374	3.324651
63	1	0	-3.090314	1.115626	-2.546238
64	1	0	-5.779869	1.027812	-2.362882
65	1	0	-6.456003	1.511268	0.203944
66	1	0	-4.202048	1.912376	1.596231
67	1	0	-3.369912	-1.183873	2.075013
68	1	0	-5.949636	-1.413436	1.459112
69	1	0	-6.144647	-1.989999	-1.170764
70	1	0	-3.651269	-2.176945	-2.163809
71	1	0	-1.116570	-0.372175	2.031114
72	1	0	-1.622326	-0.591277	4.419673
73	1	0	-2.319749	1.411009	5.732818
74	1	0	-2.498854	3.614854	4.602030
75	1	0	-2.046904	3.812841	2.187675
76	1	0	0.623098	3.554883	1.169620
77	1	0	1.264148	5.885524	0.644212
78	1	0	0.019403	7.162635	-1.083770
79	1	0	-1.873764	6.096429	-2.282569
80	1	0	-2.531891	3.777732	-1.748698
81	1	0	-0.378599	-1.809403	-3.210529
82	1	0	-0.255260	-3.604371	-4.908960
83	1	0	-0.927512	-5.921898	-4.325486
84	1	0	-1.710497	-6.437524	-2.025068
85	1	0	-1.806361	-4.653334	-0.322667
86	1	0	1.373576	-3.009921	-0.092160
87	1	0	2.638017	-4.013568	1.751707
88	1	0	1.550402	-4.370567	3.965053
89	1	0	-0.827915	-3.723790	4.275129
90	1	0	-2.081467	-2.694916	2.439518
91	45	0	0.101045	0.318202	-0.889708
92	6	0	1.377646	1.866008	-1.491429
93	6	0	2.402816	1.095444	-2.296105
94	1	0	0.802331	2.545770	-2.120177
95	1	0	1.797798	2.398733	-0.640790
96	1	0	2.077226	1.035650	-3.338525
97	6	0	3.859122	1.460342	-2.206532
98	6	0	4.418937	1.981855	-1.037305
99	6	0	4.695253	1.221549	-3.301687
100	6	0	5.783192	2.244552	-0.962387
101	1	0	3.791507	2.172812	-0.172705
102	6	0	6.057712	1.488414	-3.230770
103	1	0	4.270564	0.815493	-4.216970
104	6	0	6.606881	1.998357	-2.056588
105	1	0	6.203304	2.639579	-0.042099
106	1	0	6.691235	1.297079	-4.091998
107	1	0	7.671725	2.202995	-1.995358

Zero-point correction= 0.858504 (Hartree/Particle)
Thermal correction to Energy= 0.912083
Thermal correction to Enthalpy= 0.913027
Thermal correction to Gibbs Free Energy= 0.771260
Sum of electronic and zero-point Energies= -3970.277878
Sum of electronic and thermal Energies= -3970.224299
Sum of electronic and thermal Enthalpies= -3970.223355
Sum of electronic and thermal Free Energies= -3970.365122

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4968566

INT9a''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.457443	2.649774	1.473820
2	6	0	-2.625749	-0.703083	-0.308869
3	6	0	-1.419176	-0.688773	-0.891072
4	16	0	-2.655268	0.635938	0.897741
5	6	0	-3.825996	-1.519318	-0.562619
6	6	0	-4.606172	-1.989005	0.501422
7	6	0	-4.200120	-1.853477	-1.869550
8	6	0	-5.711448	-2.798817	0.265931
9	1	0	-4.341113	-1.720441	1.521005
10	6	0	-5.303419	-2.668080	-2.103170
11	1	0	-3.626622	-1.464537	-2.705414
12	6	0	-6.060079	-3.147230	-1.037550
13	1	0	-6.302734	-3.158748	1.102875
14	1	0	-5.576396	-2.919206	-3.124068
15	1	0	-6.923855	-3.779199	-1.221239
16	6	0	-1.111208	-1.579812	-2.033419
17	8	0	-1.013421	-1.206520	-3.186235
18	8	0	-0.974710	-2.849669	-1.642603
19	6	0	-0.742774	-3.833781	-2.659436
20	6	0	-2.053600	-4.324553	-3.245215
21	1	0	-0.214887	-4.634534	-2.136946
22	1	0	-0.091669	-3.410223	-3.427304
23	1	0	-1.865117	-5.157212	-3.931294
24	1	0	-2.727186	-4.663519	-2.452760
25	1	0	-2.547123	-3.524246	-3.803017
26	26	0	3.936623	0.422389	0.962384
27	15	0	1.473981	0.888811	-1.379209
28	15	0	0.724478	-0.820371	1.717873
29	6	0	1.799417	3.419545	-2.566164
30	6	0	1.946506	-0.615561	-2.318617
31	6	0	2.439699	-2.986505	-2.257116
32	6	0	1.220250	2.154247	-2.669648
33	6	0	2.996345	-2.911889	-3.530594
34	6	0	2.503044	-0.547984	-3.599061
35	6	0	1.913399	-1.844841	-1.663107
36	6	0	3.017799	-1.691561	-4.202350
37	6	0	0.352977	1.874309	-3.733973
38	6	0	0.092702	2.847405	-4.692273
39	6	0	2.543469	-0.771980	1.935419
40	6	0	3.137855	0.161575	2.842860
41	6	0	0.198034	-0.601010	3.470037
42	6	0	5.383610	1.190260	-0.283692
43	6	0	3.614026	-1.543927	1.369898
44	6	0	4.540643	-0.056644	2.864357
45	6	0	1.526318	4.393120	-3.524080
46	6	0	4.835539	-1.113929	1.960660
47	6	0	0.599496	-1.548159	4.422236
48	6	0	3.107342	1.281519	-0.679881
49	6	0	-0.594261	0.474573	3.867841
50	6	0	4.835055	2.223602	0.525807
51	6	0	4.329178	0.611021	-1.033396
52	6	0	3.439466	2.288379	0.285421
53	6	0	0.223578	-2.583463	1.502933
54	6	0	1.045739	-3.653622	1.147521
55	6	0	-0.985011	0.599067	5.201480
56	6	0	0.212806	-1.419309	5.748961
57	6	0	-0.584751	-0.343295	6.140572
58	6	0	0.677411	4.108222	-4.588756
59	6	0	-1.692652	-4.072934	1.382821
60	6	0	-1.150575	-2.822537	1.640921
61	6	0	-0.865300	-5.124272	0.994778
62	6	0	0.504717	-4.913717	0.892979
63	1	0	2.725599	2.923140	0.788159
64	1	0	5.375693	2.821026	1.247440
65	1	0	6.414069	0.861343	-0.288066
66	1	0	4.425020	-0.219947	-1.716482
67	1	0	3.541407	-2.281200	0.585072
68	1	0	5.819506	-1.489013	1.713931
69	1	0	5.259791	0.518130	3.431476
70	1	0	2.597107	0.920359	3.391816
71	1	0	1.449427	-1.924288	-0.689207
72	1	0	2.392793	-3.933865	-1.727081
73	1	0	3.407052	-3.800374	-4.001104
74	1	0	3.446715	-1.624909	-5.197643
75	1	0	2.549259	0.400748	-4.123068
76	1	0	-0.120845	0.897348	-3.805026
77	1	0	-0.576776	2.621296	-5.516857
78	1	0	0.467022	4.868230	-5.335502
79	1	0	1.981198	5.374945	-3.434556
80	1	0	2.464851	3.650925	-1.741156
81	1	0	-0.878417	1.231219	3.146855
82	1	0	-1.600010	1.442824	5.499730
83	1	0	-0.888317	-0.241856	7.178656
84	1	0	0.531073	-2.157939	6.478698
85	1	0	1.215860	-2.390972	4.120652
86	1	0	-1.807117	-2.016703	1.953600
87	1	0	-2.764416	-4.220423	1.473827

88	1	0	-1.286614	-6.103738	0.788526
89	1	0	1.165656	-5.732624	0.621980
90	1	0	2.117722	-3.525574	1.078115
91	45	0	-0.343726	0.734992	0.066853
92	6	0	-1.495768	2.116633	-1.024856
93	6	0	-2.877971	2.016170	-0.398722
94	1	0	-1.022134	3.086036	-0.866792
95	1	0	-1.529996	1.878850	-2.086425
96	1	0	-3.604097	1.578890	-1.088989
97	6	0	-3.487904	3.234424	0.241593
98	6	0	-2.745290	4.092888	1.057405
99	6	0	-4.844266	3.500739	0.034709
100	6	0	-3.353741	5.195688	1.648350
101	1	0	-1.692836	3.890054	1.236260
102	6	0	-5.450260	4.607631	0.621306
103	1	0	-5.432526	2.835820	-0.593852
104	6	0	-4.704341	5.458647	1.431937
105	1	0	-2.764604	5.852942	2.281377
106	1	0	-6.504051	4.803218	0.444943
107	1	0	-5.173503	6.323346	1.892605

Zero-point correction= 0.858540 (Hartree/Particle)
Thermal correction to Energy= 0.913134
Thermal correction to Enthalpy= 0.914078
Thermal correction to Gibbs Free Energy= 0.769020
Sum of electronic and zero-point Energies= -3970.270982
Sum of electronic and thermal Energies= -3970.216388
Sum of electronic and thermal Enthalpies= -3970.215444
Sum of electronic and thermal Free Energies= -3970.360502

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4889042

INT10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.232877	0.585840	-3.208407
2	16	0	1.700477	-1.124755	-2.133719
3	6	0	3.703637	-1.532542	-0.287668
4	6	0	3.860635	-2.879224	-0.643992
5	6	0	4.714658	-0.902284	0.450260
6	6	0	4.988214	-3.585471	-0.247442
7	1	0	3.088919	-3.373009	-1.227041
8	6	0	5.852313	-1.604435	0.825099
9	1	0	4.624964	0.149225	0.701510
10	6	0	5.987085	-2.948917	0.488390
11	1	0	5.092401	-4.631913	-0.517233
12	1	0	6.634731	-1.098255	1.381744
13	1	0	6.872651	-3.499547	0.791769
14	6	0	2.091194	0.475342	1.428968
15	8	0	2.219397	1.494527	2.081219
16	8	0	1.986435	-0.744649	1.979845
17	6	0	2.149309	-0.868947	3.395600
18	6	0	3.576850	-1.263345	3.724042
19	1	0	1.446153	-1.652454	3.687320
20	1	0	1.869030	0.072333	3.872040
21	1	0	3.680928	-1.432451	4.801113
22	1	0	3.852768	-2.180401	3.194647
23	1	0	4.272313	-0.471423	3.430270
24	26	0	-4.206228	0.240082	0.086763
25	15	0	-1.206469	1.876899	0.118353
26	15	0	-1.305644	-1.711831	-0.270552
27	6	0	-1.409566	4.308315	-1.250051
28	6	0	-1.130261	1.755166	1.950256
29	6	0	-0.957574	0.361579	3.925713
30	6	0	-0.780071	3.628358	-0.203966
31	6	0	-1.309725	1.439413	4.730868
32	6	0	-1.474037	2.837460	2.769978
33	6	0	-0.856497	0.526418	2.547198
34	6	0	-1.556394	2.681556	4.149448
35	6	0	0.251488	4.258569	0.501581
36	6	0	0.638826	5.552663	0.167698
37	6	0	-3.057062	-1.468795	0.219581
38	6	0	-4.143059	-1.666870	-0.689332
39	6	0	-1.528069	-3.053789	-1.519683
40	6	0	-5.279540	1.984746	0.288921
41	6	0	-3.632692	-1.102807	1.485070
42	6	0	-5.362951	-1.457688	0.006735
43	6	0	-1.018936	5.602511	-1.579894
44	6	0	-5.049842	-1.120041	1.352066
45	6	0	-1.975358	-4.319330	-1.115068
46	6	0	-3.009120	1.858430	-0.130278
47	6	0	-1.287048	-2.818029	-2.873121
48	6	0	-5.101562	1.680034	-1.088992
49	6	0	-3.997029	2.102895	0.883093
50	6	0	-3.711511	1.605863	-1.355624
51	6	0	-0.588807	-2.733369	1.097157
52	6	0	-1.217848	-3.062789	2.300305
53	6	0	-1.482088	-3.835262	-3.807748
54	6	0	-2.168621	-5.329361	-2.048007
55	6	0	-1.918792	-5.089451	-3.399261
56	6	0	0.005116	6.226766	-0.872980
57	6	0	1.355766	-4.000842	1.816399

58	6	0	0.700759	-3.224809	0.870332
59	6	0	0.726370	-4.306757	3.021203
60	6	0	-0.562762	-3.839549	3.256198
61	1	0	-3.242875	1.339281	-2.291727
62	1	0	-5.888081	1.481666	-1.804395
63	1	0	-6.224421	2.056148	0.810674
64	1	0	-3.804519	2.279216	1.931086
65	1	0	-3.096285	-0.812735	2.376618
66	1	0	-5.757927	-0.854050	2.125100
67	1	0	-6.352161	-1.498477	-0.428149
68	1	0	-4.037963	-1.908600	-1.738030
69	1	0	-0.545152	-0.312563	1.937636
70	1	0	-0.754387	-0.612621	4.361217
71	1	0	-1.386973	1.316269	5.807072
72	1	0	-1.822940	3.531277	4.770940
73	1	0	-1.688560	3.805170	2.327424
74	1	0	0.754050	3.739854	1.314400
75	1	0	1.441257	6.031664	0.720715
76	1	0	0.310430	7.235910	-1.133291
77	1	0	-1.513357	6.119806	-2.396490
78	1	0	-2.197391	3.823001	-1.817525
79	1	0	-0.982945	-1.831227	-3.206284
80	1	0	-1.293476	-3.635599	-4.858272
81	1	0	-2.068547	-5.879977	-4.129218
82	1	0	-2.514270	-6.305813	-1.720904
83	1	0	-2.169953	-4.516517	-0.064851
84	1	0	1.195668	-2.997315	-0.065443
85	1	0	2.362825	-4.353260	1.612666
86	1	0	1.235069	-4.910326	3.767255
87	1	0	-1.072929	-4.086937	4.182877
88	1	0	-2.232868	-2.742053	2.495787
89	45	0	0.066362	0.327584	-1.118664
90	6	0	2.537618	-0.755595	-0.733377
91	6	0	1.982876	0.411494	-0.051796
92	6	0	1.277883	1.829363	-1.883726
93	6	0	2.277005	1.787858	-0.758310
94	1	0	1.642640	1.518083	-2.862208
95	1	0	0.737871	2.769040	-1.982360
96	1	0	1.974833	2.517896	-0.008495
97	6	0	3.747880	2.018211	-1.038848
98	6	0	4.375501	1.551116	-2.196330
99	6	0	4.528509	2.657055	-0.068656
100	6	0	5.748744	1.700391	-2.370283
101	1	0	3.791617	1.060167	-2.968789
102	6	0	5.901370	2.809458	-0.241286
103	1	0	4.049952	3.013264	0.839819
104	6	0	6.517591	2.325999	-1.392802
105	1	0	6.218702	1.325029	-3.274801
106	1	0	6.489525	3.307821	0.524506
107	1	0	7.588385	2.443366	-1.531596

Zero-point correction= 0.859470 (Hartree/Particle)
Thermal correction to Energy= 0.912784
Thermal correction to Enthalpy= 0.913728
Thermal correction to Gibbs Free Energy= 0.773448
Sum of electronic and zero-point Energies= -3970.286516
Sum of electronic and thermal Energies= -3970.233201
Sum of electronic and thermal Enthalpies= -3970.232257
Sum of electronic and thermal Free Energies= -3970.372537

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.5009724

INT10a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.221639	1.621676	2.166194
2	16	0	0.664865	0.152884	-2.376227
3	6	0	3.018489	-1.272517	-2.000004
4	6	0	2.408332	-2.418868	-2.526385
5	6	0	4.418821	-1.223506	-1.959719
6	6	0	3.163930	-3.501541	-2.947611
7	1	0	1.328524	-2.461302	-2.583161
8	6	0	5.176230	-2.310885	-2.385045
9	1	0	4.920168	-0.328695	-1.614355
10	6	0	4.554556	-3.455406	-2.870700
11	1	0	2.665608	-4.388194	-3.326621
12	1	0	6.259830	-2.250886	-2.345552
13	1	0	5.148137	-4.304163	-3.198226
14	6	0	3.652600	0.680977	0.340218
15	8	0	4.832309	0.877787	0.150047
16	8	0	3.142664	0.336930	1.524982
17	6	0	4.038632	0.334464	2.646619
18	6	0	4.734229	-1.007153	2.789582
19	1	0	3.391633	0.550575	3.498733
20	1	0	4.757612	1.147150	2.517880
21	1	0	5.399075	-0.991683	3.659505
22	1	0	4.004666	-1.811329	2.928552
23	1	0	5.335477	-1.218175	1.900223
24	26	0	-3.174199	-1.464225	-1.654107
25	15	0	-2.046302	1.422613	-0.237553
26	15	0	-0.354911	-1.771023	0.513489
27	6	0	-2.701245	3.600126	-1.924982

28	6	0	-3.123505	1.292066	1.241370
29	6	0	-3.763444	0.144729	3.274185
30	6	0	-2.245750	3.186659	-0.672987
31	6	0	-4.914391	0.922106	3.359426
32	6	0	-4.277034	2.079556	1.338419
33	6	0	-2.874098	0.336554	2.221624
34	6	0	-5.166101	1.893561	2.392092
35	6	0	-1.894305	4.144322	0.286636
36	6	0	-2.005192	5.497495	-0.006643
37	6	0	-1.769623	-2.422288	-0.449130
38	6	0	-1.691286	-2.862976	-1.808460
39	6	0	0.931926	-3.061551	0.232888
40	6	0	-4.839969	-0.547707	-2.442524
41	6	0	-3.106280	-2.675409	-0.002742
42	6	0	-2.945475	-3.425347	-2.174753
43	6	0	-2.808905	4.959177	-2.214764
44	6	0	-3.821364	-3.306407	-1.059231
45	6	0	2.222786	-2.748798	0.664578
46	6	0	-3.067503	0.556675	-1.456752
47	6	0	0.666243	-4.350131	-0.235904
48	6	0	-3.770504	-0.509055	-3.380288
49	6	0	-4.416683	0.111610	-1.260639
50	6	0	-2.678905	0.170188	-2.780368
51	6	0	-0.735106	-2.310686	2.242383
52	6	0	-1.427446	-3.491998	2.532906
53	6	0	1.683210	-5.298658	-0.293621
54	6	0	3.236579	-3.698316	0.611951
55	6	0	2.970507	-4.974670	0.125993
56	6	0	-2.462286	5.907644	-1.258279
57	6	0	-0.352445	-1.990103	4.611792
58	6	0	-0.179357	-1.575216	3.292797
59	6	0	-1.069924	-3.147446	4.894823
60	6	0	-1.601995	-3.901272	3.849983
61	1	0	-1.715269	0.336538	-3.237128
62	1	0	-3.765165	-0.968004	-4.359533
63	1	0	-5.791027	-1.043418	-2.582129
64	1	0	-4.988113	0.211515	-0.349573
65	1	0	-3.504866	-2.412812	0.967775
66	1	0	-4.865102	-3.588709	-1.034844
67	1	0	-3.202889	-3.816849	-3.149436
68	1	0	-0.826995	-2.766416	-2.449866
69	1	0	-1.965447	-0.242180	2.185113
70	1	0	-3.538050	-0.603836	4.028137
71	1	0	-5.611002	0.780629	4.180705
72	1	0	-6.057414	2.510563	2.457339
73	1	0	-4.488968	2.833870	0.586983
74	1	0	-1.526704	3.822432	1.258146
75	1	0	-1.728857	6.233558	0.741908
76	1	0	-2.548479	6.966131	-1.485250
77	1	0	-3.168462	5.273446	-3.190125
78	1	0	-2.981563	2.867276	-2.675124
79	1	0	-0.334747	-4.622668	-0.554799
80	1	0	1.466763	-6.295671	-0.666899
81	1	0	3.763578	-5.714473	0.072000
82	1	0	4.239344	-3.431865	0.931891
83	1	0	2.433157	-1.751167	1.037465
84	1	0	0.357648	-0.655636	3.080379
85	1	0	0.073209	-1.398559	5.416872
86	1	0	-1.208403	-3.468062	5.923381
87	1	0	-2.145584	-4.817917	4.060146
88	1	0	-1.824045	-4.105799	1.730517
89	45	0	0.180828	0.765896	-0.127270
90	6	0	2.213337	-0.083068	-1.619820
91	6	0	2.559493	0.884491	-0.677316
92	6	0	0.763005	2.645726	-0.713619
93	6	0	2.234588	2.392879	-0.986109
94	1	0	0.229113	2.988915	-1.600490
95	1	0	0.587402	3.318545	0.123608
96	1	0	2.415824	2.490166	-2.062127
97	6	0	3.166937	3.352930	-0.271000
98	6	0	4.172615	4.003404	-0.985645
99	6	0	3.051115	3.595813	1.101816
100	6	0	5.046957	4.881218	-0.350470
101	1	0	4.279452	3.815618	-2.051327
102	6	0	3.929417	4.466088	1.738755
103	1	0	2.272769	3.094785	1.671951
104	6	0	4.929308	5.113353	1.016228
105	1	0	5.822910	5.379775	-0.924443
106	1	0	3.825968	4.642964	2.805791
107	1	0	5.611566	5.795338	1.515694

Zero-point correction= 0.858246 (Hartree/Particle)
Thermal correction to Energy= 0.913003
Thermal correction to Enthalpy= 0.913947
Thermal correction to Gibbs Free Energy= 0.768210
Sum of electronic and zero-point Energies= -3970.274137
Sum of electronic and thermal Energies= -3970.219379
Sum of electronic and thermal Enthalpies= -3970.218435
Sum of electronic and thermal Free Energies= -3970.364172

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4874025

INT11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.872635	-0.034824	2.559296
2	15	0	2.757514	0.828435	-0.674490
3	15	0	0.193288	-1.380348	0.839382
4	6	0	3.542849	2.498010	-2.807856
5	6	0	4.205171	-0.153007	-1.206462
6	6	0	5.100523	-2.264876	-1.984624
7	6	0	2.978811	2.436670	-1.529841
8	6	0	6.386537	-1.733812	-1.959922
9	6	0	5.499441	0.379869	-1.209825
10	6	0	4.014883	-1.474305	-1.616242
11	6	0	6.584506	-0.407662	-1.579267
12	6	0	2.511249	3.612109	-0.935239
13	6	0	2.619256	4.829513	-1.600032
14	6	0	1.543887	-1.472397	2.061724
15	6	0	1.491207	-1.238813	3.475930
16	6	0	-1.232328	-1.096248	1.949804
17	6	0	4.116568	1.505266	3.132233
18	6	0	2.874726	-1.904079	1.753932
19	6	0	2.779487	-1.493642	4.015450
20	6	0	3.655764	3.717598	-3.466277
21	6	0	3.631184	-1.907625	2.954137
22	6	0	-1.274291	0.105199	2.667474
23	6	0	3.150934	1.269839	1.044221
24	6	0	-2.259939	-2.023600	2.120587
25	6	0	2.756322	1.911592	3.233125
26	6	0	4.364514	1.116382	1.787664
27	6	0	2.161592	1.771912	1.951312
28	6	0	0.130670	-3.162131	0.389725
29	6	0	0.084239	-4.133400	1.399655
30	6	0	-3.304537	-1.759620	3.003673
31	6	0	-2.314967	0.366418	3.547891
32	6	0	-3.331407	-0.570755	3.721773
33	6	0	3.195554	4.885893	-2.865198
34	6	0	0.255901	-4.930593	-1.261174
35	6	0	0.231399	-3.574249	-0.940194
36	6	0	0.180575	-5.885617	-0.254676
37	6	0	0.097967	-5.484264	1.078731
38	1	0	1.130808	1.971472	1.687145
39	1	0	2.250927	2.225599	4.136249
40	1	0	4.825867	1.447028	3.946620
41	1	0	5.287590	0.700112	1.410022
42	1	0	3.253915	-2.144414	0.770650
43	1	0	4.685749	-2.133351	3.033316
44	1	0	3.068391	-1.352606	5.048002
45	1	0	0.631526	-0.889502	4.028565
46	1	0	3.009161	-1.884539	-1.664562
47	1	0	4.937570	-3.290426	-2.301312
48	1	0	7.233819	-2.347570	-2.251265
49	1	0	7.584035	0.016741	-1.578285
50	1	0	5.654473	1.420604	-0.938791
51	1	0	2.057021	3.587522	0.049916
52	1	0	2.248742	5.733587	-1.126346
53	1	0	3.281657	5.836598	-3.383043
54	1	0	4.098022	3.751367	-4.457328
55	1	0	3.884667	1.591341	-3.294721
56	1	0	-2.266131	-2.950313	1.557405
57	1	0	-4.107174	-2.482106	3.107439
58	1	0	-4.151023	-0.363146	4.402987
59	1	0	-2.343854	1.310449	4.082976
60	1	0	-0.486273	0.838506	2.533837
61	1	0	0.294554	-2.843719	-1.738892
62	1	0	0.332899	-5.232135	-2.301109
63	1	0	0.194532	-6.942527	-0.503430
64	1	0	0.051494	-6.226594	1.869577
65	1	0	0.037920	-3.828877	2.441536
66	17	0	1.170341	0.154346	-3.423657
67	45	0	0.514364	-0.192110	-1.135220
68	6	0	-2.340366	1.388769	-0.176619
69	6	0	-3.045943	0.240953	-0.354685
70	16	0	-0.656486	1.683883	-0.562584
71	6	0	-2.910114	2.663500	0.358313
72	6	0	-2.375303	3.294753	1.482555
73	6	0	-3.962408	3.280610	-0.326720
74	6	0	-2.912751	4.492393	1.944868
75	1	0	-1.539962	2.839349	2.002889
76	6	0	-4.493501	4.480116	0.128477
77	1	0	-4.368386	2.799845	-1.211658
78	6	0	-3.974899	5.087048	1.271787
79	1	0	-2.495133	4.963780	2.829969
80	1	0	-5.312867	4.945933	-0.411325
81	1	0	-4.392305	6.023924	1.629063
82	6	0	-4.322406	-0.038812	0.359022
83	8	0	-4.910172	-1.098909	0.266970
84	8	0	-4.738506	0.940065	1.181050
85	6	0	-5.978400	0.732357	1.854665
86	6	0	-7.146455	1.113080	0.960967
87	1	0	-5.922629	1.379834	2.733314
88	1	0	-6.048115	-0.310572	2.174627
89	1	0	-8.090176	1.026182	1.509849
90	1	0	-7.035514	2.145606	0.615424

91	1	0	-7.188408	0.449762	0.092662
92	6	0	-1.312875	-0.711401	-1.994040
93	6	0	-2.580307	-0.941567	-1.185732
94	1	0	-1.477554	0.076010	-2.733117
95	1	0	-1.079966	-1.618527	-2.561726
96	1	0	-2.449520	-1.806340	-0.523774
97	6	0	-3.639306	-1.345196	-2.210766
98	6	0	-4.265583	-0.390708	-3.013561
99	6	0	-3.924265	-2.693116	-2.426980
100	6	0	-5.171217	-0.774473	-3.997593
101	1	0	-4.040347	0.662596	-2.864063
102	6	0	-4.824756	-3.081841	-3.413074
103	1	0	-3.440771	-3.443707	-1.805453
104	6	0	-5.454977	-2.122278	-4.201563
105	1	0	-5.653444	-0.017961	-4.610588
106	1	0	-5.038160	-4.136565	-3.563683
107	1	0	-6.161620	-2.423006	-4.969617

Zero-point correction= 0.858058 (Hartree/Particle)
Thermal correction to Energy= 0.912990
Thermal correction to Enthalpy= 0.913935
Thermal correction to Gibbs Free Energy= 0.766234
Sum of electronic and zero-point Energies= -3970.264639
Sum of electronic and thermal Energies= -3970.209707
Sum of electronic and thermal Enthalpies= -3970.208763
Sum of electronic and thermal Free Energies= -3970.356463

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = - 3973.4944457

INT11a''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	4.244555	-0.066973	-1.012626
2	15	0	1.366756	-1.724647	-0.858064
3	15	0	1.729807	1.394402	0.918666
4	6	0	-0.597126	-3.632553	-1.263883
5	6	0	1.946842	-2.724835	0.569567
6	6	0	2.263909	-2.986215	2.959195
7	6	0	0.512624	-3.004417	-1.840571
8	6	0	2.855349	-4.228229	2.752433
9	6	0	2.513408	-3.990602	0.375581
10	6	0	1.809931	-2.242240	1.872548
11	6	0	2.974402	-4.732199	1.458002
12	6	0	0.903694	-3.345204	-3.133856
13	6	0	0.193978	-4.310740	-3.846012
14	6	0	3.480526	1.013283	0.550624
15	6	0	4.378283	1.826043	-0.217912
16	6	0	1.694019	3.169592	0.449515
17	6	0	5.055899	-1.195329	-2.534310
18	6	0	4.236715	-0.108484	1.028618
19	6	0	5.655071	1.207592	-0.217036
20	6	0	-1.299551	-4.595614	-1.975654
21	6	0	5.569398	0.019022	0.558600
22	6	0	1.672398	3.487958	-0.914699
23	6	0	2.879415	-1.358556	-1.782625
24	6	0	1.651986	4.198102	1.389046
25	6	0	4.323601	-0.103203	-3.079932
26	6	0	4.169741	-1.973708	-1.741537
27	6	0	2.984059	-0.201798	-2.623374
28	6	0	1.697447	1.417576	2.746549
29	6	0	2.866930	1.597328	3.496328
30	6	0	1.593313	5.526663	0.970516
31	6	0	1.620443	4.812110	-1.330592
32	6	0	1.578319	5.835753	-0.384988
33	6	0	-0.906018	-4.936189	-3.269403
34	6	0	0.412813	1.395700	4.796806
35	6	0	0.468195	1.323611	3.407539
36	6	0	1.579144	1.564354	5.536349
37	6	0	2.805769	1.667772	4.883885
38	1	0	2.172168	0.477010	-2.852916
39	1	0	4.727007	0.688350	-3.696490
40	1	0	6.116067	-1.371814	-2.656223
41	1	0	4.439292	-2.834774	-1.146033
42	1	0	3.857478	-0.922408	1.628189
43	1	0	6.360800	-0.701488	0.713780
44	1	0	6.526362	1.559723	-0.752032
45	1	0	4.121585	2.741116	-0.730800
46	1	0	1.343139	-1.279533	2.051680
47	1	0	2.145837	-2.590887	3.963534
48	1	0	3.208819	-4.811391	3.597650
49	1	0	3.417525	-5.709783	1.292787
50	1	0	2.578533	-4.404284	-0.627277
51	1	0	1.757972	-2.855614	-3.592480
52	1	0	0.501178	-4.568151	-4.855436
53	1	0	-1.459842	-5.685732	-3.827175
54	1	0	-2.160900	-5.077680	-1.522099
55	1	0	-0.915417	-3.356271	-0.261884
56	1	0	1.656124	3.970829	2.450216
57	1	0	1.553923	6.319450	1.711213
58	1	0	1.525599	6.871250	-0.707275
59	1	0	1.594609	5.042774	-2.391003
60	1	0	1.681650	2.695468	-1.660319

61	1	0	-0.442598	1.168397	2.840720
62	1	0	-0.546666	1.312289	5.297489
63	1	0	1.533581	1.617933	6.620134
64	1	0	3.719310	1.805489	5.454388
65	1	0	3.826372	1.688679	2.997916
66	17	0	-1.197084	-0.230995	-2.310246
67	45	0	0.073831	0.349720	-0.409825
68	6	0	-2.868225	-0.329811	0.914990
69	6	0	-3.401007	0.772001	0.363030
70	16	0	-1.172987	-0.721206	1.174801
71	6	0	-3.697460	-1.417746	1.518703
72	6	0	-3.856040	-2.637612	0.854027
73	6	0	-4.294938	-1.232614	2.765930
74	6	0	-4.618840	-3.648679	1.424631
75	1	0	-3.392174	-2.769168	-0.119642
76	6	0	-5.052995	-2.250469	3.340654
77	1	0	-4.170067	-0.282316	3.277416
78	6	0	-5.216820	-3.459095	2.671508
79	1	0	-4.750069	-4.589660	0.897840
80	1	0	-5.518603	-2.095940	4.309682
81	1	0	-5.808253	-4.253497	3.117615
82	6	0	-4.889269	0.939779	0.375969
83	8	0	-5.445910	1.909105	0.844842
84	8	0	-5.532324	-0.080237	-0.211150
85	6	0	-6.963900	-0.043243	-0.180733
86	6	0	-7.492136	-0.620282	1.120332
87	1	0	-7.269568	-0.648049	-1.037235
88	1	0	-7.297007	0.987091	-0.326944
89	1	0	-8.586416	-0.664025	1.093326
90	1	0	-7.100343	-1.629693	1.277043
91	1	0	-7.189435	0.005362	1.964429
92	6	0	-1.140305	2.017553	-0.003721
93	6	0	-2.670275	2.001962	-0.127582
94	1	0	-0.886306	2.388089	0.994858
95	1	0	-0.750261	2.744409	-0.723491
96	6	0	-3.161311	2.498013	-1.487033
97	6	0	-3.821130	1.691345	-2.413167
98	6	0	-2.955605	3.843622	-1.806567
99	6	0	-4.261794	2.216176	-3.625437
100	1	0	-3.976300	0.640484	-2.196849
101	6	0	-3.385364	4.370381	-3.019569
102	1	0	-2.455502	4.490136	-1.087492
103	6	0	-4.044954	3.554851	-3.935931
104	1	0	-4.770288	1.568177	-4.333847
105	1	0	-3.216749	5.420519	-3.242759
106	1	0	-4.390090	3.961915	-4.882330
107	1	0	-3.012590	2.779212	0.575215

Zero-point correction=	0.857652 (Hartree/Particle)
Thermal correction to Energy=	0.912039
Thermal correction to Enthalpy=	0.912983
Thermal correction to Gibbs Free Energy=	0.765197
Sum of electronic and zero-point Energies=	-3970.254369
Sum of electronic and thermal Energies=	-3970.199982
Sum of electronic and thermal Enthalpies=	-3970.199038
Sum of electronic and thermal Free Energies=	-3970.346825

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4876861

TS7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.626066	1.537133	-2.990134
2	16	0	2.151888	-0.624912	-1.675334
3	26	0	-4.214211	-0.025453	-0.451270
4	15	0	-1.397208	1.691039	0.440756
5	15	0	-1.142372	-1.645260	-0.695343
6	6	0	-1.436678	4.231634	-0.735904
7	6	0	-1.577149	1.342896	2.230114
8	6	0	-1.587710	-0.290337	4.019111
9	6	0	-0.962092	3.465726	0.333778
10	6	0	-2.060659	0.672609	4.905299
11	6	0	-2.050429	2.306939	3.128218
12	6	0	-1.338270	0.047854	2.691789
13	6	0	-2.284571	1.974186	4.458378
14	6	0	-0.061019	4.035567	1.240054
15	6	0	0.340150	5.359057	1.088259
16	6	0	-2.964893	-1.638274	-0.560575
17	6	0	-3.912195	-1.678714	-1.628832
18	6	0	-0.863615	-2.544078	-2.274607
19	6	0	-5.432380	1.592825	-0.079781
20	6	0	-3.706387	-1.641916	0.668279
21	6	0	-5.217716	-1.706855	-1.066309
22	6	0	-1.029445	5.553744	-0.883153
23	6	0	-5.090620	-1.691528	0.351015
24	6	0	-0.410640	-3.865486	-2.323787
25	6	0	-3.124058	1.645075	-0.111723
26	6	0	-1.079263	-1.849102	-3.471173
27	6	0	-5.009442	1.595733	-1.438423
28	6	0	-4.276381	1.628846	0.742507
29	6	0	-3.591386	1.628045	-1.467490
30	6	0	-0.752578	-2.929437	0.565885

31	6	0	-1.608911	-4.016932	0.791996
32	6	0	-0.875488	-2.480215	-4.693166
33	6	0	-0.196383	-4.487904	-3.551530
34	6	0	-0.435019	-3.801104	-4.737404
35	6	0	-0.143655	6.121220	0.028733
36	6	0	0.792954	-3.849331	2.190117
37	6	0	0.447355	-2.858603	1.272862
38	6	0	-0.064919	-4.920015	2.413879
39	6	0	-1.268100	-5.001126	1.712164
40	1	0	-2.948845	1.594545	-2.338137
41	1	0	-5.653811	1.525522	-2.304278
42	1	0	-6.452550	1.515480	0.271424
43	1	0	-4.266142	1.589189	1.822405
44	1	0	-3.283484	-1.598954	1.662319
45	1	0	-5.903069	-1.665212	1.064366
46	1	0	-6.144837	-1.694053	-1.622988
47	1	0	-3.673438	-1.655584	-2.682743
48	1	0	-0.939465	-0.700625	2.017949
49	1	0	-1.400418	-1.306288	4.354723
50	1	0	-2.249914	0.414813	5.943186
51	1	0	-2.646726	2.731593	5.146928
52	1	0	-2.239351	3.319710	2.785251
53	1	0	0.350007	3.445943	2.051246
54	1	0	1.040828	5.788084	1.798266
55	1	0	0.173523	7.153158	-0.090914
56	1	0	-1.402565	6.136939	-1.719354
57	1	0	-2.107130	3.795614	-1.467135
58	1	0	-1.359887	-0.799058	-3.448160
59	1	0	-1.043513	-1.927842	-5.612724
60	1	0	-0.266808	-4.288705	-5.693252
61	1	0	0.161154	-5.513298	-3.576646
62	1	0	-0.217430	-4.415650	-1.409155
63	1	0	1.114502	-2.021505	1.119055
64	1	0	1.738625	-3.773518	2.718183
65	1	0	0.200156	-5.692871	3.129602
66	1	0	-1.942386	-5.835886	1.879805
67	1	0	-2.542890	-4.096517	0.244282
68	45	0	0.122054	0.391777	-0.713116
69	6	0	2.580314	-0.567885	0.053921
70	6	0	1.742486	0.403808	0.545941
71	6	0	3.679716	-1.303822	0.671307
72	6	0	4.496284	-0.698795	1.640532
73	6	0	3.923518	-2.644083	0.338747
74	6	0	5.493867	-1.421529	2.281344
75	1	0	4.359465	0.353873	1.872558
76	6	0	4.934446	-3.360812	0.971353
77	1	0	3.298598	-3.129667	-0.406529
78	6	0	5.716898	-2.758165	1.953004
79	1	0	6.114997	-0.932575	3.026576
80	1	0	5.103252	-4.399753	0.702994
81	1	0	6.502415	-3.320014	2.449438
82	6	0	1.789074	0.797862	1.982251
83	8	0	1.927951	1.926670	2.404789
84	8	0	1.683301	-0.272873	2.773264
85	6	0	1.863745	-0.052677	4.177114
86	6	0	1.959878	-1.419111	4.820470
87	1	0	1.017138	0.528134	4.555533
88	1	0	2.776184	0.532294	4.326600
89	1	0	2.091256	-1.315939	5.902063
90	1	0	1.052143	-1.999981	4.630343
91	1	0	2.815187	-1.967256	4.412933
92	6	0	1.891974	1.821940	-0.656632
93	6	0	2.574286	1.200006	-1.876824
94	1	0	1.146670	2.565617	-0.959233
95	1	0	2.565032	2.327834	0.037900
96	1	0	2.028924	1.499198	-2.776079
97	6	0	4.048523	1.509002	-1.999670
98	6	0	4.393472	2.846215	-2.232397
99	6	0	5.068391	0.568096	-1.870447
100	6	0	5.725055	3.231727	-2.329078
101	1	0	3.605811	3.588749	-2.337616
102	6	0	6.404154	0.953686	-1.967037
103	1	0	4.834297	-0.475876	-1.689604
104	6	0	6.737799	2.283890	-2.194789
105	1	0	5.971297	4.273657	-2.512027
106	1	0	7.183581	0.205006	-1.860191
107	1	0	7.779527	2.581680	-2.270072

Zero-point correction= 0.856403 (Hartree/Particle)
Thermal correction to Energy= 0.909938
Thermal correction to Enthalpy= 0.910882
Thermal correction to Gibbs Free Energy= 0.767779
Sum of electronic and zero-point Energies= -3970.235916
Sum of electronic and thermal Energies= -3970.182381
Sum of electronic and thermal Enthalpies= -3970.181437
Sum of electronic and thermal Free Energies= -3970.324539

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.451778

TS7a''

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

1	17	0	1.110453	2.620139	1.299811
2	16	0	-2.477046	1.212318	0.743379
3	26	0	3.685819	-0.760736	1.431841
4	15	0	1.774561	0.392913	-1.187864
5	15	0	0.188711	-0.927617	1.710863
6	6	0	2.748459	2.923701	-1.921808
7	6	0	1.834749	-1.115362	-2.226422
8	6	0	1.469786	-3.507958	-2.345196
9	6	0	2.022350	1.801049	-2.332519
10	6	0	2.163815	-3.559482	-3.550781
11	6	0	2.537016	-1.175536	-3.434630
12	6	0	1.297242	-2.289583	-1.696006
13	6	0	2.688874	-2.389634	-4.097551
14	6	0	1.359193	1.831006	-3.565016
15	6	0	1.441355	2.956051	-4.379439
16	6	0	1.884878	-1.300101	2.275686
17	6	0	2.665527	-0.535300	3.194360
18	6	0	-0.695563	-0.394718	3.238912
19	6	0	5.411390	-0.635713	0.317461
20	6	0	2.659465	-2.451730	1.910158
21	6	0	3.892273	-1.220613	3.413784
22	6	0	2.823265	4.047655	-2.738890
23	6	0	3.887815	-2.405387	2.625121
24	6	0	-1.740272	-1.146107	3.788415
25	6	0	3.360949	0.221824	-0.317328
26	6	0	-0.384390	0.847930	3.805828
27	6	0	5.195401	0.572286	1.037977
28	6	0	4.289888	-0.853982	-0.522974
29	6	0	3.936169	1.102868	0.657667
30	6	0	-0.480999	-2.631496	1.506967
31	6	0	-0.151774	-3.660028	2.402724
32	6	0	-1.077692	1.304753	4.920447
33	6	0	-2.438788	-0.677247	4.899118
34	6	0	-2.105023	0.543755	5.473576
35	6	0	2.173744	4.066537	-3.969867
36	6	0	-2.038819	-4.130456	0.412199
37	6	0	-1.430942	-2.880503	0.517649
38	6	0	-1.694603	-5.148739	1.292905
39	6	0	-0.747028	-4.910377	2.289146
40	1	0	3.438427	1.963501	1.081331
41	1	0	5.847308	0.984813	1.796064
42	1	0	6.255957	-1.302601	0.426022
43	1	0	4.144028	-1.703310	-1.174497
44	1	0	2.360364	-3.217042	1.207620
45	1	0	4.697145	-3.117468	2.538134
46	1	0	4.707049	-0.870900	4.032934
47	1	0	2.385808	0.419443	3.615577
48	1	0	0.737677	-2.255043	-0.769915
49	1	0	1.052371	-4.410074	-1.907601
50	1	0	2.296530	-4.507441	-4.063919
51	1	0	3.229646	-2.423519	-5.038503
52	1	0	2.976352	-0.275991	-3.853589
53	1	0	0.751197	0.991411	-3.882749
54	1	0	0.920815	2.963399	-5.332306
55	1	0	2.231408	4.946715	-4.603565
56	1	0	3.388089	4.912856	-2.405346
57	1	0	3.239614	2.935152	-0.957182
58	1	0	0.359664	1.486685	3.338955
59	1	0	-0.824550	2.271888	5.344119
60	1	0	-2.650636	0.908457	6.339006
61	1	0	-3.248051	-1.273184	5.311141
62	1	0	-2.022861	-2.099656	3.357048
63	1	0	-1.703456	-2.099927	-0.177893
64	1	0	-2.788970	-4.290601	-0.355855
65	1	0	-2.166320	-6.123909	1.213055
66	1	0	-0.479496	-5.697459	2.988005
67	1	0	0.562945	-3.478471	3.199215
68	45	0	-0.171506	0.734589	0.011453
69	6	0	-2.751543	0.052552	-0.580168
70	6	0	-1.608236	0.192459	-1.338761
71	6	0	-3.990132	-0.688023	-0.786487
72	6	0	-4.508678	-0.910331	-2.073392
73	6	0	-4.667565	-1.250372	0.306922
74	6	0	-5.643745	-1.689888	-2.258506
75	1	0	-4.026791	-0.451535	-2.932799
76	6	0	-5.810917	-2.017877	0.118623
77	1	0	-4.273700	-1.098674	1.308769
78	6	0	-6.301069	-2.250236	-1.164384
79	1	0	-6.029265	-1.845006	-3.262452
80	1	0	-6.314702	-2.446913	0.980095
81	1	0	-7.192465	-2.852799	-1.310530
82	6	0	-1.434846	-0.540654	-2.626630
83	8	0	-1.169972	-0.033071	-3.697831
84	8	0	-1.632419	-1.851619	-2.477052
85	6	0	-1.602374	-2.638755	-3.674620
86	6	0	-2.052483	-4.031651	-3.293429
87	1	0	-0.586011	-2.625259	-4.079019
88	1	0	-2.270541	-2.182476	-4.411273
89	1	0	-2.039787	-4.683742	-4.172405
90	1	0	-1.390141	-4.455387	-2.532907
91	1	0	-3.070592	-4.002874	-2.892173
92	6	0	-1.306949	2.033472	-1.500779
93	6	0	-2.371147	2.600378	-0.578316

94	1	0	-0.358679	2.576768	-1.429975
95	1	0	-1.559676	2.017652	-2.560896
96	1	0	-3.357864	2.543076	-1.048121
97	6	0	-2.209071	3.967947	0.031313
98	6	0	-1.047416	4.733819	-0.064698
99	6	0	-3.308689	4.503650	0.714205
100	6	0	-0.985338	5.997476	0.517531
101	1	0	-0.171597	4.351494	-0.573197
102	6	0	-3.247837	5.762626	1.296718
103	1	0	-4.223874	3.919979	0.791272
104	6	0	-2.079273	6.515845	1.200213
105	1	0	-0.066431	6.570569	0.440801
106	1	0	-4.112472	6.157134	1.822432
107	1	0	-2.024308	7.500699	1.654911

Zero-point correction= 0.856929 (Hartree/Particle)
Thermal correction to Energy= 0.910330
Thermal correction to Enthalpy= 0.911274
Thermal correction to Gibbs Free Energy= 0.768237
Sum of electronic and zero-point Energies= -3970.225790
Sum of electronic and thermal Energies= -3970.172389
Sum of electronic and thermal Enthalpies= -3970.171444
Sum of electronic and thermal Free Energies= -3970.314481

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4419522

TS8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.937914	-0.617236	2.568178
2	15	0	-2.901141	-0.572854	-0.813491
3	15	0	-0.305280	0.921667	1.049505
4	6	0	-4.197568	-1.251722	-3.214017
5	6	0	-4.012472	0.882028	-0.900375
6	6	0	-4.248023	3.292079	-1.015014
7	6	0	-3.678866	-1.728487	-2.006582
8	6	0	-5.632112	3.163610	-0.956917
9	6	0	-5.407118	0.761399	-0.880972
10	6	0	-3.445228	2.154065	-0.993759
11	6	0	-6.210854	1.896032	-0.899655
12	6	0	-3.735024	-3.095942	-1.731501
13	6	0	-4.312019	-3.973107	-2.645726
14	6	0	-1.537140	0.818870	2.399258
15	6	0	-1.398684	0.159773	3.665242
16	6	0	1.190940	0.451099	2.005413
17	6	0	-4.306188	-2.156786	2.695498
18	6	0	-2.845257	1.404740	2.369629
19	6	0	-2.615967	0.311457	4.381190
20	6	0	-4.780440	-2.128319	-4.120943
21	6	0	-3.505064	1.083852	3.583963
22	6	0	1.337804	-0.896757	2.352688
23	6	0	-3.312510	-1.391669	0.753618
24	6	0	2.152453	1.367481	2.430097
25	6	0	-2.982889	-2.679058	2.646585
26	6	0	-4.516150	-1.371908	1.529940
27	6	0	-2.372997	-2.220510	1.449454
28	6	0	-0.190592	2.759010	0.921948
29	6	0	-0.273489	3.548905	2.077258
30	6	0	3.235184	0.946882	3.199238
31	6	0	2.411679	-1.313703	3.128314
32	6	0	3.363464	-0.389962	3.554495
33	6	0	-4.839139	-3.490900	-3.839402
34	6	0	0.055213	4.782879	-0.393862
35	6	0	-0.030797	3.394521	-0.310619
36	6	0	-0.018089	5.554404	0.760423
37	6	0	-0.183835	4.933421	1.997338
38	1	0	-1.360421	-2.410424	1.116483
39	1	0	-2.508167	-3.280649	3.409663
40	1	0	-5.012194	-2.285343	3.504778
41	1	0	-5.404129	-0.796793	1.311413
42	1	0	-3.271977	1.960712	1.547269
43	1	0	-4.527077	1.337670	3.830156
44	1	0	-2.836578	-0.122082	5.346997
45	1	0	-0.534106	-0.395313	3.998224
46	1	0	-2.365517	2.254618	-1.046812
47	1	0	-3.786679	4.272711	-1.080718
48	1	0	-6.262660	4.047754	-0.972565
49	1	0	-7.291550	1.791112	-0.879236
50	1	0	-5.865256	-0.223405	-0.875721
51	1	0	-3.329590	-3.486049	-0.803068
52	1	0	-4.349869	-5.034966	-2.421374
53	1	0	-5.289422	-4.175860	-4.551918
54	1	0	-5.179754	-1.745515	-5.055273
55	1	0	-4.136227	-0.194819	-3.451547
56	1	0	2.078902	2.412769	2.150644
57	1	0	3.987174	1.669472	3.498785
58	1	0	4.213127	-0.718659	4.145253
59	1	0	2.523942	-2.364312	3.376551
60	1	0	0.610365	-1.621986	2.000460
61	1	0	0.017888	2.809909	-1.221969
62	1	0	0.182952	5.253429	-1.363897
63	1	0	0.051668	6.636274	0.698427

64	1	0	-0.244946	5.528756	2.903344
65	1	0	-0.405775	3.075811	3.045879
66	17	0	-0.953705	-0.674592	-3.356087
67	45	0	-0.603332	-0.084576	-1.059289
68	6	0	2.791024	-1.404594	-0.502882
69	6	0	3.351129	-0.172310	-0.450050
70	16	0	1.160390	-1.661568	-1.095948
71	6	0	3.453859	-2.698190	-0.187596
72	6	0	2.867323	-3.646469	0.653140
73	6	0	4.660709	-3.013849	-0.822353
74	6	0	3.495970	-4.866042	0.891414
75	1	0	1.915058	-3.427804	1.124416
76	6	0	5.283772	-4.232121	-0.591687
77	1	0	5.106278	-2.288418	-1.495737
78	6	0	4.706430	-5.161011	0.273203
79	1	0	3.032424	-5.589092	1.556308
80	1	0	6.220358	-4.460837	-1.091726
81	1	0	5.193250	-6.115064	0.452949
82	6	0	4.558843	0.208608	0.308403
83	8	0	4.926899	1.362286	0.420880
84	8	0	5.182306	-0.814784	0.918123
85	6	0	6.353679	-0.496346	1.668624
86	6	0	7.577218	-0.455680	0.769385
87	1	0	6.430642	-1.296425	2.408962
88	1	0	6.207420	0.458855	2.179304
89	1	0	8.479244	-0.273232	1.363102
90	1	0	7.693804	-1.408487	0.243672
91	1	0	7.478864	0.347270	0.033799
92	6	0	1.423019	0.473484	-1.884914
93	6	0	2.594584	0.980667	-1.067779
94	1	0	1.707874	0.015224	-2.828624
95	1	0	0.723506	1.284779	-2.147238
96	1	0	2.239340	1.647204	-0.274032
97	6	0	3.443468	1.828268	-2.007622
98	6	0	4.210161	1.232217	-3.010399
99	6	0	3.415032	3.219329	-1.917387
100	6	0	4.942934	2.012208	-3.898863
101	1	0	4.236259	0.147795	-3.090750
102	6	0	4.144801	4.002553	-2.806180
103	1	0	2.829434	3.690246	-1.131353
104	6	0	4.911978	3.401247	-3.800387
105	1	0	5.538179	1.534051	-4.671627
106	1	0	4.119064	5.085115	-2.717086
107	1	0	5.485073	4.011123	-4.492656

Zero-point correction=	0.857567 (Hartree/Particle)
Thermal correction to Energy=	0.911814
Thermal correction to Enthalpy=	0.912758
Thermal correction to Gibbs Free Energy=	0.766653
Sum of electronic and zero-point Energies=	-3970.248672
Sum of electronic and thermal Energies=	-3970.194425
Sum of electronic and thermal Enthalpies=	-3970.193481
Sum of electronic and thermal Free Energies=	-3970.339586

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4754629

INT12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.212344	2.791679	-1.973068
2	16	0	2.255506	0.561717	-1.325423
3	26	0	-4.160451	-0.644447	-1.011007
4	15	0	-2.047168	1.486137	0.397494
5	15	0	-0.812028	-1.477463	-0.583520
6	6	0	-2.795343	4.186959	0.024293
7	6	0	-2.364069	0.846211	2.091834
8	6	0	-1.751714	-0.644451	3.902887
9	6	0	-2.011259	3.283903	0.740315
10	6	0	-2.836176	-0.195896	4.648732
11	6	0	-3.421766	1.331329	2.872037
12	6	0	-1.512682	-0.112785	2.637467
13	6	0	-3.661920	0.805658	4.136592
14	6	0	-1.133301	3.759751	1.718564
15	6	0	-1.039390	5.122170	1.975374
16	6	0	-2.587747	-1.914040	-0.719059
17	6	0	-3.277067	-2.253094	-1.926047
18	6	0	-0.227087	-2.186323	-2.188621
19	6	0	-5.744939	0.666714	-1.146046
20	6	0	-3.531865	-2.022188	0.353706
21	6	0	-4.626262	-2.558785	-1.601692
22	6	0	-2.703448	5.551469	0.285852
23	6	0	-4.781806	-2.421570	-0.193727
24	6	0	0.089662	-3.536636	-2.365342
25	6	0	-3.600344	1.225420	-0.495892
26	6	0	-0.131217	-1.320079	-3.284574
27	6	0	-4.940574	0.756279	-2.317375
28	6	0	-4.926845	0.961403	-0.022527
29	6	0	-3.623185	1.104244	-1.924474
30	6	0	-0.279821	-2.728839	0.658740
31	6	0	-0.895766	-3.979405	0.795147
32	6	0	0.282584	-1.793666	-4.527151
33	6	0	0.505311	-4.007476	-3.607314

34	6	0	0.604710	-3.137378	-4.690789
35	6	0	-1.825198	6.021408	1.257042
36	6	0	1.321160	-3.365428	2.361871
37	6	0	0.811927	-2.425063	1.471518
38	6	0	0.716352	-4.612574	2.476532
39	6	0	-0.401866	-4.913362	1.700489
40	1	0	-2.757315	1.224917	-2.562261
41	1	0	-5.263916	0.545758	-3.327645
42	1	0	-6.784644	0.370460	-1.108443
43	1	0	-5.238844	0.908198	1.010068
44	1	0	-3.331095	-1.811518	1.395353
45	1	0	-5.703705	-2.542559	0.358910
46	1	0	-5.405828	-2.807248	-2.308838
47	1	0	-2.846212	-2.240288	-2.917417
48	1	0	-0.654259	-0.440165	2.065302
49	1	0	-1.086676	-1.408598	4.294148
50	1	0	-3.030535	-0.609826	5.633869
51	1	0	-4.490309	1.183417	4.728700
52	1	0	-4.046211	2.137543	2.497378
53	1	0	-0.524345	3.060858	2.287290
54	1	0	-0.352090	5.482922	2.735045
55	1	0	-1.749282	7.086901	1.453243
56	1	0	-3.314344	6.248132	-0.280445
57	1	0	-3.467670	3.828696	-0.748873
58	1	0	-0.368177	-0.265366	-3.159777
59	1	0	0.359602	-1.104515	-5.362546
60	1	0	0.936084	-3.506372	-5.656982
61	1	0	0.753413	-5.058247	-3.728102
62	1	0	0.038282	-4.224164	-1.527722
63	1	0	1.267964	-1.443338	1.410612
64	1	0	2.201676	-3.119110	2.946743
65	1	0	1.108966	-5.348776	3.172100
66	1	0	-0.888428	-5.879535	1.797088
67	1	0	-1.765556	-4.224805	0.192188
68	45	0	-0.226387	0.723557	-0.678149
69	6	0	3.068609	-0.191359	0.095428
70	6	0	3.179968	0.687418	1.104134
71	6	0	3.513078	-1.592956	0.035808
72	6	0	4.444991	-2.097338	0.954728
73	6	0	3.000601	-2.460137	-0.934277
74	6	0	4.789943	-3.442851	0.945313
75	1	0	4.933124	-1.435926	1.662481
76	6	0	3.345380	-3.805779	-0.941815
77	1	0	2.308675	-2.090650	-1.683262
78	6	0	4.229672	-4.307342	0.007363
79	1	0	5.512533	-3.813655	1.666366
80	1	0	2.915256	-4.458320	-1.695362
81	1	0	4.497137	-5.359727	0.005161
82	6	0	3.670364	0.416511	2.481994
83	8	0	4.685332	0.882094	2.950027
84	8	0	2.803622	-0.341530	3.167859
85	6	0	3.124329	-0.614382	4.541476
86	6	0	1.838849	-1.000647	5.242911
87	1	0	3.581448	0.274608	4.982447
88	1	0	3.864636	-1.421934	4.563672
89	1	0	2.041690	-1.211320	6.297644
90	1	0	1.110173	-0.186603	5.184530
91	1	0	1.394618	-1.891355	4.789159
92	6	0	2.728221	2.092449	0.794515
93	6	0	2.788508	2.241234	-0.724167
94	1	0	1.688715	2.227460	1.129916
95	1	0	3.350288	2.840111	1.297079
96	1	0	2.018130	2.923162	-1.086130
97	6	0	4.131124	2.609803	-1.307754
98	6	0	4.158959	3.172572	-2.587899
99	6	0	5.337459	2.412749	-0.630166
100	6	0	5.363911	3.525905	-3.182744
101	1	0	3.220913	3.331814	-3.114852
102	6	0	6.544882	2.766683	-1.227641
103	1	0	5.348314	1.984980	0.368306
104	6	0	6.563186	3.321426	-2.503323
105	1	0	5.366933	3.966582	-4.175356
106	1	0	7.474994	2.608018	-0.689710
107	1	0	7.506585	3.597255	-2.965445

Zero-point correction= 0.859100 (Hartree/Particle)
Thermal correction to Energy= 0.913341
Thermal correction to Enthalpy= 0.914285
Thermal correction to Gibbs Free Energy= 0.768156
Sum of electronic and zero-point Energies= -3970.301390
Sum of electronic and thermal Energies= -3970.247148
Sum of electronic and thermal Enthalpies= -3970.246204
Sum of electronic and thermal Free Energies= -3970.392333

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.5214975

INT12a''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.153340	-0.674990	-2.459552
2	16	0	-0.843465	-2.308835	-1.795944
3	26	0	1.340747	3.839781	-0.167827

4	15	0	1.947486	0.673352	0.559836
5	15	0	-1.164888	1.426291	-0.392505
6	6	0	4.540763	-0.233089	-0.064466
7	6	0	1.463320	0.882365	2.321880
8	6	0	-0.227220	0.693156	4.050346
9	6	0	3.426741	-0.391184	0.762655
10	6	0	0.661395	1.209400	4.986875
11	6	0	2.367539	1.351950	3.283753
12	6	0	0.182828	0.515631	2.730412
13	6	0	1.966689	1.521833	4.603859
14	6	0	3.432633	-1.395962	1.735338
15	6	0	4.544254	-2.219360	1.890812
16	6	0	-0.578962	3.143491	-0.121049
17	6	0	-0.446475	4.153477	-1.124767
18	6	0	-1.983519	1.646389	-2.034317
19	6	0	3.292140	4.489385	-0.052087
20	6	0	-0.224812	3.740806	1.132702
21	6	0	-0.011061	5.353241	-0.499130
22	6	0	5.652299	-1.053244	0.096282
23	6	0	0.119125	5.099801	0.895074
24	6	0	-3.308059	2.069266	-2.178579
25	6	0	2.610022	2.285381	0.058591
26	6	0	-1.224969	1.386405	-3.183844
27	6	0	3.004667	4.052064	-1.375780
28	6	0	3.058678	3.404631	0.834366
29	6	0	2.590176	2.697781	-1.315427
30	6	0	-2.572296	1.411541	0.799541
31	6	0	-3.283532	2.565246	1.153212
32	6	0	-1.786102	1.540189	-4.449155
33	6	0	-3.864144	2.226069	-3.444838
34	6	0	-3.106705	1.958815	-4.582920
35	6	0	5.659143	-2.044220	1.075180
36	6	0	-4.006298	0.113356	2.268608
37	6	0	-2.943496	0.197082	1.374715
38	6	0	-4.709117	1.265396	2.607611
39	6	0	-4.344927	2.490139	2.049731
40	1	0	2.271062	2.069017	-2.136485
41	1	0	3.044044	4.660937	-2.268711
42	1	0	3.581978	5.490162	0.239109
43	1	0	3.127065	3.455852	1.910700
44	1	0	-0.205599	3.236081	2.089146
45	1	0	0.473313	5.800562	1.639034
46	1	0	0.223308	6.280902	-1.003192
47	1	0	-0.613698	4.009409	-2.183021
48	1	0	-0.494030	0.084086	2.005249
49	1	0	-1.243076	0.430365	4.331496
50	1	0	0.348581	1.354819	6.016788
51	1	0	2.675334	1.892796	5.338489
52	1	0	3.396905	1.559307	3.006780
53	1	0	2.570280	-1.533803	2.382402
54	1	0	4.539455	-2.993623	2.652320
55	1	0	6.530381	-2.681076	1.199761
56	1	0	6.513729	-0.920971	-0.551270
57	1	0	4.534615	0.523823	-0.841116
58	1	0	-0.192383	1.052961	-3.092351
59	1	0	-1.186674	1.324773	-5.328423
60	1	0	-3.546168	2.075248	-5.569230
61	1	0	-4.895702	2.553307	-3.541272
62	1	0	-3.919099	2.258415	-1.302358
63	1	0	-2.385549	-0.694993	1.122651
64	1	0	-4.269643	-0.853452	2.685771
65	1	0	-5.537169	1.213264	3.308716
66	1	0	-4.887479	3.392859	2.315573
67	1	0	-3.006692	3.526534	0.730181
68	45	0	0.426917	-0.150344	-0.844818
69	6	0	-1.981310	-2.612757	-0.437285
70	6	0	-1.317601	-3.089015	0.649738
71	6	0	-3.399156	-2.280508	-0.658151
72	6	0	-4.424087	-2.977327	-0.005482
73	6	0	-3.747900	-1.284345	-1.580599
74	6	0	-5.754957	-2.646270	-0.232359
75	1	0	-4.176458	-3.769265	0.686707
76	6	0	-5.076958	-0.949962	-1.797920
77	1	0	-2.977453	-0.751286	-2.127682
78	6	0	-6.086818	-1.625573	-1.118146
79	1	0	-6.536000	-3.194947	0.285384
80	1	0	-5.316379	-0.162016	-2.504809
81	1	0	-7.128045	-1.368848	-1.289826
82	6	0	-1.804081	-3.068312	2.045417
83	8	0	-2.951071	-3.086132	2.446492
84	8	0	-0.748487	-2.949853	2.876580
85	6	0	-1.040888	-2.807687	4.273012
86	6	0	-1.250423	-4.159115	4.932055
87	1	0	-1.923515	-2.172835	4.386359
88	1	0	-0.170818	-2.287844	4.678919
89	1	0	-1.397706	-4.028565	6.009166
90	1	0	-2.135056	-4.650610	4.519379
91	1	0	-0.379363	-4.802929	4.777307
92	6	0	0.144911	-3.382088	0.400569
93	6	0	0.233762	-3.656235	-1.092570
94	1	0	0.754410	-2.506612	0.672639
95	1	0	0.500017	-4.238327	0.982437
96	1	0	-0.364004	-4.551577	-1.305303

97	6	0	1.582737	-3.839398	-1.727200
98	6	0	2.765385	-3.676231	-1.011391
99	6	0	1.648273	-4.254337	-3.060148
100	6	0	3.994545	-3.909186	-1.620692
101	1	0	2.743935	-3.344846	0.020515
102	6	0	2.873467	-4.473664	-3.673829
103	1	0	0.727828	-4.390671	-3.623585
104	6	0	4.053328	-4.300605	-2.952719
105	1	0	4.906016	-3.763308	-1.050172
106	1	0	2.909428	-4.779842	-4.715239
107	1	0	5.013871	-4.470253	-3.430556

Zero-point correction= 0.858720 (Hartree/Particle)
Thermal correction to Energy= 0.912892
Thermal correction to Enthalpy= 0.913836
Thermal correction to Gibbs Free Energy= 0.768608
Sum of electronic and zero-point Energies= -3970.291707
Sum of electronic and thermal Energies= -3970.237535
Sum of electronic and thermal Enthalpies= -3970.236591
Sum of electronic and thermal Free Energies= -3970.381819

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.505928

INT13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	3.409523	-0.189766	-2.678959
2	15	0	3.301999	-0.657050	0.688457
3	15	0	0.716640	0.775078	-0.918046
4	6	0	4.246928	-1.605861	3.135539
5	6	0	4.242968	0.883896	1.027829
6	6	0	4.279458	3.277793	1.392369
7	6	0	4.181709	-1.854799	1.760499
8	6	0	5.667925	3.248831	1.482122
9	6	0	5.637374	0.858537	1.152725
10	6	0	3.571193	2.098448	1.173538
11	6	0	6.345286	2.035514	1.370263
12	6	0	4.797210	-2.993590	1.239654
13	6	0	5.478710	-3.869276	2.082830
14	6	0	1.837540	1.034378	-2.328113
15	6	0	1.711033	0.446180	-3.626925
16	6	0	-0.753696	0.078074	-1.780960
17	6	0	5.036724	-1.427681	-2.938685
18	6	0	3.059240	1.783726	-2.312783
19	6	0	2.851779	0.811142	-4.391245
20	6	0	4.933296	-2.475965	3.971655
21	6	0	3.679119	1.639746	-3.582762
22	6	0	-0.929488	-1.310557	-1.741856
23	6	0	3.863894	-1.152844	-0.966160
24	6	0	-1.672020	0.859616	-2.487603
25	6	0	3.829565	-2.175475	-3.038936
26	6	0	5.066213	-0.802821	-1.663118
27	6	0	3.110217	-2.015794	-1.825490
28	6	0	0.244316	2.502120	-0.504535
29	6	0	0.237524	3.529687	-1.454387
30	6	0	-2.741388	0.261199	-3.146014
31	6	0	-1.999557	-1.905886	-2.402780
32	6	0	-2.910269	-1.120271	-3.102232
33	6	0	5.550660	-3.610358	3.446768
34	6	0	-0.494264	4.085535	1.176571
35	6	0	-0.117171	2.795532	0.814748
36	6	0	-0.508855	5.097813	0.221309
37	6	0	-0.140479	4.819134	-1.093272
38	1	0	2.135217	-2.421426	-1.591862
39	1	0	3.492983	-2.725231	-3.907220
40	1	0	5.776357	-1.305991	-3.718472
41	1	0	5.826146	-0.120481	-1.310086
42	1	0	3.461235	2.322780	-1.465910
43	1	0	4.638960	2.050455	-3.865006
44	1	0	3.069314	0.482380	-5.398254
45	1	0	0.909151	-0.206049	-3.944265
46	1	0	2.487491	2.116192	1.123414
47	1	0	3.741288	4.214585	1.501514
48	1	0	6.221349	4.166942	1.656083
49	1	0	7.426702	2.004156	1.465108
50	1	0	6.167942	-0.088127	1.097027
51	1	0	4.751217	-3.204259	0.175992
52	1	0	5.953045	-4.753649	1.667713
53	1	0	6.083750	-4.292192	4.102906
54	1	0	4.976340	-2.275636	5.037779
55	1	0	3.747888	-0.736720	3.552425
56	1	0	-1.572084	1.939973	-2.507857
57	1	0	-3.457904	0.882453	-3.674379
58	1	0	-3.762529	-1.580784	-3.591738
59	1	0	-2.128506	-2.982648	-2.358107
60	1	0	-0.237167	-1.920919	-1.165516
61	1	0	-0.090143	2.010424	1.567733
62	1	0	-0.784417	4.291250	2.201909
63	1	0	-0.802089	6.105485	0.500730
64	1	0	-0.144223	5.607990	-1.839380
65	1	0	0.536624	3.323826	-2.478423
66	17	0	0.931878	-1.814019	2.880817

67	45	0	1.104281	-0.511375	0.921912
68	6	0	-4.033207	-1.366861	0.582901
69	6	0	-3.954002	-0.051347	0.284148
70	16	0	-2.776794	-1.934578	1.680504
71	6	0	-5.029986	-2.374307	0.159591
72	6	0	-4.617537	-3.580787	-0.411173
73	6	0	-6.393549	-2.154126	0.378986
74	6	0	-5.555778	-4.535156	-0.793824
75	1	0	-3.557938	-3.766088	-0.557561
76	6	0	-7.327841	-3.111587	0.007019
77	1	0	-6.711463	-1.225879	0.842692
78	6	0	-6.911856	-4.302274	-0.587345
79	1	0	-5.223738	-5.464827	-1.246197
80	1	0	-8.383947	-2.931541	0.184876
81	1	0	-7.643651	-5.049586	-0.879390
82	6	0	-4.738044	0.700657	-0.708864
83	8	0	-4.608176	1.896336	-0.890436
84	8	0	-5.574379	-0.061268	-1.433987
85	6	0	-6.399742	0.613020	-2.385598
86	6	0	-7.647034	1.171986	-1.723097
87	1	0	-6.650500	-0.154091	-3.121611
88	1	0	-5.823175	1.406731	-2.868074
89	1	0	-8.305165	1.621114	-2.474234
90	1	0	-8.195880	0.374391	-1.212677
91	1	0	-7.376588	1.940873	-0.994611
92	6	0	-1.902446	-0.336582	1.583594
93	6	0	-2.886196	0.718662	1.044057
94	1	0	-1.478263	-0.093591	2.557390
95	1	0	-1.085734	-0.478105	0.854905
96	1	0	-2.354562	1.368585	0.343232
97	6	0	-3.487045	1.605652	2.125093
98	6	0	-3.907536	1.080650	3.350876
99	6	0	-3.644055	2.973052	1.891054
100	6	0	-4.457053	1.908825	4.325181
101	1	0	-3.803618	0.017077	3.549685
102	6	0	-4.192591	3.802432	2.865090
103	1	0	-3.347028	3.381477	0.930689
104	6	0	-4.598932	3.273421	4.087150
105	1	0	-4.773585	1.484276	5.273550
106	1	0	-4.307002	4.864395	2.665941
107	1	0	-5.024280	3.920110	4.849276

Zero-point correction= 0.859410 (Hartree/Particle)
Thermal correction to Energy= 0.913660
Thermal correction to Enthalpy= 0.914604
Thermal correction to Gibbs Free Energy= 0.766903
Sum of electronic and zero-point Energies= -3970.292291
Sum of electronic and thermal Energies= -3970.238041
Sum of electronic and thermal Enthalpies= -3970.237096
Sum of electronic and thermal Free Energies= -3970.384797

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.5180352

TS9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	3.395577	-1.177104	-1.806624
2	15	0	0.398002	-1.905255	-0.263731
3	15	0	2.080837	1.307253	0.317340
4	6	0	-1.875210	-3.414632	0.280739
5	6	0	1.162386	-2.738430	1.188027
6	6	0	2.685254	-2.603578	3.071839
7	6	0	-0.921961	-3.095127	-0.693361
8	6	0	2.544104	-3.970097	3.294205
9	6	0	1.031885	-4.113286	1.413621
10	6	0	1.996666	-2.002800	2.024421
11	6	0	1.717908	-4.721408	2.461449
12	6	0	-1.008474	-3.682569	-1.953624
13	6	0	-2.044242	-4.566579	-2.243053
14	6	0	3.413154	0.567510	-0.695782
15	6	0	3.717506	0.830861	-2.066493
16	6	0	2.113409	3.100043	-0.132769
17	6	0	3.535286	-3.084600	-2.560969
18	6	0	4.390123	-0.367491	-0.215384
19	6	0	4.881714	0.092486	-2.415385
20	6	0	-2.908111	-4.294850	-0.011163
21	6	0	5.297846	-0.645352	-1.272692
22	6	0	1.811280	3.499175	-1.441749
23	6	0	1.670538	-2.216774	-1.514640
24	6	0	2.282718	4.088689	0.843787
25	6	0	2.861152	-2.239129	-3.487279
26	6	0	2.802133	-3.081786	-1.347158
27	6	0	1.712724	-1.702702	-2.850715
28	6	0	2.928183	1.384069	1.956852
29	6	0	4.261491	1.807063	2.052115
30	6	0	2.177422	5.437916	0.515506
31	6	0	1.717180	4.847765	-1.767655
32	6	0	1.901467	5.823007	-0.791654
33	6	0	-2.998055	-4.868399	-1.278247
34	6	0	2.860878	1.189536	4.375183
35	6	0	2.237949	1.082922	3.132630
36	6	0	4.185496	1.603885	4.455153

37	6	0	4.884832	1.913807	3.288906
38	1	0	1.015514	-0.985030	-3.257930
39	1	0	3.197490	-1.996500	-4.486301
40	1	0	4.473456	-3.595528	-2.730673
41	1	0	3.070304	-3.601901	-0.438683
42	1	0	4.424011	-0.793123	0.778075
43	1	0	6.123662	-1.342246	-1.229246
44	1	0	5.335564	0.058145	-3.396308
45	1	0	3.142772	1.449581	-2.738036
46	1	0	2.108176	-0.943865	1.857159
47	1	0	3.319476	-1.996859	3.712192
48	1	0	3.071951	-4.449078	4.113692
49	1	0	1.603058	-5.788509	2.626560
50	1	0	0.399588	-4.715509	0.770481
51	1	0	-0.279166	-3.443496	-2.719785
52	1	0	-2.107898	-5.012718	-3.230864
53	1	0	-3.807672	-5.554599	-1.509391
54	1	0	-3.645673	-4.526726	0.751448
55	1	0	-1.807548	-2.979319	1.272801
56	1	0	2.492841	3.817566	1.872469
57	1	0	2.308925	6.187624	1.290083
58	1	0	1.815704	6.875378	-1.045068
59	1	0	1.481167	5.132265	-2.788679
60	1	0	1.581033	2.756514	-2.195286
61	1	0	1.212900	0.731340	3.084801
62	1	0	2.306713	0.942529	5.275540
63	1	0	4.673822	1.687895	5.421406
64	1	0	5.918392	2.242138	3.344377
65	1	0	4.810669	2.061044	1.150451
66	45	0	-0.268161	0.354933	0.060925
67	17	0	-0.219443	0.949271	-2.290507
68	6	0	-2.581148	-0.352869	1.249878
69	6	0	-2.192476	-0.186220	-0.023026
70	16	0	-1.148880	-0.067795	2.268333
71	6	0	-3.907016	-0.665186	1.809453
72	6	0	-4.812490	-1.447206	1.080142
73	6	0	-4.291150	-0.183391	3.065338
74	6	0	-6.076982	-1.718001	1.590163
75	1	0	-4.514640	-1.860698	0.121475
76	6	0	-5.556479	-0.457436	3.573526
77	1	0	-3.592055	0.415122	3.644182
78	6	0	-6.455859	-1.223434	2.836184
79	1	0	-6.766997	-2.326059	1.012098
80	1	0	-5.840732	-0.069453	4.547471
81	1	0	-7.443593	-1.437945	3.233432
82	6	0	-3.000635	-0.342305	-1.260238
83	8	0	-2.928692	-1.286673	-2.015927
84	8	0	-3.835200	0.683703	-1.433169
85	6	0	-4.625689	0.678422	-2.628182
86	6	0	-3.809926	1.098797	-3.837607
87	1	0	-5.420677	1.395744	-2.415843
88	1	0	-5.057684	-0.317327	-2.766464
89	1	0	-4.461068	1.165422	-4.716682
90	1	0	-3.351395	2.074775	-3.659071
91	1	0	-3.017713	0.373978	-4.035827
92	6	0	-0.991265	2.290413	1.928573
93	6	0	-1.133444	2.533494	0.561413
94	1	0	-1.814923	2.458733	2.613146
95	1	0	-0.006509	2.382465	2.376030
96	1	0	-0.258673	2.910771	0.044695
97	6	0	-2.411740	2.990681	-0.021102
98	6	0	-3.642626	2.853765	0.630945
99	6	0	-2.383590	3.651980	-1.254153
100	6	0	-4.806264	3.363347	0.070456
101	1	0	-3.709649	2.316128	1.572124
102	6	0	-3.547519	4.164138	-1.815581
103	1	0	-1.435524	3.753901	-1.774558
104	6	0	-4.766122	4.022857	-1.155975
105	1	0	-5.751515	3.234291	0.590009
106	1	0	-3.501859	4.675778	-2.773197
107	1	0	-5.675884	4.425015	-1.592977

Zero-point correction= 0.857450 (Hartree/Particle)
Thermal correction to Energy= 0.911091
Thermal correction to Enthalpy= 0.912035
Thermal correction to Gibbs Free Energy= 0.770675
Sum of electronic and zero-point Energies= -3970.239030
Sum of electronic and thermal Energies= -3970.185390
Sum of electronic and thermal Enthalpies= -3970.184445
Sum of electronic and thermal Free Energies= -3970.325805

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.5180352

TS10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.602772	1.038462	2.367613
2	6	0	-4.156248	0.600639	-0.264667
3	6	0	-4.924423	-0.370231	0.386478
4	6	0	-4.762495	1.415355	-1.227077
5	6	0	-6.266342	-0.537414	0.062180
6	1	0	-4.455339	-0.999248	1.137704

7	6	0	-6.106576	1.254041	-1.542316
8	1	0	-4.175460	2.181801	-1.726444
9	6	0	-6.861186	0.272681	-0.902466
10	1	0	-6.850159	-1.301988	0.566222
11	1	0	-6.566636	1.897967	-2.286422
12	1	0	-7.910894	0.144938	-1.150031
13	6	0	-1.743462	0.866576	-2.264756
14	8	0	-1.155274	1.582256	-3.058322
15	8	0	-2.530020	-0.145102	-2.674486
16	6	0	-2.691952	-0.312790	-4.088719
17	6	0	-3.789955	0.588262	-4.624068
18	1	0	-2.948664	-1.368443	-4.205192
19	1	0	-1.736050	-0.120558	-4.580759
20	1	0	-3.950361	0.388362	-5.688821
21	1	0	-4.727299	0.413006	-4.087967
22	1	0	-3.507577	1.638625	-4.510323
23	26	0	3.416426	-1.977007	0.321916
24	15	0	1.759572	0.659762	-1.080936
25	15	0	-0.059202	-1.625818	1.096986
26	6	0	3.410162	2.927242	-0.925481
27	6	0	1.363822	-0.215166	-2.643987
28	6	0	0.235371	-2.077938	-3.709675
29	6	0	2.360445	2.309977	-1.614568
30	6	0	0.871922	-1.784492	-4.911816
31	6	0	2.006089	0.068980	-3.853197
32	6	0	0.480324	-1.291084	-2.589495
33	6	0	1.753963	-0.707154	-4.980342
34	6	0	1.693931	3.021118	-2.619853
35	6	0	2.080282	4.321076	-2.932651
36	6	0	1.554161	-2.500076	1.042947
37	6	0	2.534894	-2.569288	2.079664
38	6	0	-0.644399	-1.946000	2.826938
39	6	0	5.120773	-1.616407	-0.784542
40	6	0	1.984401	-3.384797	-0.004296
41	6	0	3.534162	-3.502835	1.691711
42	6	0	3.787981	4.229386	-1.238732
43	6	0	3.192336	-4.011288	0.407152
44	6	0	-1.814668	-2.680597	3.055281
45	6	0	3.300674	-0.198667	-0.643052
46	6	0	0.036261	-1.417771	3.928776
47	6	0	5.191987	-0.931053	0.460178
48	6	0	3.966054	-1.163919	-1.472706
49	6	0	4.078666	-0.057795	0.554439
50	6	0	-1.088951	-2.861953	0.188785
51	6	0	-0.903199	-4.238171	0.392646
52	6	0	-0.422898	-1.648040	5.221885
53	6	0	-2.272690	-2.904087	4.349686
54	6	0	-1.574889	-2.395885	5.440055
55	6	0	3.125121	4.929385	-2.242978
56	6	0	-2.945381	-3.372871	-1.286016
57	6	0	-2.126057	-2.446358	-0.642567
58	6	0	-2.740403	-4.733304	-1.094268
59	6	0	-1.717807	-5.163132	-0.247193
60	1	0	3.800142	0.542508	1.407462
61	1	0	5.930765	-1.091971	1.233546
62	1	0	5.796176	-2.388438	-1.127535
63	1	0	3.620045	-1.524996	-2.429928
64	1	0	1.475222	-3.545887	-0.944162
65	1	0	3.778271	-4.702891	-0.182731
66	1	0	4.427265	-3.738948	2.253964
67	1	0	2.536626	-1.982131	2.985083
68	1	0	-0.040266	-1.509746	-1.667905
69	1	0	-0.464139	-2.905826	-3.634772
70	1	0	0.682382	-2.389207	-5.793871
71	1	0	2.254339	-0.472457	-5.915103
72	1	0	2.711552	0.891236	-3.916710
73	1	0	0.864237	2.562964	-3.149828
74	1	0	1.555890	4.859918	-3.716158
75	1	0	3.420213	5.946079	-2.484729
76	1	0	4.602934	4.696227	-0.693853
77	1	0	3.931369	2.397843	-0.135548
78	1	0	0.898248	-0.780708	3.778508
79	1	0	0.122072	-1.224197	6.060071
80	1	0	-1.933372	-2.570525	6.450320
81	1	0	-3.183987	-3.475476	4.500531
82	1	0	-2.388978	-3.077278	2.226880
83	1	0	-2.297932	-1.395712	-0.810333
84	1	0	-3.745871	-3.013173	-1.925574
85	1	0	-3.376280	-5.460110	-1.591598
86	1	0	-1.558697	-6.224153	-0.079077
87	1	0	-0.127004	-4.588754	1.064968
88	45	0	-0.034664	0.770033	0.515139
89	6	0	-2.727359	0.763025	0.061305
90	6	0	-1.673148	0.957241	-0.793872
91	16	0	-2.138282	0.727833	1.688025
92	6	0	-0.940240	2.900344	-0.453166
93	6	0	0.011603	3.069759	0.560272
94	1	0	-0.617688	2.938030	-1.486061
95	1	0	-1.951252	3.246503	-0.271584
96	1	0	1.044614	3.151841	0.242513
97	6	0	-0.253496	3.756812	1.844193
98	6	0	0.846599	4.248930	2.556210
99	6	0	-1.535867	4.024821	2.338541

100	6	0	0.675799	4.976686	3.728361
101	1	0	1.846752	4.044404	2.186979
102	6	0	-1.708489	4.749822	3.510232
103	1	0	-2.410431	3.644153	1.822532
104	6	0	-0.603747	5.228087	4.212740
105	1	0	1.545875	5.342063	4.266110
106	1	0	-2.712468	4.938723	3.879265
107	1	0	-0.741932	5.792661	5.130386

Zero-point correction= 0.856707 (Hartree/Particle)
Thermal correction to Energy= 0.911257
Thermal correction to Enthalpy= 0.912202
Thermal correction to Gibbs Free Energy= 0.767527
Sum of electronic and zero-point Energies= -3970.245068
Sum of electronic and thermal Energies= -3970.190518
Sum of electronic and thermal Enthalpies= -3970.189573
Sum of electronic and thermal Free Energies= -3970.334248

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4597366

INT14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	3.367621	-0.889941	-1.992170
2	15	0	0.469238	-1.920801	-0.387734
3	15	0	1.985374	1.256163	0.420502
4	6	0	-1.927577	-3.411363	-0.283593
5	6	0	1.199000	-2.591507	1.169603
6	6	0	3.070454	-2.854134	2.694303
7	6	0	-0.660632	-3.298021	-0.865547
8	6	0	2.250724	-3.495371	3.616067
9	6	0	0.381891	-3.232404	2.108586
10	6	0	2.544559	-2.392272	1.492010
11	6	0	0.901586	-3.673674	3.321787
12	6	0	-0.256702	-4.273658	-1.781627
13	6	0	-1.097493	-5.335229	-2.102859
14	6	0	3.282244	0.778538	-0.780805
15	6	0	3.313694	1.136831	-2.167181
16	6	0	2.035404	3.103931	0.377357
17	6	0	3.632235	-2.748331	-2.848102
18	6	0	4.474464	0.023758	-0.518203
19	6	0	4.515268	0.633731	-2.734241
20	6	0	-2.761449	-4.478992	-0.594033
21	6	0	5.228643	-0.060617	-1.719469
22	6	0	1.798298	3.783743	-0.823559
23	6	0	1.783449	-2.110293	-1.620000
24	6	0	2.140306	3.851195	1.556257
25	6	0	2.813834	-1.928880	-3.675814
26	6	0	2.995668	-2.876753	-1.586648
27	6	0	1.673513	-1.539006	-2.929144
28	6	0	2.811779	0.944396	2.030975
29	6	0	4.102715	1.428689	2.289697
30	6	0	2.037560	5.240211	1.530427
31	6	0	1.704125	5.170773	-0.847676
32	6	0	1.825556	5.905654	0.328465
33	6	0	-2.349901	-5.444327	-1.507619
34	6	0	2.705047	0.119296	4.307246
35	6	0	2.123956	0.290263	3.051608
36	6	0	3.987340	0.594985	4.550045
37	6	0	4.688638	1.248789	3.535631
38	1	0	0.885802	-0.869817	-3.246320
39	1	0	3.048368	-1.606743	-4.681234
40	1	0	4.594730	-3.164551	-3.113419
41	1	0	3.370233	-3.442562	-0.746525
42	1	0	4.759927	-0.400586	0.433808
43	1	0	6.160028	-0.595838	-1.844421
44	1	0	4.798144	0.710127	-3.775223
45	1	0	2.516815	1.623576	-2.708099
46	1	0	3.189682	-1.859914	0.804853
47	1	0	4.119719	-2.684632	2.917338
48	1	0	2.658112	-3.851899	4.557565
49	1	0	0.248725	-4.171952	4.032496
50	1	0	-0.665425	-3.412647	1.890821
51	1	0	0.715672	-4.209451	-2.257022
52	1	0	-0.768124	-6.078508	-2.822975
53	1	0	-3.005529	-6.272400	-1.760934
54	1	0	-3.741688	-4.541123	-0.131040
55	1	0	-2.284194	-2.651885	0.400980
56	1	0	2.299071	3.356640	2.508552
57	1	0	2.122227	5.798464	2.458127
58	1	0	1.741956	6.988129	0.308604
59	1	0	1.519414	5.675335	-1.791264
60	1	0	1.632812	3.231157	-1.739091
61	1	0	1.142123	-0.127282	2.858674
62	1	0	2.156149	-0.405213	5.083016
63	1	0	4.444801	0.459275	5.525719
64	1	0	5.689205	1.628238	3.720444
65	1	0	4.642699	1.963388	1.513534
66	45	0	-0.344819	0.429328	0.034949
67	17	0	-0.169697	1.243238	-2.230319
68	6	0	-2.739804	-0.316906	1.083130
69	6	0	-2.275698	-0.094081	-0.151954

70	16	0	-1.327560	-0.010303	2.174987
71	6	0	-4.043254	-0.747631	1.613604
72	6	0	-5.230865	-0.359475	0.978038
73	6	0	-4.118144	-1.568203	2.745742
74	6	0	-6.458885	-0.798103	1.460807
75	1	0	-5.180005	0.299160	0.116846
76	6	0	-5.349119	-1.999416	3.227880
77	1	0	-3.204183	-1.876460	3.247359
78	6	0	-6.524059	-1.617814	2.585258
79	1	0	-7.371680	-0.488506	0.960121
80	1	0	-5.389622	-2.638460	4.105239
81	1	0	-7.485409	-1.954603	2.961792
82	6	0	-2.960839	-0.254960	-1.458766
83	8	0	-2.796741	-1.200445	-2.194878
84	8	0	-3.750831	0.788842	-1.727737
85	6	0	-4.351000	0.839370	-3.030412
86	6	0	-3.366540	1.343553	-4.068703
87	1	0	-5.184761	1.533116	-2.903906
88	1	0	-4.734398	-0.152258	-3.286503
89	1	0	-3.876607	1.469507	-5.030390
90	1	0	-2.950747	2.303907	-3.753091
91	1	0	-2.543189	0.636709	-4.191648
92	6	0	-1.138343	2.297937	0.795229
93	6	0	-1.293782	1.857455	2.233094
94	1	0	-0.298757	2.979811	0.694648
95	1	0	-2.162017	2.227443	2.784499
96	1	0	-0.388737	2.069698	2.811715
97	6	0	-2.331539	2.910307	0.139800
98	6	0	-3.637644	2.782884	0.626851
99	6	0	-2.139637	3.693560	-1.007575
100	6	0	-4.711760	3.389808	-0.016833
101	1	0	-3.841309	2.183310	1.508424
102	6	0	-3.209546	4.296349	-1.655668
103	1	0	-1.134460	3.807491	-1.400007
104	6	0	-4.506430	4.143672	-1.166970
105	1	0	-5.713522	3.265049	0.386123
106	1	0	-3.030020	4.890800	-2.547635
107	1	0	-5.343953	4.618298	-1.670778

Zero-point correction=	0.858242 (Hartree/Particle)
Thermal correction to Energy=	0.912833
Thermal correction to Enthalpy=	0.913777
Thermal correction to Gibbs Free Energy=	0.769252
Sum of electronic and zero-point Energies=	-3970.257251
Sum of electronic and thermal Energies=	-3970.202660
Sum of electronic and thermal Enthalpies=	-3970.201715
Sum of electronic and thermal Free Energies=	-3970.346241

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4741265

INT15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.680530	0.172323	-2.458605
2	6	0	-2.743029	-2.780093	0.140585
3	6	0	-3.773908	-2.176436	-0.586463
4	6	0	-3.068303	-3.671389	1.170997
5	6	0	-5.102055	-2.421319	-0.260801
6	1	0	-3.524353	-1.499945	-1.397061
7	6	0	-4.396148	-3.932632	1.481646
8	1	0	-2.277105	-4.175756	1.718108
9	6	0	-5.416508	-3.296678	0.775035
10	1	0	-5.891094	-1.925819	-0.817897
11	1	0	-4.636259	-4.636489	2.272979
12	1	0	-6.454942	-3.493983	1.024571
13	6	0	-0.373832	-2.323598	2.154948
14	8	0	0.433720	-2.710150	2.980537
15	8	0	-1.465844	-1.628039	2.495926
16	6	0	-1.689964	-1.399965	3.893891
17	6	0	-2.360320	-2.595156	4.545909
18	1	0	-2.331223	-0.517529	3.918567
19	1	0	-0.737575	-1.158455	4.369586
20	1	0	-2.570284	-2.372613	5.597348
21	1	0	-3.303985	-2.829387	4.043890
22	1	0	-1.706989	-3.471211	4.506013
23	26	0	1.072789	3.603130	-0.504835
24	15	0	1.729232	0.517066	1.008232
25	15	0	-1.398797	1.114773	-0.991533
26	6	0	4.557618	0.409825	1.166548
27	6	0	0.876854	0.886848	2.600072
28	6	0	-1.053547	1.926976	3.644771
29	6	0	3.345120	-0.159791	1.559593
30	6	0	-0.448536	1.813802	4.893930
31	6	0	1.476486	0.777244	3.857579
32	6	0	-0.393317	1.458612	2.516013
33	6	0	0.812174	1.231846	4.995659
34	6	0	3.362169	-1.331305	2.331411
35	6	0	4.569082	-1.910746	2.704469
36	6	0	-0.732971	2.815395	-1.163906
37	6	0	0.039144	3.312222	-2.257377
38	6	0	-2.236667	0.839815	-2.620876
39	6	0	2.538943	4.491095	0.632912

40	6	0	-0.930280	3.908259	-0.254967
41	6	0	0.281639	4.696467	-2.042970
42	6	0	5.765248	-0.180264	1.535078
43	6	0	-0.318416	5.066908	-0.807468
44	6	0	-3.628452	0.767736	-2.752057
45	6	0	2.161200	2.214193	0.519484
46	6	0	-1.447737	0.611561	-3.755633
47	6	0	3.083889	4.014111	-0.592614
48	6	0	1.980287	3.387530	1.326131
49	6	0	2.855529	2.616406	-0.669814
50	6	0	-2.862574	1.448015	0.083957
51	6	0	-3.700402	2.559005	-0.096986
52	6	0	-2.036491	0.353490	-4.988582
53	6	0	-4.214373	0.496870	-3.986617
54	6	0	-3.421935	0.296035	-5.111198
55	6	0	5.774764	-1.339748	2.302499
56	6	0	-4.323975	0.686748	1.864250
57	6	0	-3.188709	0.521124	1.072364
58	6	0	-5.142528	1.794919	1.682347
59	6	0	-4.825787	2.733827	0.699465
60	1	0	3.092366	1.966843	-1.498791
61	1	0	3.536822	4.619589	-1.366009
62	1	0	2.507611	5.521963	0.958826
63	1	0	1.475165	3.431207	2.279915
64	1	0	-1.450514	3.858596	0.691277
65	1	0	-0.267894	6.040193	-0.338595
66	1	0	0.871813	5.338512	-2.682538
67	1	0	0.413288	2.722418	-3.080843
68	1	0	-0.865153	1.563587	1.551383
69	1	0	-2.041282	2.367238	3.539862
70	1	0	-0.955065	2.176470	5.783564
71	1	0	1.292567	1.138575	5.965012
72	1	0	2.468494	0.353259	3.959749
73	1	0	2.429905	-1.801398	2.636383
74	1	0	4.564015	-2.818386	3.300381
75	1	0	6.717055	-1.799935	2.584390
76	1	0	6.699623	0.273056	1.218080
77	1	0	4.568681	1.316455	0.572336
78	1	0	-0.366126	0.596516	-3.667431
79	1	0	-1.402762	0.179143	-5.853033
80	1	0	-3.879979	0.086829	-6.073466
81	1	0	-5.296676	0.443505	-4.064144
82	1	0	-4.272690	0.914858	-1.892606
83	1	0	-2.544263	-0.331214	1.242936
84	1	0	-4.564232	-0.060945	2.614780
85	1	0	-6.027658	1.929950	2.297357
86	1	0	-5.463226	3.599860	0.547208
87	1	0	-3.476508	3.284783	-0.872892
88	45	0	0.529437	-0.812715	-0.569444
89	6	0	-1.327700	-2.556450	-0.223694
90	6	0	-0.222766	-2.526019	0.688337
91	16	0	-0.893279	-2.298754	-1.846954
92	6	0	1.034776	-3.323986	0.276200
93	6	0	1.950469	-2.366694	-0.451871
94	1	0	1.502149	-3.715788	1.183766
95	1	0	0.731367	-4.171682	-0.343593
96	1	0	2.698529	-1.979393	0.227884
97	6	0	2.657618	-2.794264	-1.691671
98	6	0	3.933472	-2.261696	-1.923407
99	6	0	2.161753	-3.726628	-2.608794
100	6	0	4.682765	-2.634225	-3.031156
101	1	0	4.332530	-1.533541	-1.220930
102	6	0	2.910603	-4.105168	-3.718621
103	1	0	1.174783	-4.154288	-2.468750
104	6	0	4.172250	-3.559574	-3.938195
105	1	0	5.666009	-2.199544	-3.188153
106	1	0	2.503133	-4.830448	-4.417732
107	1	0	4.752917	-3.854727	-4.807666

Zero-point correction= 0.859918 (Hartree/Particle)
Thermal correction to Energy= 0.913278
Thermal correction to Enthalpy= 0.914222
Thermal correction to Gibbs Free Energy= 0.774172
Sum of electronic and zero-point Energies= -3970.280681
Sum of electronic and thermal Energies= -3970.227321
Sum of electronic and thermal Enthalpies= -3970.226377
Sum of electronic and thermal Free Energies= -3970.366427

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4939101

INT16a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.037847	1.883518	2.268269
2	15	0	0.533072	2.132529	-0.165028
3	15	0	-2.551344	-0.965884	0.218174
4	6	0	0.827372	3.326499	-2.705375
5	6	0	2.142334	2.087228	0.696830
6	6	0	3.483770	1.432392	2.599923
7	6	0	0.745386	3.526387	-1.328344
8	6	0	4.613988	1.981217	2.000787
9	6	0	3.283353	2.628533	0.097485

10	6	0	2.256843	1.471765	1.948192
11	6	0	4.512916	2.570252	0.745921
12	6	0	0.887713	4.818959	-0.809845
13	6	0	1.117876	5.893168	-1.660341
14	6	0	-2.663901	-0.050584	1.796113
15	6	0	-3.741439	0.711334	2.342017
16	6	0	-4.201639	-0.796531	-0.544210
17	6	0	-1.633705	3.803348	2.884472
18	6	0	-1.619611	-0.070697	2.781557
19	6	0	-3.369880	1.142721	3.643771
20	6	0	1.064094	4.403671	-3.555800
21	6	0	-2.063421	0.649663	3.917362
22	6	0	-4.749802	0.472821	-0.763961
23	6	0	-0.643771	2.825515	1.041392
24	6	0	-4.898173	-1.925426	-0.986725
25	6	0	-2.576902	3.823023	1.818820
26	6	0	-0.443859	3.191093	2.410705
27	6	0	-1.979485	3.216200	0.688833
28	6	0	-2.512636	-2.699418	0.782058
29	6	0	-3.258555	-3.128885	1.885120
30	6	0	-6.130349	-1.787049	-1.619620
31	6	0	-5.987675	0.605079	-1.382708
32	6	0	-6.681025	-0.523879	-1.812393
33	6	0	1.210726	5.685160	-3.035331
34	6	0	-1.746357	-4.961901	0.427801
35	6	0	-1.751890	-3.619225	0.059600
36	6	0	-2.489986	-5.386279	1.524140
37	6	0	-3.244527	-4.468584	2.255059
38	1	0	-2.429299	3.054833	-0.280853
39	1	0	-3.594128	4.185917	1.876588
40	1	0	-1.805010	4.147209	3.895620
41	1	0	0.453460	3.024305	2.988161
42	1	0	-0.660659	-0.557581	2.665438
43	1	0	-1.485935	0.839994	4.811860
44	1	0	-3.963001	1.774349	4.291272
45	1	0	-4.672169	0.937032	1.841499
46	1	0	1.387977	1.005074	2.401665
47	1	0	3.562391	0.956390	3.572504
48	1	0	5.573017	1.937914	2.508221
49	1	0	5.392267	2.987238	0.264644
50	1	0	3.216849	3.101939	-0.876537
51	1	0	0.820167	4.984027	0.261913
52	1	0	1.225650	6.892379	-1.249295
53	1	0	1.391879	6.524072	-3.700828
54	1	0	1.123945	4.237855	-4.626822
55	1	0	0.678552	2.337773	-3.119936
56	1	0	-4.481780	-2.916200	-0.834944
57	1	0	-6.661223	-2.672182	-1.957408
58	1	0	-7.644352	-0.417439	-2.302366
59	1	0	-6.403511	1.595078	-1.543700
60	1	0	-4.199958	1.359037	-0.468405
61	1	0	-1.152014	-3.284853	-0.778426
62	1	0	-1.148943	-5.667233	-0.141651
63	1	0	-2.479932	-6.432725	1.815536
64	1	0	-3.822152	-4.798433	3.113538
65	1	0	-3.850149	-2.414964	2.451974
66	45	0	-0.554805	0.230603	-0.707122
67	17	0	-1.992614	1.521356	-2.205136
68	6	0	2.379824	-1.296244	0.080587
69	6	0	2.890945	-0.730970	-1.041758
70	16	0	0.707831	-1.271295	0.577772
71	6	0	3.193908	-2.171509	0.976175
72	6	0	3.193066	-2.018097	2.364484
73	6	0	3.921832	-3.228978	0.420782
74	6	0	3.945637	-2.863206	3.172257
75	1	0	2.601532	-1.225475	2.808161
76	6	0	4.665188	-4.083236	1.227394
77	1	0	3.906186	-3.376259	-0.655634
78	6	0	4.688310	-3.897096	2.607244
79	1	0	3.946592	-2.718008	4.248940
80	1	0	5.223889	-4.898395	0.776377
81	1	0	5.270948	-4.560962	3.239287
82	6	0	4.354991	-0.597595	-1.266586
83	8	0	4.860739	-0.502359	-2.369510
84	8	0	5.065382	-0.492359	-0.130924
85	6	0	6.481321	-0.367591	-0.264124
86	6	0	7.145039	-1.723827	-0.429376
87	1	0	6.797646	0.117750	0.662498
88	1	0	6.706704	0.286904	-1.110387
89	1	0	8.233210	-1.605118	-0.470802
90	1	0	6.891969	-2.379027	0.409119
91	1	0	6.814034	-2.194564	-1.359224
92	6	0	0.614811	-0.346247	-2.331789
93	6	0	2.113107	-0.137831	-2.196665
94	1	0	2.309183	0.942784	-2.231912
95	1	0	2.583783	-0.527583	-3.111328
96	1	0	0.233388	0.364991	-3.066797
97	6	0	0.100982	-1.702153	-2.685963
98	6	0	-1.208124	-1.820752	-3.185067
99	6	0	0.868770	-2.869079	-2.560180
100	6	0	-1.733741	-3.062107	-3.529547
101	1	0	-1.814733	-0.925582	-3.292073
102	6	0	0.345803	-4.107151	-2.915532

103	1	0	1.882748	-2.805220	-2.180705
104	6	0	-0.959082	-4.211365	-3.396373
105	1	0	-2.750663	-3.126939	-3.905311
106	1	0	0.960734	-4.996944	-2.814307
107	1	0	-1.366822	-5.181244	-3.666060

Zero-point correction= 0.858286 (Hartree/Particle)
Thermal correction to Energy= 0.912357
Thermal correction to Enthalpy= 0.913301
Thermal correction to Gibbs Free Energy= 0.769180
Sum of electronic and zero-point Energies= -3970.291170
Sum of electronic and thermal Energies= -3970.237100
Sum of electronic and thermal Enthalpies= -3970.236156
Sum of electronic and thermal Free Energies= -3970.380277

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.5096906

TS11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	3.880433	-0.727213	-1.432995
2	15	0	0.742150	-1.912881	-0.320432
3	15	0	1.919127	1.495644	0.350539
4	6	0	-1.593842	-3.220751	-1.087374
5	6	0	1.016401	-2.572748	1.365591
6	6	0	2.207268	-2.478337	3.475260
7	6	0	-0.199723	-3.252329	-1.138913
8	6	0	1.288316	-3.358228	4.043192
9	6	0	0.095926	-3.452385	1.944171
10	6	0	2.066239	-2.081546	2.150105
11	6	0	0.231950	-3.838906	3.275679
12	6	0	0.439690	-4.328249	-1.766764
13	6	0	-0.312440	-5.346404	-2.341885
14	6	0	3.430714	1.108416	-0.589897
15	6	0	3.626405	1.215112	-2.002325
16	6	0	1.500395	3.249899	-0.033542
17	6	0	4.510083	-2.664293	-1.718191
18	6	0	4.637932	0.569434	-0.033373
19	6	0	4.948510	0.784296	-2.301376
20	6	0	-2.344346	-4.240189	-1.666352
21	6	0	5.571010	0.380204	-1.088322
22	6	0	1.268658	3.649500	-1.356100
23	6	0	2.353807	-2.067390	-1.141842
24	6	0	1.188636	4.146991	0.996575
25	6	0	3.861699	-2.173746	-2.887207
26	6	0	3.582692	-2.610833	-0.644374
27	6	0	2.538379	-1.800594	-2.537281
28	6	0	2.610192	1.673704	2.045833
29	6	0	3.704787	2.515091	2.296604
30	6	0	0.669903	5.407799	0.712762
31	6	0	0.762816	4.914349	-1.637026
32	6	0	0.457088	5.797759	-0.605001
33	6	0	-1.705256	-5.303148	-2.295164
34	6	0	2.514931	1.155258	4.412692
35	6	0	2.021217	1.003257	3.116875
36	6	0	3.603154	1.986342	4.647992
37	6	0	4.198756	2.667858	3.585126
38	1	0	1.797809	-1.348944	-3.181818
39	1	0	4.317251	-2.044167	-3.859441
40	1	0	5.541700	-2.980994	-1.644927
41	1	0	3.776930	-2.921377	0.371569
42	1	0	4.808325	0.347000	1.010551
43	1	0	6.560824	-0.043783	-0.988068
44	1	0	5.379657	0.715313	-3.290790
45	1	0	2.876687	1.500904	-2.724354
46	1	0	2.772083	-1.370562	1.730052
47	1	0	3.029421	-2.085128	4.066297
48	1	0	1.394827	-3.663784	5.079807
49	1	0	-0.491782	-4.523298	3.708676
50	1	0	-0.730850	-3.840277	1.357177
51	1	0	1.523259	-4.371414	-1.813168
52	1	0	0.191030	-6.175252	-2.831116
53	1	0	-2.288036	-6.097640	-2.752545
54	1	0	-3.427230	-4.181108	-1.629040
55	1	0	-2.107113	-2.400115	-0.604888
56	1	0	1.351171	3.869815	2.033359
57	1	0	0.430837	6.084084	1.528094
58	1	0	0.047488	6.778809	-0.825643
59	1	0	0.591902	5.200097	-2.670706
60	1	0	1.432615	2.956033	-2.170224
61	1	0	1.185783	0.335298	2.942627
62	1	0	2.044203	0.619219	5.231403
63	1	0	3.990645	2.107813	5.655309
64	1	0	5.047324	3.321433	3.764060
65	1	0	4.167395	3.053152	1.474015
66	45	0	-0.224232	0.245970	-0.131658
67	17	0	0.141448	0.631146	-2.484852
68	6	0	-2.581718	-0.507273	1.040185
69	6	0	-2.273113	0.113853	-0.159939
70	16	0	-1.176544	-0.045542	2.018979
71	6	0	-3.715938	-1.238012	1.600350
72	6	0	-5.018891	-1.102224	1.091949

73	6	0	-3.519876	-2.118078	2.678185
74	6	0	-6.074032	-1.818624	1.641539
75	1	0	-5.204929	-0.431448	0.261970
76	6	0	-4.581610	-2.823817	3.231441
77	1	0	-2.518818	-2.258979	3.078092
78	6	0	-5.866620	-2.681838	2.715314
79	1	0	-7.070678	-1.694515	1.227285
80	1	0	-4.399196	-3.497614	4.064143
81	1	0	-6.696308	-3.236406	3.143269
82	6	0	-3.076263	-0.071482	-1.409301
83	8	0	-3.711396	-1.079212	-1.651589
84	8	0	-3.003484	0.967979	-2.229504
85	6	0	-3.739598	0.888488	-3.454433
86	6	0	-2.960075	0.142830	-4.522468
87	1	0	-3.906075	1.932709	-3.727847
88	1	0	-4.702709	0.409382	-3.258598
89	1	0	-3.522238	0.152586	-5.463012
90	1	0	-1.986064	0.612021	-4.681380
91	1	0	-2.799181	-0.895312	-4.221225
92	6	0	-1.820570	1.932068	0.325236
93	6	0	-1.515958	1.793733	1.804931
94	1	0	-1.011812	2.470597	-0.181615
95	1	0	-2.335366	2.066907	2.474128
96	1	0	-0.610222	2.331915	2.092076
97	6	0	-3.092479	2.650434	-0.012390
98	6	0	-4.297854	2.365739	0.635370
99	6	0	-3.077021	3.652827	-0.987901
100	6	0	-5.462675	3.051673	0.301557
101	1	0	-4.335257	1.590918	1.395973
102	6	0	-4.238781	4.336358	-1.323338
103	1	0	-2.142587	3.878419	-1.495173
104	6	0	-5.439814	4.035620	-0.682101
105	1	0	-6.390901	2.811828	0.812446
106	1	0	-4.207851	5.108535	-2.086931
107	1	0	-6.349133	4.568994	-0.943461

Zero-point correction= 0.856197 (Hartree/Particle)
Thermal correction to Energy= 0.910706
Thermal correction to Enthalpy= 0.911650
Thermal correction to Gibbs Free Energy= 0.764555
Sum of electronic and zero-point Energies= -3970.214462
Sum of electronic and thermal Energies= -3970.159953
Sum of electronic and thermal Enthalpies= -3970.159009
Sum of electronic and thermal Free Energies= -3970.306104

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4282492

TS12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.131011	1.824233	-2.205549
2	15	0	-0.240420	2.225751	0.332406
3	15	0	2.489279	-1.056580	-0.199843
4	6	0	-0.552027	3.225667	2.918508
5	6	0	-1.858945	2.330122	-0.518540
6	6	0	-3.242519	1.767626	-2.426998
7	6	0	-0.366650	3.556851	1.575805
8	6	0	-4.330446	2.401440	-1.832544
9	6	0	-2.961934	2.945698	0.079339
10	6	0	-2.019407	1.725585	-1.769652
11	6	0	-4.190603	2.978893	-0.575617
12	6	0	-0.339019	4.902086	1.194820
13	6	0	-0.503348	5.901640	2.146938
14	6	0	2.555395	-0.185019	-1.803914
15	6	0	3.654509	0.445546	-2.461874
16	6	0	4.216650	-0.978657	0.400534
17	6	0	1.994175	3.804875	-2.726330
18	6	0	1.419417	-0.059186	-2.667627
19	6	0	3.203044	0.937394	-3.717026
20	6	0	-0.725822	4.227108	3.869704
21	6	0	1.821482	0.618729	-3.846050
22	6	0	4.818318	0.269119	0.601262
23	6	0	0.941554	2.903995	-0.879143
24	6	0	4.941590	-2.136941	0.693728
25	6	0	2.970179	3.638985	-1.702920
26	6	0	0.743811	3.355873	-2.221333
27	6	0	2.329458	3.077933	-0.571226
28	6	0	2.306309	-2.805382	-0.705041
29	6	0	2.746498	-3.283056	-1.942893
30	6	0	6.246838	-2.047871	1.171272
31	6	0	6.125968	0.354060	1.064491
32	6	0	6.843085	-0.804515	1.353589
33	6	0	-0.701513	5.564372	3.484783
34	6	0	1.604901	-5.042429	-0.105057
35	6	0	1.731330	-3.692816	0.208220
36	6	0	2.043708	-5.512267	-1.339716
37	6	0	2.612400	-4.631415	-2.258194
38	1	0	2.780790	2.809730	0.374815
39	1	0	4.027220	3.850278	-1.791786
40	1	0	2.175813	4.166720	-3.729478
41	1	0	-0.189612	3.340481	-2.765788
42	1	0	0.431528	-0.431149	-2.436335

43	1	0	1.178489	0.892976	-4.671667
44	1	0	3.795971	1.502808	-4.423283
45	1	0	4.650919	0.553243	-2.056951
46	1	0	-1.174361	1.220517	-2.228477
47	1	0	-3.352674	1.287416	-3.394362
48	1	0	-5.288378	2.431116	-2.343110
49	1	0	-5.039046	3.458676	-0.096894
50	1	0	-2.865413	3.410270	1.055330
51	1	0	-0.187758	5.164936	0.151283
52	1	0	-0.475456	6.944774	1.846058
53	1	0	-0.828511	6.345625	4.228548
54	1	0	-0.865288	3.961661	4.913045
55	1	0	-0.528275	2.184646	3.223851
56	1	0	4.493008	-3.114076	0.546854
57	1	0	6.797376	-2.956735	1.395927
58	1	0	7.861344	-0.736483	1.725423
59	1	0	6.579319	1.329206	1.214790
60	1	0	4.259075	1.174723	0.401001
61	1	0	1.369573	-3.326240	1.164277
62	1	0	1.151101	-5.717863	0.613828
63	1	0	1.937353	-6.563860	-1.590034
64	1	0	2.954158	-4.996612	-3.222361
65	1	0	3.192678	-2.599602	-2.659928
66	45	0	0.719594	0.198006	0.743020
67	17	0	2.193722	1.268405	2.357760
68	6	0	-2.490335	-1.157118	-0.161546
69	6	0	-3.140795	-0.579371	0.867818
70	16	0	-0.748304	-1.420554	-0.021992
71	6	0	-3.091472	-1.814848	-1.349859
72	6	0	-2.600300	-1.592426	-2.637980
73	6	0	-4.113842	-2.754420	-1.176336
74	6	0	-3.150940	-2.250926	-3.732794
75	1	0	-1.785518	-0.892251	-2.785075
76	6	0	-4.660382	-3.418923	-2.266605
77	1	0	-4.479249	-2.961501	-0.174999
78	6	0	-4.185319	-3.163812	-3.551572
79	1	0	-2.760432	-2.058376	-4.727720
80	1	0	-5.451988	-4.146453	-2.111931
81	1	0	-4.610746	-3.683705	-4.404756
82	6	0	-4.575493	-0.209451	0.911982
83	8	0	-5.139304	0.099767	1.943559
84	8	0	-5.173292	-0.209609	-0.285522
85	6	0	-6.568850	0.098826	-0.310233
86	6	0	-7.401183	-1.135899	-0.010524
87	1	0	-6.747818	0.462801	-1.324182
88	1	0	-6.772624	0.899473	0.405325
89	1	0	-8.466984	-0.907481	-0.114572
90	1	0	-7.147925	-1.940614	-0.707636
91	1	0	-7.219880	-1.477424	1.012237
92	6	0	-0.982750	-0.859134	2.186511
93	6	0	-2.364178	-0.233454	2.107720
94	1	0	-2.262173	0.856582	2.180196
95	1	0	-2.946022	-0.541577	2.986193
96	1	0	-0.296708	-0.173104	2.686940
97	6	0	-0.795543	-2.213026	2.764843
98	6	0	0.419003	-2.501004	3.399216
99	6	0	-1.780245	-3.205975	2.700510
100	6	0	0.650113	-3.760429	3.945381
101	1	0	1.188159	-1.732272	3.443177
102	6	0	-1.549989	-4.460211	3.250683
103	1	0	-2.724404	-2.996510	2.205396
104	6	0	-0.332308	-4.744009	3.869508
105	1	0	1.598611	-3.969902	4.430855
106	1	0	-2.321276	-5.222719	3.194673
107	1	0	-0.155981	-5.725933	4.298775

Zero-point correction=	0.857822 (Hartree/Particle)
Thermal correction to Energy=	0.912518
Thermal correction to Enthalpy=	0.913463
Thermal correction to Gibbs Free Energy=	0.766448
Sum of electronic and zero-point Energies=	-3970.247369
Sum of electronic and thermal Energies=	-3970.192672
Sum of electronic and thermal Enthalpies=	-3970.191728
Sum of electronic and thermal Free Energies=	-3970.338743

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.467938

INT17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-3.725014	-1.278427	-1.294984
2	15	0	-1.887795	1.404727	0.006460
3	15	0	-0.617139	-1.999423	0.141486
4	6	0	-0.748857	3.455501	-1.521847
5	6	0	-2.455414	1.763868	1.713212
6	6	0	-3.232385	0.898221	3.843163
7	6	0	-1.880957	3.039133	-0.822171
8	6	0	-3.084775	2.158091	4.419440
9	6	0	-2.312580	3.024127	2.300536
10	6	0	-2.912807	0.703117	2.504439
11	6	0	-2.622841	3.217765	3.644900
12	6	0	-3.017538	3.859169	-0.798126

13	6	0	-3.005936	5.090416	-1.440330
14	6	0	-2.143455	-2.492147	-0.736558
15	6	0	-2.347415	-2.510981	-2.153184
16	6	0	0.650461	-3.202274	-0.448145
17	6	0	-5.454299	-0.169269	-1.265751
18	6	0	-3.366888	-2.930668	-0.128916
19	6	0	-3.660869	-2.992063	-2.408950
20	6	0	-0.740131	4.691024	-2.167177
21	6	0	-4.293558	-3.243439	-1.159889
22	6	0	0.925568	-3.309067	-1.815081
23	6	0	-3.360650	0.676205	-0.781311
24	6	0	1.457752	-3.909191	0.451368
25	6	0	-4.761964	0.020631	-2.494225
26	6	0	-4.597743	0.239978	-0.208413
27	6	0	-3.472820	0.537184	-2.201334
28	6	0	-0.987864	-2.666217	1.819905
29	6	0	-1.304597	-4.020853	2.004051
30	6	0	2.493257	-4.721129	-0.004386
31	6	0	1.944006	-4.139045	-2.270012
32	6	0	2.733610	-4.847196	-1.368953
33	6	0	-1.862599	5.509095	-2.123333
34	6	0	-1.250824	-2.326642	4.209137
35	6	0	-0.965129	-1.832055	2.936468
36	6	0	-1.558387	-3.670920	4.378035
37	6	0	-1.584914	-4.518912	3.269705
38	1	0	-2.682295	0.748892	-2.907647
39	1	0	-5.129919	-0.237909	-3.477882
40	1	0	-6.441915	-0.594392	-1.148225
41	1	0	-4.843308	0.215887	0.842898
42	1	0	-3.556393	-3.005120	0.932287
43	1	0	-5.314527	-3.569374	-1.014788
44	1	0	-4.118551	-3.084940	-3.384405
45	1	0	-1.652328	-2.145538	-2.894269
46	1	0	-3.008834	-0.289713	2.073964
47	1	0	-3.587047	0.060137	4.436507
48	1	0	-3.325913	2.312214	5.466958
49	1	0	-2.503267	4.202925	4.085957
50	1	0	-1.966616	3.863528	1.704703
51	1	0	-3.911640	3.529692	-0.274640
52	1	0	-3.888944	5.722497	-1.414794
53	1	0	-1.854472	6.472442	-2.625360
54	1	0	0.152376	5.006702	-2.698112
55	1	0	0.121366	2.810181	-1.572221
56	1	0	1.284928	-3.830652	1.520174
57	1	0	3.105662	-5.261497	0.711824
58	1	0	3.532035	-5.490345	-1.727384
59	1	0	2.131837	-4.218437	-3.336843
60	1	0	0.368510	-2.712913	-2.527478
61	1	0	-0.745487	-0.778021	2.810051
62	1	0	-1.232895	-1.653147	5.061007
63	1	0	-1.776477	-4.062526	5.367233
64	1	0	-1.823608	-5.570849	3.394648
65	1	0	-1.326252	-4.688175	1.147126
66	45	0	0.214718	0.267777	-0.031464
67	17	0	-0.021262	0.146158	-2.443185
68	6	0	1.836706	1.474779	0.476637
69	6	0	2.355985	0.228969	-0.070111
70	16	0	1.123673	0.916571	2.034938
71	6	0	2.187723	2.906220	0.336588
72	6	0	3.406834	3.318335	-0.210245
73	6	0	1.304575	3.882625	0.814042
74	6	0	3.713598	4.672980	-0.302369
75	1	0	4.105296	2.578936	-0.578978
76	6	0	1.613742	5.232395	0.728312
77	1	0	0.355110	3.577331	1.245040
78	6	0	2.820861	5.634671	0.160453
79	1	0	4.660577	4.974296	-0.740443
80	1	0	0.904561	5.970294	1.091434
81	1	0	3.062649	6.690542	0.081047
82	6	0	2.939274	0.188410	-1.439519
83	8	0	3.160194	1.137951	-2.157984
84	8	0	3.230786	-1.078178	-1.779966
85	6	0	3.891922	-1.265544	-3.034853
86	6	0	2.941576	-1.182284	-4.216123
87	1	0	4.337636	-2.259870	-2.949990
88	1	0	4.689413	-0.522172	-3.125806
89	1	0	3.489118	-1.398854	-5.140649
90	1	0	2.128557	-1.905231	-4.112165
91	1	0	2.502547	-0.185844	-4.285301
92	6	0	2.974161	-0.741577	0.945414
93	6	0	2.278434	-0.483636	2.295897
94	1	0	2.762028	-1.762254	0.624593
95	1	0	2.978063	-0.210104	3.088935
96	1	0	1.683681	-1.338339	2.625923
97	6	0	4.481864	-0.578227	1.023440
98	6	0	5.057671	0.603002	1.500502
99	6	0	5.318846	-1.597338	0.567611
100	6	0	6.439437	0.758296	1.528625
101	1	0	4.420991	1.417372	1.840198
102	6	0	6.702759	-1.445259	0.595350
103	1	0	4.875123	-2.508936	0.175045
104	6	0	7.267153	-0.267628	1.077201
105	1	0	6.870295	1.683255	1.900867

106	1	0	7.341504	-2.247644	0.237028
107	1	0	8.346271	-0.146633	1.098221

Zero-point correction= 0.859580 (Hartree/Particle)
Thermal correction to Energy= 0.912804
Thermal correction to Enthalpy= 0.913748
Thermal correction to Gibbs Free Energy= 0.772802
Sum of electronic and zero-point Energies= -3970.302294
Sum of electronic and thermal Energies= -3970.249070
Sum of electronic and thermal Enthalpies= -3970.248126
Sum of electronic and thermal Free Energies= -3970.389073

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.5198697

INT18a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.886144	1.689203	-1.799021
2	15	0	0.085264	2.277151	0.256170
3	15	0	2.318166	-1.336384	0.116049
4	6	0	-0.397636	3.427814	2.737126
5	6	0	-1.326231	2.395596	-0.911595
6	6	0	-2.336366	1.590552	-2.965218
7	6	0	-0.163671	3.689648	1.386855
8	6	0	-3.406505	2.464977	-2.785465
9	6	0	-2.412927	3.252197	-0.729701
10	6	0	-1.312254	1.552284	-2.028806
11	6	0	-3.450777	3.280855	-1.660232
12	6	0	-0.135765	5.014469	0.936821
13	6	0	-0.362664	6.059293	1.825043
14	6	0	3.020364	-0.373015	-1.271862
15	6	0	4.302057	0.247988	-1.317167
16	6	0	3.798067	-1.919051	1.030167
17	6	0	2.734346	3.577167	-2.587562
18	6	0	2.409990	-0.172203	-2.553099
19	6	0	4.508222	0.763267	-2.627285
20	6	0	-0.627014	4.474851	3.626518
21	6	0	3.341125	0.493161	-3.396585
22	6	0	3.795332	-1.850641	2.423847
23	6	0	1.462577	2.847570	-0.802999
24	6	0	4.888884	-2.499560	0.372489
25	6	0	3.554014	3.599603	-1.424433
26	6	0	1.445729	3.116865	-2.207665
27	6	0	2.781223	3.141070	-0.329323
28	6	0	1.801884	-2.900311	-0.705741
29	6	0	2.276494	-3.327976	-1.950378
30	6	0	5.967191	-2.989846	1.098751
31	6	0	4.874936	-2.348351	3.150901
32	6	0	5.960673	-2.913971	2.491338
33	6	0	-0.613394	5.789075	3.170092
34	6	0	0.487803	-4.931841	-0.544008
35	6	0	0.914559	-3.723166	-0.004018
36	6	0	0.951306	-5.340407	-1.790757
37	6	0	1.853386	-4.540768	-2.487500
38	1	0	3.122833	2.986833	0.683992
39	1	0	4.603978	3.857315	-1.389408
40	1	0	3.045379	3.820562	-3.594799
41	1	0	0.605277	2.979417	-2.872173
42	1	0	1.426905	-0.514408	-2.846174
43	1	0	3.166255	0.795541	-4.420235
44	1	0	5.378974	1.311149	-2.961372
45	1	0	4.989554	0.315374	-0.485161
46	1	0	-0.480134	0.868180	-2.162322
47	1	0	-2.310125	0.920437	-3.819024
48	1	0	-4.211541	2.496144	-3.513803
49	1	0	-4.294233	3.945350	-1.500385
50	1	0	-2.455554	3.904268	0.137053
51	1	0	0.062037	5.223421	-0.111384
52	1	0	-0.339679	7.085557	1.470285
53	1	0	-0.787488	6.606165	3.864264
54	1	0	-0.801621	4.263482	4.677069
55	1	0	-0.358923	2.402559	3.093669
56	1	0	4.894934	-2.572001	-0.711771
57	1	0	6.811192	-3.435954	0.580739
58	1	0	6.803979	-3.296993	3.058931
59	1	0	4.868097	-2.281492	4.234723
60	1	0	2.959844	-1.380744	2.931896
61	1	0	0.546164	-3.412423	0.968564
62	1	0	-0.212063	-5.550182	0.009557
63	1	0	0.612169	-6.279274	-2.218389
64	1	0	2.230774	-4.860124	-3.455069
65	1	0	2.976450	-2.713368	-2.507948
66	45	0	0.798931	0.200175	0.912831
67	17	0	2.452003	1.231672	2.333965
68	6	0	-2.473684	-0.965074	-0.247724
69	6	0	-3.440479	-0.137046	0.192989
70	16	0	-1.118988	-1.117057	0.918353
71	6	0	-2.376989	-1.832595	-1.438816
72	6	0	-1.184545	-1.892321	-2.165657
73	6	0	-3.425731	-2.687441	-1.792789
74	6	0	-1.058450	-2.744636	-3.256029
75	1	0	-0.345490	-1.278925	-1.855831

76	6	0	-3.297194	-3.546305	-2.877028
77	1	0	-4.340579	-2.678415	-1.210889
78	6	0	-2.117238	-3.571342	-3.617931
79	1	0	-0.120323	-2.781284	-3.800183
80	1	0	-4.118743	-4.206349	-3.139639
81	1	0	-2.018114	-4.247205	-4.462193
82	6	0	-4.686697	0.276340	-0.494568
83	8	0	-5.509431	0.993532	0.038062
84	8	0	-4.810240	-0.194963	-1.740038
85	6	0	-5.989377	0.185618	-2.457056
86	6	0	-7.168043	-0.698956	-2.090368
87	1	0	-5.714818	0.068377	-3.507585
88	1	0	-6.205905	1.237263	-2.253182
89	1	0	-8.038057	-0.433435	-2.699983
90	1	0	-6.929849	-1.752107	-2.269713
91	1	0	-7.430434	-0.564543	-1.038032
92	6	0	-2.122963	-0.316386	2.264677
93	6	0	-3.182604	0.508455	1.532498
94	1	0	-2.824932	1.533188	1.375430
95	1	0	-4.102179	0.586336	2.118469
96	1	0	-1.419936	0.325277	2.798363
97	6	0	-2.632785	-1.392219	3.193242
98	6	0	-1.828453	-1.796177	4.262601
99	6	0	-3.861486	-2.026835	2.995651
100	6	0	-2.242152	-2.811077	5.118628
101	1	0	-0.867417	-1.311000	4.419598
102	6	0	-4.276757	-3.042204	3.852418
103	1	0	-4.501905	-1.730523	2.169783
104	6	0	-3.469572	-3.437368	4.915393
105	1	0	-1.606469	-3.110574	5.946597
106	1	0	-5.236207	-3.524204	3.689055
107	1	0	-3.796619	-4.227133	5.585134

Zero-point correction=	0.858390 (Hartree/Particle)
Thermal correction to Energy=	0.913576
Thermal correction to Enthalpy=	0.914520
Thermal correction to Gibbs Free Energy=	0.765057
Sum of electronic and zero-point Energies=	-3970.284246
Sum of electronic and thermal Energies=	-3970.229060
Sum of electronic and thermal Enthalpies=	-3970.228116
Sum of electronic and thermal Free Energies=	-3970.377579

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.5052622

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.206772	-0.000001	0.000032
2	6	0	-1.509251	-1.205432	0.000020
3	6	0	-0.119729	-1.209412	-0.000001
4	6	0	0.587723	0.000001	-0.000009
5	6	0	-0.119730	1.209412	0.000003
6	6	0	-1.509253	1.205432	0.000024
7	1	0	-3.292697	-0.000002	0.000048
8	1	0	-2.049189	-2.147461	0.000026
9	1	0	0.428907	-2.145754	-0.000010
10	1	0	0.428904	2.145756	-0.000003
11	1	0	-2.049191	2.147460	0.000033
12	6	0	2.021900	-0.000001	-0.000029
13	6	0	3.228163	0.000001	-0.000046
14	1	0	4.294956	-0.000002	-0.000062

Zero-point correction=	0.110874 (Hartree/Particle)
Thermal correction to Energy=	0.117276
Thermal correction to Enthalpy=	0.118220
Thermal correction to Gibbs Free Energy=	0.080474
Sum of electronic and zero-point Energies=	-308.167440
Sum of electronic and thermal Energies=	-308.161038
Sum of electronic and thermal Enthalpies=	-308.160094
Sum of electronic and thermal Free Energies=	-308.197840

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -308.3740067

INT8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.528813	1.947993	1.673132
2	6	0	-2.802989	0.447807	-0.029902
3	6	0	-1.772896	0.074504	-0.806920
4	16	0	-2.150685	1.150986	1.453559
5	6	0	-4.253538	0.415814	-0.299179
6	6	0	-5.152859	0.100336	0.724939
7	6	0	-4.759927	0.713270	-1.568847
8	6	0	-6.519459	0.042757	0.476183
9	1	0	-4.769800	-0.101181	1.721158
10	6	0	-6.126736	0.655649	-1.818430
11	1	0	-4.077935	1.011499	-2.359375
12	6	0	-7.011413	0.312566	-0.798909
13	1	0	-7.203915	-0.211785	1.280477
14	1	0	-6.502175	0.889788	-2.810725

15	1	0	-8.079122	0.268408	-0.993102
16	6	0	-1.886457	-0.398855	-2.191181
17	8	0	-1.403043	0.159586	-3.166749
18	8	0	-2.580221	-1.542744	-2.284955
19	6	0	-2.796886	-2.068479	-3.601035
20	6	0	-3.973643	-1.397868	-4.286685
21	1	0	-2.990187	-3.130471	-3.432096
22	1	0	-1.879386	-1.956561	-4.183971
23	1	0	-4.181907	-1.898310	-5.238430
24	1	0	-4.866851	-1.449825	-3.657326
25	1	0	-3.748239	-0.348138	-4.492867
26	26	0	3.462711	-1.758222	0.762852
27	15	0	1.702826	0.276465	-1.289010
28	15	0	0.026565	-1.205060	1.507575
29	6	0	3.048687	2.697352	-1.700505
30	6	0	1.452422	-1.016574	-2.564263
31	6	0	0.457963	-3.149076	-3.142314
32	6	0	2.156359	1.770039	-2.244200
33	6	0	1.189680	-3.177816	-4.325787
34	6	0	2.184631	-1.051672	-3.755232
35	6	0	0.588165	-2.068676	-2.276099
36	6	0	2.048071	-2.123243	-4.632287
37	6	0	1.525360	2.054972	-3.459758
38	6	0	1.799311	3.243096	-4.129579
39	6	0	1.595891	-2.162744	1.524256
40	6	0	2.550017	-1.990580	2.580638
41	6	0	-0.180760	-0.998739	3.326627
42	6	0	5.202052	-1.573206	-0.318461
43	6	0	2.081403	-3.236486	0.699882
44	6	0	3.578655	-2.955161	2.427330
45	6	0	3.316712	3.886238	-2.372954
46	6	0	3.287192	-3.728885	1.270647
47	6	0	-0.288770	-2.165443	4.096283
48	6	0	3.298462	-0.292720	-0.616000
49	6	0	-0.205545	0.242054	3.958675
50	6	0	5.164171	-0.594126	0.712032
51	6	0	4.064890	-1.387046	-1.145107
52	6	0	4.000907	0.196970	0.535725
53	6	0	-1.308901	-2.430169	1.153853
54	6	0	-1.175139	-3.508317	0.276675
55	6	0	-0.342457	0.315044	5.344066
56	6	0	-0.429893	-2.088039	5.475554
57	6	0	-0.458224	-0.843568	6.103133
58	6	0	2.695218	4.160863	-3.588496
59	6	0	-3.639173	-3.035892	1.453541
60	6	0	-2.555791	-2.221289	1.757697
61	6	0	-3.499418	-4.087677	0.553133
62	6	0	-2.258875	-4.328969	-0.022785
63	1	0	3.645066	0.976184	1.192658
64	1	0	5.867386	-0.502665	1.528671
65	1	0	5.939117	-2.357241	-0.428217
66	1	0	3.793577	-2.006034	-1.987088
67	1	0	1.665427	-3.587265	-0.231368
68	1	0	3.904543	-4.512851	0.853613
69	1	0	4.457116	-3.045131	3.051301
70	1	0	2.494094	-1.231799	3.348210
71	1	0	-0.014924	-2.028195	-1.378033
72	1	0	-0.231899	-3.951884	-2.896577
73	1	0	1.088208	-4.013009	-5.012534
74	1	0	2.618022	-2.137095	-5.556496
75	1	0	2.872527	-0.246680	-3.994756
76	1	0	0.805030	1.355239	-3.875005
77	1	0	1.304603	3.452717	-5.073220
78	1	0	2.904871	5.090395	-4.109429
79	1	0	4.014637	4.599435	-1.943973
80	1	0	3.521899	2.502836	-0.744030
81	1	0	-0.092150	1.149934	3.379432
82	1	0	-0.358048	1.288491	5.824265
83	1	0	-0.570112	-0.780134	7.181742
84	1	0	-0.518053	-2.999693	6.058914
85	1	0	-0.263985	-3.139261	3.615595
86	1	0	-2.680179	-1.407990	2.463176
87	1	0	-4.599593	-2.841995	1.920822
88	1	0	-4.348982	-4.719566	0.312235
89	1	0	-2.124601	-5.160150	-0.709231
90	1	0	-0.225098	-3.737266	-0.181297
91	45	0	-0.117197	0.741390	0.212575
92	6	0	0.776509	5.037487	0.616657
93	6	0	0.914937	6.081164	1.521154
94	6	0	-0.149576	6.431858	2.349585
95	6	0	-1.357791	5.741289	2.273099
96	6	0	-1.507347	4.696813	1.369936
97	6	0	-0.437356	4.341190	0.538755
98	1	0	1.596887	4.738691	-0.026457
99	1	0	1.857566	6.615403	1.588659
100	1	0	-0.036166	7.244960	3.061036
101	1	0	-2.184004	6.015638	2.921787
102	1	0	-2.433291	4.136238	1.307065
103	6	0	-0.582683	3.292717	-0.417995
104	6	0	-0.690583	2.459491	-1.307795
105	1	0	-0.895684	1.999899	-2.256355

Zero-point correction= 0.833521 (Hartree/Particle)

Thermal correction to Energy= 0.888458
Thermal correction to Enthalpy= 0.889403
Thermal correction to Gibbs Free Energy= 0.744169
Sum of electronic and zero-point Energies= -3969.030111
Sum of electronic and thermal Energies= -3968.975174
Sum of electronic and thermal Enthalpies= -3968.974230
Sum of electronic and thermal Free Energies= -3969.119463

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.225867

TS5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.392776	2.694997	1.602852
2	6	0	-2.619764	-0.626844	-0.226040
3	6	0	-1.458266	-0.576992	-0.898019
4	16	0	-2.471762	0.371575	1.226308
5	6	0	-3.887442	-1.293709	-0.576132
6	6	0	-4.675153	-1.881979	0.420533
7	6	0	-4.333877	-1.346487	-1.901686
8	6	0	-5.858798	-2.536029	0.097200
9	1	0	-4.351374	-1.824435	1.456494
10	6	0	-5.516917	-2.002875	-2.225278
11	1	0	-3.754670	-0.857552	-2.679552
12	6	0	-6.281219	-2.604893	-1.228708
13	1	0	-6.453908	-2.992363	0.883181
14	1	0	-5.846426	-2.035845	-3.260063
15	1	0	-7.206305	-3.114654	-1.481643
16	6	0	-1.217650	-1.251143	-2.184641
17	8	0	-0.950689	-0.698322	-3.235951
18	8	0	-1.321942	-2.584686	-2.062877
19	6	0	-1.160405	-3.365674	-3.252522
20	6	0	-2.448244	-3.429927	-4.054292
21	1	0	-0.873047	-4.352592	-2.882038
22	1	0	-0.342347	-2.949275	-3.845933
23	1	0	-2.336156	-4.139331	-4.881356
24	1	0	-3.278859	-3.754815	-3.420905
25	1	0	-2.687016	-2.448219	-4.471887
26	26	0	3.954375	0.164617	1.045657
27	15	0	1.593092	0.954244	-1.252289
28	15	0	0.656164	-0.949159	1.601945
29	6	0	1.991934	3.579952	-2.183335
30	6	0	2.050768	-0.471596	-2.313717
31	6	0	2.163037	-2.874702	-2.604533
32	6	0	1.441995	2.325739	-2.454124
33	6	0	2.903979	-2.708219	-3.770491
34	6	0	2.789085	-0.311343	-3.490930
35	6	0	1.736199	-1.759940	-1.890620
36	6	0	3.209193	-1.423090	-4.214818
37	6	0	0.688170	2.137834	-3.620530
38	6	0	0.512015	3.190955	-4.512363
39	6	0	2.480961	-1.078478	1.769791
40	6	0	3.173294	-0.438324	2.847920
41	6	0	0.203816	-0.823045	3.381684
42	6	0	5.449736	1.167424	0.044329
43	6	0	3.470054	-1.797246	1.011934
44	6	0	4.549050	-0.778349	2.772772
45	6	0	1.808042	4.630657	-3.079145
46	6	0	4.732004	-1.624805	1.645319
47	6	0	0.473093	-1.918276	4.213667
48	6	0	3.195825	1.281173	-0.456148
49	6	0	-0.349555	0.333528	3.927379
50	6	0	4.831320	2.030960	0.990286
51	6	0	4.452134	0.710597	-0.854596
52	6	0	3.448650	2.110288	0.687934
53	6	0	0.059241	-2.661893	1.248016
54	6	0	0.831880	-3.696333	0.715737
55	6	0	-0.630831	0.392887	5.291857
56	6	0	0.190796	-1.854544	5.571732
57	6	0	-0.363984	-0.695685	6.113883
58	6	0	1.074184	4.437903	-4.245609
59	6	0	-1.877934	-4.120929	1.145201
60	6	0	-1.298844	-2.907655	1.490383
61	6	0	-1.105963	-5.129522	0.575250
62	6	0	0.253605	-4.919285	0.380144
63	1	0	2.689309	2.636434	1.248278
64	1	0	5.316408	2.501786	1.834577
65	1	0	6.487478	0.862134	0.040579
66	1	0	4.602160	-0.000585	-1.653788
67	1	0	3.322084	-2.319524	0.079213
68	1	0	5.672956	-2.017762	1.284973
69	1	0	5.325363	-0.413996	3.431413
70	1	0	2.716017	0.215666	3.577273
71	1	0	1.124082	-1.902398	-1.009547
72	1	0	1.894270	-3.866718	-2.251844
73	1	0	3.234600	-3.573538	-4.337435
74	1	0	3.776734	-1.283951	-5.130073
75	1	0	3.040999	0.684162	-3.843177
76	1	0	0.223611	1.173823	-3.813510
77	1	0	-0.069124	3.035597	-5.416459
78	1	0	0.935534	5.257987	-4.944054
79	1	0	2.242498	5.601825	-2.862228

80	1	0	2.559448	3.741345	-1.272645
81	1	0	-0.537185	1.194082	3.295226
82	1	0	-1.060455	1.299701	5.706532
83	1	0	-0.584608	-0.644346	7.176347
84	1	0	0.403727	-2.709222	6.207101
85	1	0	0.905058	-2.824058	3.797686
86	1	0	-1.906940	-2.137158	1.950946
87	1	0	-2.939560	-4.271798	1.314844
88	1	0	-1.559249	-6.078178	0.303206
89	1	0	0.878329	-5.709573	-0.027080
90	1	0	1.895286	-3.572829	0.568408
91	45	0	-0.307778	0.721530	0.159825
92	6	0	-2.890055	4.405238	1.183521
93	6	0	-3.831971	5.190333	1.836826
94	6	0	-5.189809	4.908747	1.700633
95	6	0	-5.617636	3.831660	0.921053
96	6	0	-4.687202	3.030039	0.279529
97	6	0	-3.318385	3.322010	0.399766
98	1	0	-1.824793	4.587558	1.283273
99	1	0	-3.507091	6.022946	2.452837
100	1	0	-5.922339	5.528173	2.210246
101	1	0	-6.677088	3.615798	0.825815
102	1	0	-4.994451	2.168892	-0.305386
103	6	0	-2.349405	2.555866	-0.301698
104	6	0	-1.388665	2.151321	-1.002513
105	1	0	-1.020011	2.453752	-1.971411

Zero-point correction=	0.830583 (Hartree/Particle)
Thermal correction to Energy=	0.884728
Thermal correction to Enthalpy=	0.885672
Thermal correction to Gibbs Free Energy=	0.741117
Sum of electronic and zero-point Energies=	-3969.022043
Sum of electronic and thermal Energies=	-3968.967899
Sum of electronic and thermal Enthalpies=	-3968.966954
Sum of electronic and thermal Free Energies=	-3969.111510

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.21367

TS6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.580505	0.229734	-3.165350
2	6	0	2.365866	-1.013527	-0.699618
3	6	0	1.665396	-0.042214	-0.044643
4	16	0	1.453354	-1.493900	-2.105222
5	6	0	3.675905	-1.606572	-0.369508
6	6	0	3.971164	-2.921184	-0.751149
7	6	0	4.655775	-0.872126	0.307776
8	6	0	5.196656	-3.495747	-0.435004
9	1	0	3.228006	-3.494217	-1.298505
10	6	0	5.884906	-1.443067	0.616025
11	1	0	4.471447	0.163964	0.571495
12	6	0	6.158106	-2.759590	0.254570
13	1	0	5.402761	-4.520088	-0.731506
14	1	0	6.633324	-0.850574	1.134666
15	1	0	7.117776	-3.206554	0.497158
16	6	0	1.999953	0.576053	1.244837
17	8	0	2.024086	1.772528	1.476359
18	8	0	2.243699	-0.349605	2.188711
19	6	0	2.632776	0.126376	3.481730
20	6	0	4.124103	0.407136	3.539571
21	1	0	2.352656	-0.684185	4.158481
22	1	0	2.052387	1.019643	3.724351
23	1	0	4.408966	0.695647	4.557122
24	1	0	4.694553	-0.481314	3.253332
25	1	0	4.384178	1.227367	2.863575
26	26	0	-4.200521	0.113858	0.383984
27	15	0	-1.305052	1.821687	-0.056052
28	15	0	-1.235006	-1.750344	-0.080258
29	6	0	-1.696237	4.023432	-1.756011
30	6	0	-1.065359	2.040640	1.748228
31	6	0	-0.679337	1.020235	3.910968
32	6	0	-0.913181	3.468722	-0.742838
33	6	0	-0.911397	2.240899	4.537769
34	6	0	-1.292454	3.265161	2.383741
35	6	0	-0.747406	0.930071	2.524989
36	6	0	-1.211062	3.364217	3.769602
37	6	0	0.256069	4.122835	-0.335587
38	6	0	0.620009	5.328805	-0.922683
39	6	0	-2.937246	-1.504144	0.570446
40	6	0	-4.083234	-1.847873	-0.216976
41	6	0	-1.555871	-3.218530	-1.143665
42	6	0	-5.333589	1.825622	0.547043
43	6	0	-3.430942	-1.052520	1.843553
44	6	0	-5.251493	-1.642449	0.561745
45	6	0	-1.321792	5.228117	-2.347036
46	6	0	-4.849654	-1.160763	1.837395
47	6	0	-1.918135	-4.427049	-0.534546
48	6	0	-3.121654	1.749441	-0.120233
49	6	0	-1.499041	-3.140932	-2.534321
50	6	0	-5.296462	1.393115	-0.807797
51	6	0	-4.000774	2.057898	0.972963

52	6	0	-3.942948	1.345825	-1.225852
53	6	0	-0.276677	-2.539748	1.285728
54	6	0	-0.570837	-2.440067	2.648185
55	6	0	-1.795933	-4.263447	-3.306470
56	6	0	-2.207484	-5.544066	-1.307720
57	6	0	-2.145196	-5.463618	-2.698578
58	6	0	-0.167423	5.883563	-1.930252
59	6	0	1.743412	-3.758385	1.862871
60	6	0	0.879272	-3.235510	0.909758
61	6	0	1.459268	-3.617507	3.217506
62	6	0	0.290005	-2.972662	3.605168
63	1	0	-3.567916	1.000456	-2.178520
64	1	0	-6.147588	1.091137	-1.402973
65	1	0	-6.216341	1.910540	1.166491
66	1	0	-3.699787	2.349129	1.968725
67	1	0	-2.856605	-0.628542	2.652684
68	1	0	-5.505817	-0.861226	2.643278
69	1	0	-6.268604	-1.781368	0.222004
70	1	0	-4.051271	-2.185319	-1.243492
71	1	0	-0.521418	-0.013449	2.044494
72	1	0	-0.424267	0.137080	4.490606
73	1	0	-0.850363	2.321873	5.619090
74	1	0	-1.385685	4.321969	4.250596
75	1	0	-1.540478	4.144256	1.796812
76	1	0	0.883058	3.673907	0.430248
77	1	0	1.526765	5.832047	-0.599624
78	1	0	0.121792	6.822766	-2.392641
79	1	0	-1.936439	5.651923	-3.135438
80	1	0	-2.593449	3.514778	-2.093495
81	1	0	-1.247643	-2.201909	-3.015649
82	1	0	-1.748588	-4.189676	-4.388700
83	1	0	-2.371314	-6.337137	-3.303611
84	1	0	-2.480341	-6.477777	-0.824815
85	1	0	-1.971153	-4.496165	0.548319
86	1	0	1.102514	-3.368020	-0.142897
87	1	0	2.648103	-4.263724	1.539283
88	1	0	2.137298	-4.020171	3.964374
89	1	0	0.035555	-2.885842	4.658057
90	1	0	-1.480838	-1.964321	2.984888
91	45	0	-0.079914	0.102281	-1.151734
92	6	0	4.501211	1.166160	-2.223416
93	6	0	5.866329	1.350226	-2.050742
94	6	0	6.331164	2.239054	-1.084029
95	6	0	5.432244	2.954222	-0.290934
96	6	0	4.065296	2.785014	-0.459835
97	6	0	3.589954	1.881820	-1.425849
98	1	0	4.117532	0.463569	-2.956032
99	1	0	6.566837	0.789166	-2.660518
100	1	0	7.399520	2.377207	-0.945907
101	1	0	5.800634	3.648826	0.457706
102	1	0	3.354721	3.318251	0.158397
103	6	0	2.199316	1.680921	-1.639669
104	6	0	1.039308	1.582666	-2.119324
105	1	0	0.524859	2.086832	-2.926150

Zero-point correction= 0.831760 (Hartree/Particle)
Thermal correction to Energy= 0.885070
Thermal correction to Enthalpy= 0.886014
Thermal correction to Gibbs Free Energy= 0.746352
Sum of electronic and zero-point Energies= -3969.026389
Sum of electronic and thermal Energies= -3968.973079
Sum of electronic and thermal Enthalpies= -3968.972135
Sum of electronic and thermal Free Energies= -3969.111796

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.1487915

INT9b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.428170	1.276397	-2.826591
2	6	0	2.523008	-0.792518	0.475712
3	6	0	1.428333	-0.219479	0.990086
4	16	0	2.440965	-0.567289	-1.327595
5	6	0	3.727567	-1.371058	1.096167
6	6	0	4.326851	-2.508865	0.541793
7	6	0	4.299456	-0.793605	2.237284
8	6	0	5.458968	-3.067336	1.124547
9	1	0	3.896121	-2.960312	-0.348110
10	6	0	5.428742	-1.358131	2.820898
11	1	0	3.871305	0.113720	2.652304
12	6	0	6.011320	-2.496208	2.268755
13	1	0	5.909668	-3.952044	0.684599
14	1	0	5.864694	-0.896085	3.701838
15	1	0	6.897078	-2.930962	2.722258
16	6	0	1.304477	0.040802	2.443226
17	8	0	1.412206	1.143892	2.940490
18	8	0	1.098922	-1.061446	3.170570
19	6	0	0.983237	-0.858741	4.587002
20	6	0	0.593268	-2.184766	5.201286
21	1	0	0.231128	-0.087134	4.770499
22	1	0	1.944179	-0.497068	4.967146
23	1	0	0.475076	-2.071348	6.283439

24	1	0	-0.354779	-2.534924	4.781969
25	1	0	1.360028	-2.943105	5.014051
26	26	0	-3.989144	0.409023	-1.106103
27	15	0	-1.228714	1.746387	0.519134
28	15	0	-1.114305	-1.628128	-0.953173
29	6	0	-1.511425	4.553131	0.272208
30	6	0	-1.659075	1.184803	2.212945
31	6	0	-2.384006	-0.634228	3.642103
32	6	0	-0.733025	3.492554	0.741933
33	6	0	-2.564531	0.258970	4.695481
34	6	0	-1.836981	2.074558	3.274666
35	6	0	-1.928422	-0.170048	2.413197
36	6	0	-2.284101	1.610972	4.509233
37	6	0	0.470630	3.763504	1.406209
38	6	0	0.882100	5.078119	1.595170
39	6	0	-2.870561	-1.317575	-1.364414
40	6	0	-3.395553	-0.856462	-2.609453
41	6	0	-0.432686	-2.575868	-2.386968
42	6	0	-5.196791	1.901637	-0.364066
43	6	0	-3.986006	-1.531949	-0.486439
44	6	0	-4.814149	-0.825172	-2.512216
45	6	0	-1.089290	5.867457	0.458366
46	6	0	-5.179795	-1.244975	-1.202773
47	6	0	0.097141	-3.860607	-2.214990
48	6	0	-2.894140	1.862232	-0.191280
49	6	0	-0.334897	-1.974622	-3.647649
50	6	0	-4.652625	2.289943	-1.621176
51	6	0	-4.120151	1.648334	0.523729
52	6	0	-3.238439	2.267069	-1.522953
53	6	0	-1.287993	-2.995861	0.270223
54	6	0	-2.258210	-3.997994	0.120794
55	6	0	0.245622	-2.654861	-4.712332
56	6	0	0.687309	-4.533590	-3.282159
57	6	0	0.757502	-3.937250	-4.536050
58	6	0	0.106484	6.132576	1.117690
59	6	0	-0.420221	-4.176817	2.200919
60	6	0	-0.362962	-3.108548	1.307311
61	6	0	-1.403405	-5.149336	2.062414
62	6	0	-2.320302	-5.059694	1.014850
63	1	0	-2.527783	2.453046	-2.314189
64	1	0	-5.215409	2.502048	-2.520141
65	1	0	-6.246105	1.769623	-0.137296
66	1	0	-4.207324	1.313276	1.547272
67	1	0	-3.927777	-1.853166	0.543997
68	1	0	-6.182780	-1.283529	-0.799997
69	1	0	-5.491177	-0.483741	-3.283243
70	1	0	-2.811084	-0.537877	-3.459729
71	1	0	-1.781366	-0.874681	1.605873
72	1	0	-2.585823	-1.693765	3.770934
73	1	0	-2.918474	-0.097294	5.658636
74	1	0	-2.416346	2.312694	5.327308
75	1	0	-1.630024	3.130803	3.139416
76	1	0	1.072880	2.943721	1.787683
77	1	0	1.815914	5.275864	2.112742
78	1	0	0.433605	7.158352	1.260844
79	1	0	-1.700920	6.683721	0.085833
80	1	0	-2.449278	4.361986	-0.237402
81	1	0	-0.661433	-0.950889	-3.786651
82	1	0	0.312778	-2.167220	-5.680189
83	1	0	1.217987	-4.462151	-5.367988
84	1	0	1.093687	-5.528703	-3.125849
85	1	0	0.057654	-4.350767	-1.249160
86	1	0	0.412067	-2.364070	1.423422
87	1	0	0.312816	-4.240230	2.998931
88	1	0	-1.452079	-5.981016	2.759420
89	1	0	-3.080819	-5.824699	0.888810
90	1	0	-2.962584	-3.954607	-0.703568
91	45	0	0.320408	0.426065	-0.600657
92	6	0	4.199557	2.970395	-2.421606
93	6	0	5.429502	3.483492	-2.816664
94	6	0	6.596978	2.755737	-2.595721
95	6	0	6.525205	1.510561	-1.975875
96	6	0	5.297008	0.997527	-1.573043
97	6	0	4.121215	1.725086	-1.786329
98	1	0	3.284241	3.521546	-2.616897
99	1	0	5.475507	4.449749	-3.310690
100	1	0	7.556593	3.154960	-2.910926
101	1	0	7.430936	0.937804	-1.798681
102	1	0	5.250986	0.031268	-1.076619
103	6	0	2.817467	1.222301	-1.330997
104	6	0	1.736571	1.836710	-0.858612
105	1	0	1.630893	2.910264	-0.732611

Zero-point correction= 0.834513 (Hartree/Particle)
Thermal correction to Energy= 0.888140
Thermal correction to Enthalpy= 0.889084
Thermal correction to Gibbs Free Energy= 0.745659
Sum of electronic and zero-point Energies= -3969.058426
Sum of electronic and thermal Energies= -3969.004799
Sum of electronic and thermal Enthalpies= -3969.003854
Sum of electronic and thermal Free Energies= -3969.147279

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2554532

INT10b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.186189	-0.855441	-3.127572
2	6	0	-2.297079	1.403606	-0.880606
3	6	0	-2.061313	0.135884	-0.165396
4	16	0	-1.338038	1.556489	-2.234513
5	6	0	-3.268124	2.420393	-0.454489
6	6	0	-3.079699	3.779731	-0.736878
7	6	0	-4.429665	2.014908	0.216915
8	6	0	-4.016577	4.717409	-0.322519
9	1	0	-2.188038	4.097962	-1.268827
10	6	0	-5.376876	2.952693	0.606214
11	1	0	-4.602878	0.959394	0.405652
12	6	0	-5.165954	4.305786	0.350981
13	1	0	-3.853141	5.770492	-0.529641
14	1	0	-6.279241	2.626227	1.113465
15	1	0	-5.900281	5.039584	0.669399
16	6	0	-2.163367	0.119953	1.310453
17	8	0	-2.471649	-0.842282	1.989943
18	8	0	-1.816614	1.306114	1.836027
19	6	0	-1.955099	1.492773	3.247438
20	6	0	-3.275445	2.176198	3.550024
21	1	0	-1.108020	2.122961	3.529639
22	1	0	-1.873522	0.525644	3.746165
23	1	0	-3.354926	2.381313	4.622901
24	1	0	-3.355981	3.120572	3.002984
25	1	0	-4.113834	1.535978	3.258679
26	26	0	3.984466	-1.214258	0.184214
27	15	0	0.661023	-2.006747	0.203228
28	15	0	1.710352	1.438408	-0.333983
29	6	0	0.282673	-4.532330	-0.965427
30	6	0	0.556857	-1.783546	2.020902
31	6	0	0.801225	-0.327716	3.941516
32	6	0	-0.233198	-3.572595	-0.093893
33	6	0	0.734162	-1.425594	4.793622
34	6	0	0.477770	-2.881416	2.884275
35	6	0	0.698947	-0.509141	2.565946
36	6	0	0.560011	-2.701386	4.261190
37	6	0	-1.507970	-3.751914	0.458398
38	6	0	-2.247023	-4.886477	0.148079
39	6	0	3.332561	0.749512	0.171034
40	6	0	4.408647	0.570562	-0.753033
41	6	0	2.274853	2.652591	-1.605399
42	6	0	4.547065	-3.152530	0.588779
43	6	0	3.815979	0.347689	1.462631
44	6	0	5.543553	0.099953	-0.040647
45	6	0	-0.464827	-5.666458	-1.275988
46	6	0	5.182648	-0.028203	1.329212
47	6	0	3.028059	3.770247	-1.221215
48	6	0	2.407089	-2.475994	0.041437
49	6	0	1.984283	2.460027	-2.956359
50	6	0	4.496326	-2.941996	-0.817334
51	6	0	3.263025	-2.874065	1.123383
52	6	0	3.184516	-2.531911	-1.162266
53	6	0	1.277100	2.630347	1.013648
54	6	0	2.043646	2.924726	2.145220
55	6	0	2.435580	3.375323	-3.907344
56	6	0	3.474904	4.679891	-2.170440
57	6	0	3.176704	4.484679	-3.518846
58	6	0	-1.727692	-5.845116	-0.720338
59	6	0	-0.362064	4.267163	1.749518
60	6	0	0.077538	3.324275	0.830454
61	6	0	0.396643	4.534025	2.886419
62	6	0	1.601161	3.863263	3.077384
63	1	0	2.832270	-2.239633	-2.140668
64	1	0	5.328309	-3.022450	-1.503746
65	1	0	5.424315	-3.418626	1.163074
66	1	0	2.994658	-2.899726	2.169572
67	1	0	3.240104	0.291779	2.375123
68	1	0	5.812707	-0.406626	2.122763
69	1	0	6.498003	-0.161432	-0.476546
70	1	0	4.345848	0.743316	-1.818795
71	1	0	0.704620	0.358458	1.917987
72	1	0	0.922687	0.676295	4.338830
73	1	0	0.809843	-1.289003	5.868340
74	1	0	0.495203	-3.562132	4.920065
75	1	0	0.359852	-3.881482	2.479176
76	1	0	-1.928861	-2.993916	1.113614
77	1	0	-3.238133	-5.010918	0.573580
78	1	0	-2.310397	-6.727733	-0.967934
79	1	0	-0.057724	-6.407498	-1.957377
80	1	0	1.262426	-4.396010	-1.411859
81	1	0	1.439725	1.576972	-3.273162
82	1	0	2.206268	3.209299	-4.955626
83	1	0	3.524790	5.197026	-4.261392
84	1	0	4.055089	5.543428	-1.858230
85	1	0	3.261708	3.935001	-0.173502
86	1	0	-0.520128	3.123154	-0.048305
87	1	0	-1.306389	4.776582	1.579534
88	1	0	0.056371	5.264750	3.614268

89	1	0	2.211993	4.077571	3.949760
90	1	0	3.002329	2.445268	2.299356
91	45	0	-0.111893	-0.228393	-1.123912
92	6	0	-4.587142	-1.704250	-2.298441
93	6	0	-5.903552	-2.137127	-2.414233
94	6	0	-6.672270	-2.352630	-1.272850
95	6	0	-6.109679	-2.137769	-0.017576
96	6	0	-4.789338	-1.712494	0.101683
97	6	0	-4.008511	-1.487658	-1.040484
98	1	0	-3.993850	-1.516590	-3.188928
99	1	0	-6.333773	-2.296141	-3.398952
100	1	0	-7.702624	-2.684738	-1.362436
101	1	0	-6.697902	-2.312233	0.879351
102	1	0	-4.346048	-1.573187	1.081631
103	6	0	-2.595137	-1.054818	-0.972083
104	6	0	-1.569482	-1.454462	-1.707477
105	1	0	-1.484138	-2.241541	-2.449152

Zero-point correction= 0.834444 (Hartree/Particle)
Thermal correction to Energy= 0.887789
Thermal correction to Enthalpy= 0.888733
Thermal correction to Gibbs Free Energy= 0.747425
Sum of electronic and zero-point Energies= -3969.074814
Sum of electronic and thermal Energies= -3969.021469
Sum of electronic and thermal Enthalpies= -3969.020525
Sum of electronic and thermal Free Energies= -3969.161833

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2645533

INT11b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.611727	-0.984518	2.679075
2	15	0	2.165119	0.483620	-0.328160
3	15	0	-0.317532	-2.182072	0.093922
4	6	0	3.049539	2.332534	-2.184549
5	6	0	3.601439	-0.607955	-0.652701
6	6	0	4.476304	-2.730448	-1.420613
7	6	0	2.826237	2.113957	-0.820365
8	6	0	5.765508	-2.326316	-1.087208
9	6	0	4.904758	-0.196885	-0.349006
10	6	0	3.398695	-1.873342	-1.208660
11	6	0	5.979375	-1.054879	-0.556625
12	6	0	3.089751	3.135906	0.092020
13	6	0	3.582890	4.360000	-0.352572
14	6	0	0.641511	-2.440590	1.631734
15	6	0	0.131891	-2.379469	2.968279
16	6	0	-2.022353	-2.462504	0.720541
17	6	0	2.528766	0.515803	3.753600
18	6	0	2.045047	-2.728059	1.732681
19	6	0	1.202362	-2.617320	3.870762
20	6	0	3.547273	3.553228	-2.623690
21	6	0	2.380698	-2.841280	3.107471
22	6	0	-2.623560	-1.429138	1.442607
23	6	0	2.090396	0.585271	1.483338
24	6	0	-2.725525	-3.652904	0.525995
25	6	0	1.142976	0.796471	3.585938
26	6	0	3.113739	0.387002	2.464655
27	6	0	0.870295	0.835065	2.192835
28	6	0	-0.007196	-3.729348	-0.842293
29	6	0	0.693372	-4.816038	-0.310271
30	6	0	-4.007005	-3.803342	1.054915
31	6	0	-3.897462	-1.582263	1.975528
32	6	0	-4.594126	-2.772914	1.782074
33	6	0	3.814278	4.568854	-1.707815
34	6	0	-0.455959	-5.033824	-2.834405
35	6	0	-0.585329	-3.853696	-2.111463
36	6	0	0.259797	-6.104259	-2.304611
37	6	0	0.832373	-5.992740	-1.041691
38	1	0	-0.105199	0.952897	1.742551
39	1	0	0.412318	0.893563	4.377714
40	1	0	3.036916	0.365248	4.696508
41	1	0	4.140482	0.119434	2.257399
42	1	0	2.739506	-2.813554	0.910404
43	1	0	3.374086	-3.010041	3.500239
44	1	0	1.135749	-2.586378	4.949735
45	1	0	-0.889413	-2.156345	3.241428
46	1	0	2.400143	-2.183028	-1.499842
47	1	0	4.301911	-3.709210	-1.857210
48	1	0	6.606161	-2.993191	-1.255691
49	1	0	6.986488	-0.727418	-0.315439
50	1	0	5.078794	0.803902	0.037724
51	1	0	2.903260	2.984394	1.150519
52	1	0	3.774761	5.152520	0.364274
53	1	0	4.196964	5.525035	-2.053338
54	1	0	3.717225	3.714613	-3.683836
55	1	0	2.826159	1.547337	-2.901836
56	1	0	-2.280484	-4.469124	-0.032583
57	1	0	-4.543496	-4.734110	0.896349
58	1	0	-5.594934	-2.891525	2.186364
59	1	0	-4.357458	-0.759468	2.514558
60	1	0	-2.101042	-0.490468	1.579009

61	1	0	-1.129268	-3.021980	-2.541823
62	1	0	-0.907879	-5.110182	-3.818354
63	1	0	0.367109	-7.023911	-2.872261
64	1	0	1.381847	-6.826458	-0.614700
65	1	0	1.124869	-4.758871	0.682085
66	45	0	-0.100256	-0.116390	-1.237685
67	17	0	0.718468	-1.157003	-3.196048
68	6	0	-0.963168	2.391097	-1.088314
69	6	0	-2.002137	1.694876	-0.481329
70	16	0	-0.292244	1.800631	-2.586684
71	6	0	-0.382043	3.643494	-0.521521
72	6	0	-0.162400	3.831905	0.845971
73	6	0	-0.043042	4.684389	-1.394570
74	6	0	0.348467	5.030025	1.332468
75	1	0	-0.370418	3.034842	1.546580
76	6	0	0.459241	5.884471	-0.909767
77	1	0	-0.179021	4.550638	-2.462785
78	6	0	0.654473	6.065770	0.457256
79	1	0	0.512913	5.145337	2.400113
80	1	0	0.707482	6.679114	-1.606682
81	1	0	1.053338	7.002890	0.834448
82	6	0	-2.644809	2.302530	0.742366
83	8	0	-3.333701	3.291764	0.728448
84	8	0	-2.385933	1.600370	1.861900
85	6	0	-2.995240	2.065344	3.078559
86	6	0	-2.197441	3.192020	3.709936
87	1	0	-3.014211	1.180650	3.719753
88	1	0	-4.018741	2.377866	2.859326
89	1	0	-2.650370	3.470335	4.666992
90	1	0	-1.163663	2.881180	3.894840
91	1	0	-2.191891	4.069993	3.059026
92	6	0	-4.966501	1.788066	-1.388648
93	6	0	-6.355957	1.760036	-1.453159
94	6	0	-7.041564	0.552927	-1.341798
95	6	0	-6.327350	-0.629500	-1.164119
96	6	0	-4.939305	-0.602194	-1.092495
97	6	0	-4.239401	0.605729	-1.206512
98	1	0	-4.441440	2.733052	-1.480911
99	1	0	-6.903021	2.687201	-1.597537
100	1	0	-8.126573	0.534156	-1.392836
101	1	0	-6.850560	-1.576910	-1.069213
102	1	0	-4.386277	-1.523032	-0.930783
103	6	0	-2.755884	0.594654	-1.168390
104	6	0	-2.004877	-0.329128	-1.781033
105	1	0	-2.412210	-1.093853	-2.437883

Zero-point correction= 0.834108 (Hartree/Particle)
Thermal correction to Energy= 0.888670
Thermal correction to Enthalpy= 0.889614
Thermal correction to Gibbs Free Energy= 0.743387
Sum of electronic and zero-point Energies= -3969.060712
Sum of electronic and thermal Energies= -3969.006150
Sum of electronic and thermal Enthalpies= -3969.005206
Sum of electronic and thermal Free Energies= -3969.151433

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2557996

TS7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.321437	2.377433	-2.031487
2	6	0	2.659701	-0.596060	0.522707
3	6	0	1.636207	-0.021535	1.210644
4	16	0	2.786377	0.284951	-1.034437
5	6	0	3.575730	-1.691100	0.848716
6	6	0	3.857385	-2.681998	-0.102008
7	6	0	4.142775	-1.805068	2.126220
8	6	0	4.671132	-3.762261	0.220837
9	1	0	3.411504	-2.617206	-1.091721
10	6	0	4.949064	-2.890520	2.446603
11	1	0	3.961356	-1.029179	2.864397
12	6	0	5.214763	-3.876236	1.497636
13	1	0	4.871725	-4.523351	-0.527509
14	1	0	5.383409	-2.959693	3.439949
15	1	0	5.847076	-4.722116	1.750077
16	6	0	1.344833	-0.290910	2.639833
17	8	0	1.242411	0.561210	3.496711
18	8	0	1.214340	-1.597226	2.894044
19	6	0	1.006499	-1.957634	4.265827
20	6	0	1.000525	-3.469250	4.324491
21	1	0	0.060418	-1.525506	4.604399
22	1	0	1.813113	-1.528037	4.868024
23	1	0	0.846786	-3.803920	5.355139
24	1	0	0.197506	-3.874433	3.701583
25	1	0	1.954572	-3.867785	3.964701
26	26	0	-3.847660	0.068337	-1.260604
27	15	0	-1.461604	1.258959	0.975519
28	15	0	-0.634593	-1.290239	-1.444637
29	6	0	-1.665692	4.057717	0.985400
30	6	0	-1.901920	0.158754	2.374228
31	6	0	-2.254969	-2.117722	3.126689
32	6	0	-1.245492	2.928220	1.693609

33	6	0	-2.847453	-1.645857	4.294647
34	6	0	-2.505380	0.626078	3.546188
35	6	0	-1.777236	-1.217774	2.179633
36	6	0	-2.964645	-0.272721	4.504337
37	6	0	-0.540179	3.094866	2.891760
38	6	0	-0.285656	4.371993	3.382506
39	6	0	-2.400875	-1.258075	-1.907601
40	6	0	-2.978994	-0.566496	-3.013539
41	6	0	0.250083	-1.495513	-3.051234
42	6	0	-5.338681	1.069434	-0.243557
43	6	0	-3.463388	-1.935175	-1.221532
44	6	0	-4.375467	-0.836915	-3.026859
45	6	0	-1.404169	5.331907	1.479420
46	6	0	-4.674923	-1.684978	-1.923674
47	6	0	0.940823	-2.666377	-3.381812
48	6	0	-3.074042	1.339092	0.136429
49	6	0	0.310479	-0.403615	-3.926052
50	6	0	-4.811456	1.888594	-1.280784
51	6	0	-4.277180	0.732374	0.634758
52	6	0	-3.420555	2.054268	-1.058345
53	6	0	-0.498211	-2.993863	-0.756925
54	6	0	-1.201682	-4.074360	-1.309809
55	6	0	1.016398	-0.497588	-5.120310
56	6	0	1.656998	-2.750292	-4.574107
57	6	0	1.690677	-1.670673	-5.449992
58	6	0	-0.718504	5.493078	2.679847
59	6	0	0.618448	-4.536334	0.744782
60	6	0	0.411639	-3.242342	0.270208
61	6	0	-0.094287	-5.598126	0.200761
62	6	0	-1.007048	-5.363259	-0.828372
63	1	0	-2.713259	2.554726	-1.704190
64	1	0	-5.359576	2.266556	-2.133126
65	1	0	-6.358202	0.717352	-0.163268
66	1	0	-4.354396	0.097170	1.505185
67	1	0	-3.358296	-2.529589	-0.324508
68	1	0	-5.657425	-2.032509	-1.634657
69	1	0	-5.090923	-0.422947	-3.724176
70	1	0	-2.449214	0.080216	-3.698182
71	1	0	-1.300134	-1.592799	1.283708
72	1	0	-2.152346	-3.184198	2.948226
73	1	0	-3.217087	-2.343586	5.040395
74	1	0	-3.425642	0.101888	5.413249
75	1	0	-2.629086	1.691798	3.708043
76	1	0	-0.157845	2.232156	3.426629
77	1	0	0.263409	4.486011	4.312297
78	1	0	-0.514793	6.489014	3.062215
79	1	0	-1.735121	6.200157	0.917746
80	1	0	-2.181057	3.951107	0.039242
81	1	0	-0.149719	0.540572	-3.648540
82	1	0	1.053281	0.360656	-5.784525
83	1	0	2.249670	-1.737989	-6.378847
84	1	0	2.189052	-3.666347	-4.814402
85	1	0	0.930653	-3.521225	-2.714720
86	1	0	0.963800	-2.425135	0.711481
87	1	0	1.347231	-4.700585	1.532432
88	1	0	0.062568	-6.608344	0.567922
89	1	0	-1.560900	-6.189282	-1.264878
90	1	0	-1.894575	-3.908165	-2.128768
91	45	0	0.348349	0.628046	-0.247456
92	6	0	2.870445	4.327833	-0.880484
93	6	0	3.612957	5.411159	-1.334622
94	6	0	4.928277	5.230923	-1.757675
95	6	0	5.501510	3.961213	-1.725281
96	6	0	4.766708	2.877148	-1.260488
97	6	0	3.447620	3.051805	-0.823744
98	1	0	1.828712	4.444778	-0.598004
99	1	0	3.156948	6.395743	-1.378002
100	1	0	5.503514	6.077216	-2.122006
101	1	0	6.525256	3.816658	-2.057638
102	1	0	5.219344	1.890029	-1.221801
103	6	0	2.659076	1.941320	-0.291826
104	6	0	1.686187	1.912980	0.635851
105	1	0	1.460382	2.722260	1.321082

Zero-point correction= 0.831896 (Hartree/Particle)
Thermal correction to Energy= 0.886215
Thermal correction to Enthalpy= 0.887159
Thermal correction to Gibbs Free Energy= 0.741128
Sum of electronic and zero-point Energies= -3969.029498
Sum of electronic and thermal Energies= -3968.975180
Sum of electronic and thermal Enthalpies= -3968.974236
Sum of electronic and thermal Free Energies= -3969.120267

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2188648

TS8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.493960	-1.062908	2.719482
2	15	0	2.284586	0.193642	-0.321616
3	15	0	-0.525358	-2.104651	0.174306
4	6	0	3.189129	1.926330	-2.272407

5	6	0	3.650069	-0.999455	-0.560328
6	6	0	4.384692	-3.203728	-1.235211
7	6	0	3.021106	1.763657	-0.892225
8	6	0	5.691086	-2.882061	-0.878606
9	6	0	4.970796	-0.672040	-0.233461
10	6	0	3.367480	-2.264534	-1.082088
11	6	0	5.984632	-1.612206	-0.383667
12	6	0	3.384930	2.797224	-0.027489
13	6	0	3.931729	3.972603	-0.535254
14	6	0	0.380498	-2.462070	1.723909
15	6	0	-0.114848	-2.294974	3.055838
16	6	0	-2.251801	-2.134685	0.792415
17	6	0	2.516554	0.390126	3.762870
18	6	0	1.748401	-2.879407	1.835928
19	6	0	0.931497	-2.598547	3.967857
20	6	0	3.738769	3.100191	-2.774446
21	6	0	2.079135	-2.968801	3.214551
22	6	0	-2.722018	-0.982101	1.425019
23	6	0	2.166312	0.399717	1.476656
24	6	0	-3.103091	-3.236124	0.665315
25	6	0	1.172839	0.800343	3.529752
26	6	0	3.130365	0.146493	2.504230
27	6	0	0.954239	0.804245	2.127168
28	6	0	-0.425613	-3.683821	-0.747676
29	6	0	0.125702	-4.856291	-0.224064
30	6	0	-4.402418	-3.176512	1.163667
31	6	0	-4.017826	-0.924640	1.924050
32	6	0	-4.863059	-2.022305	1.791332
33	6	0	4.113182	4.123515	-1.906162
34	6	0	-1.023917	-4.892888	-2.759661
35	6	0	-1.001175	-3.714415	-2.023433
36	6	0	-0.459647	-6.053987	-2.236819
37	6	0	0.114655	-6.032969	-0.969643
38	1	0	0.014576	1.011048	1.632927
39	1	0	0.429798	1.009162	4.287494
40	1	0	2.975319	0.234192	4.729864
41	1	0	4.129855	-0.234855	2.347826
42	1	0	2.427149	-3.064822	1.016692
43	1	0	3.052662	-3.218904	3.613689
44	1	0	0.872234	-2.518416	5.044746
45	1	0	-1.107687	-1.956753	3.317163
46	1	0	2.354544	-2.507372	-1.389420
47	1	0	4.152934	-4.181895	-1.645607
48	1	0	6.484335	-3.613918	-1.000735
49	1	0	7.006884	-1.351626	-0.125345
50	1	0	5.206480	0.326208	0.126801
51	1	0	3.234713	2.691901	1.042532
52	1	0	4.203526	4.774728	0.143953
53	1	0	4.536663	5.042812	-2.300526
54	1	0	3.867693	3.219004	-3.845987
55	1	0	2.880484	1.134277	-2.950459
56	1	0	-2.755959	-4.141181	0.177387
57	1	0	-5.057228	-4.036494	1.057374
58	1	0	-5.882123	-1.973132	2.162873
59	1	0	-4.375719	-0.009429	2.385731
60	1	0	-2.080194	-0.114694	1.519017
61	1	0	-1.424853	-2.809287	-2.445100
62	1	0	-1.472079	-4.898803	-3.748338
63	1	0	-0.468719	-6.973164	-2.815393
64	1	0	0.550052	-6.935973	-0.551820
65	1	0	0.556552	-4.861703	0.771238
66	45	0	0.040299	-0.124663	-1.225533
67	17	0	0.800792	-1.246223	-3.160826
68	6	0	-0.796487	2.463032	-1.065544
69	6	0	-1.984567	1.952679	-0.501897
70	16	0	-0.265379	1.735031	-2.548672
71	6	0	-0.079903	3.665376	-0.575595
72	6	0	0.147973	3.890648	0.785799
73	6	0	0.380693	4.622747	-1.489686
74	6	0	0.787290	5.045416	1.224572
75	1	0	-0.161220	3.152962	1.514397
76	6	0	1.017165	5.775443	-1.052188
77	1	0	0.231204	4.463622	-2.553204
78	6	0	1.220770	5.996665	0.308529
79	1	0	0.950413	5.192634	2.288580
80	1	0	1.358520	6.505196	-1.780085
81	1	0	1.719278	6.899576	0.648462
82	6	0	-2.607511	2.696619	0.650338
83	8	0	-3.209547	3.737451	0.555964
84	8	0	-2.402738	2.060066	1.818283
85	6	0	-2.952307	2.671481	2.998946
86	6	0	-2.015008	3.722410	3.565708
87	1	0	-3.086716	1.839251	3.693631
88	1	0	-3.925756	3.100252	2.751288
89	1	0	-2.435407	4.130154	4.490751
90	1	0	-1.036187	3.287224	3.793648
91	1	0	-1.881296	4.540868	2.853733
92	6	0	-5.017490	1.844813	-1.203851
93	6	0	-6.393741	1.648745	-1.261143
94	6	0	-6.919789	0.365638	-1.385392
95	6	0	-6.055626	-0.724906	-1.449556
96	6	0	-4.682038	-0.532063	-1.377347
97	6	0	-4.137708	0.754002	-1.251224

98	1	0	-4.622396	2.852619	-1.139300
99	1	0	-7.057679	2.507951	-1.225174
100	1	0	-7.994593	0.216613	-1.435752
101	1	0	-6.451895	-1.732375	-1.539640
102	1	0	-4.015917	-1.390111	-1.383014
103	6	0	-2.668988	0.916966	-1.209610
104	6	0	-1.810788	0.173733	-2.013279
105	1	0	-2.182174	-0.403581	-2.858943

Zero-point correction= 0.832939 (Hartree/Particle)
Thermal correction to Energy= 0.887001
Thermal correction to Enthalpy= 0.887945
Thermal correction to Gibbs Free Energy= 0.743395
Sum of electronic and zero-point Energies= -3969.050779
Sum of electronic and thermal Energies= -3968.996717
Sum of electronic and thermal Enthalpies= -3968.995773
Sum of electronic and thermal Free Energies= -3969.140323

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.243799

INT12b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.910785	-0.452336	-2.077525
2	6	0	-2.374003	2.578062	0.086842
3	6	0	-2.552940	1.701312	1.139774
4	16	0	-3.672088	2.434932	-1.038389
5	6	0	-1.244557	3.456522	-0.291542
6	6	0	-0.548358	3.177355	-1.476057
7	6	0	-0.876539	4.573857	0.464551
8	6	0	0.513001	3.983496	-1.881844
9	1	0	-0.858815	2.330521	-2.088065
10	6	0	0.177090	5.382215	0.051734
11	1	0	-1.418812	4.799007	1.376358
12	6	0	0.879218	5.085660	-1.116559
13	1	0	1.050634	3.742901	-2.793914
14	1	0	0.451350	6.251278	0.643702
15	1	0	1.708044	5.713882	-1.428724
16	6	0	-1.714755	1.507214	2.340228
17	8	0	-1.926316	0.635778	3.160215
18	8	0	-0.733435	2.415530	2.470809
19	6	0	-0.003629	2.442457	3.704461
20	6	0	-0.177408	3.811097	4.334634
21	1	0	1.043294	2.258122	3.452957
22	1	0	-0.362155	1.640347	4.351002
23	1	0	0.412369	3.879775	5.254643
24	1	0	0.156455	4.596675	3.649127
25	1	0	-1.227977	3.992190	4.581843
26	26	0	2.870731	-2.919980	-0.832471
27	15	0	-0.065131	-1.832987	0.397510
28	15	0	2.229230	0.414740	-0.524640
29	6	0	-2.194406	-3.523079	-0.326123
30	6	0	0.576166	-1.832925	2.116085
31	6	0	1.708172	-0.688807	3.924478
32	6	0	-1.712684	-2.606053	0.611116
33	6	0	1.687249	-1.852851	4.684901
34	6	0	0.514824	-2.986987	2.907533
35	6	0	1.142169	-0.677569	2.651847
36	6	0	1.073983	-2.999042	4.179922
37	6	0	-2.504293	-2.263934	1.711129
38	6	0	-3.753575	-2.853866	1.880813
39	6	0	3.410020	-0.975734	-0.531147
40	6	0	4.074431	-1.493063	-1.687072
41	6	0	2.617332	1.246583	-2.124021
42	6	0	2.291889	-4.891111	-0.976436
43	6	0	3.795107	-1.791333	0.583980
44	6	0	4.855405	-2.612063	-1.290815
45	6	0	-3.443644	-4.110629	-0.151401
46	6	0	4.689096	-2.790896	0.111077
47	6	0	3.585699	2.247879	-2.243954
48	6	0	0.896564	-3.129544	-0.439736
49	6	0	1.871112	0.882873	-3.252708
50	6	0	1.971954	-4.203415	-2.180572
51	6	0	1.627917	-4.238413	0.096419
52	6	0	1.109437	-3.124615	-1.857417
53	6	0	2.979130	1.571217	0.689368
54	6	0	4.273756	1.436925	1.200315
55	6	0	2.082048	1.516901	-4.474602
56	6	0	3.800077	2.874759	-3.467466
57	6	0	3.046776	2.514803	-4.583627
58	6	0	-4.223166	-3.781731	0.955197
59	6	0	2.735386	3.645679	1.910056
60	6	0	2.211170	2.678763	1.058237
61	6	0	4.020244	3.501118	2.426870
62	6	0	4.786609	2.392866	2.073609
63	1	0	0.703917	-2.385643	-2.535700
64	1	0	2.359828	-4.430365	-3.164225
65	1	0	2.972329	-5.726792	-0.882498
66	1	0	1.730390	-4.490477	1.141611
67	1	0	3.440051	-1.682484	1.599929
68	1	0	5.119796	-3.583917	0.707281
69	1	0	5.439346	-3.241495	-1.948248

70	1	0	3.962819	-1.113848	-2.693531
71	1	0	1.132245	0.235856	2.068049
72	1	0	2.160778	0.216394	4.318439
73	1	0	2.129962	-1.865535	5.676473
74	1	0	1.025783	-3.901923	4.781421
75	1	0	0.011986	-3.874435	2.534070
76	1	0	-2.157389	-1.530468	2.433407
77	1	0	-4.361935	-2.580752	2.738151
78	1	0	-5.199051	-4.239198	1.089810
79	1	0	-3.807785	-4.824424	-0.884312
80	1	0	-1.598929	-3.775059	-1.197734
81	1	0	1.110434	0.107690	-3.172611
82	1	0	1.486620	1.231946	-5.336626
83	1	0	3.210602	3.012335	-5.534950
84	1	0	4.554404	3.651992	-3.547708
85	1	0	4.165971	2.550567	-1.378111
86	1	0	1.194008	2.776698	0.691705
87	1	0	2.128158	4.506628	2.173340
88	1	0	4.423729	4.249182	3.103240
89	1	0	5.789408	2.273497	2.473393
90	1	0	4.886757	0.587946	0.915014
91	45	0	0.021841	0.028258	-0.778480
92	6	0	-5.536175	-0.931734	-0.784818
93	6	0	-6.635614	-1.655215	-1.232688
94	6	0	-7.823941	-1.000793	-1.549628
95	6	0	-7.908787	0.383554	-1.418639
96	6	0	-6.813218	1.110720	-0.962680
97	6	0	-5.622302	0.456881	-0.635055
98	1	0	-4.592801	-1.425935	-0.576473
99	1	0	-6.554009	-2.732263	-1.348601
100	1	0	-8.680790	-1.566127	-1.904990
101	1	0	-8.832697	0.898442	-1.665834
102	1	0	-6.884808	2.188662	-0.843811
103	6	0	-4.439782	1.177992	-0.132779
104	6	0	-3.728513	0.905141	0.995033
105	1	0	-4.016537	0.149519	1.713507

Zero-point correction= 0.836498 (Hartree/Particle)
Thermal correction to Energy= 0.889839
Thermal correction to Enthalpy= 0.890784
Thermal correction to Gibbs Free Energy= 0.748507
Sum of electronic and zero-point Energies= -3969.120778
Sum of electronic and thermal Energies= -3969.067436
Sum of electronic and thermal Enthalpies= -3969.066492
Sum of electronic and thermal Free Energies= -3969.208768

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.3165216

INT13b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-3.398070	0.454408	2.355619
2	15	0	-2.220150	-1.360236	-0.270001
3	15	0	-1.444969	1.873984	0.108847
4	6	0	-1.052781	-3.551964	-1.524865
5	6	0	-3.792530	-1.980568	-0.980357
6	6	0	-5.756660	-1.618199	-2.342361
7	6	0	-1.128629	-2.833562	-0.326213
8	6	0	-6.233158	-2.878960	-1.997379
9	6	0	-4.270794	-3.253302	-0.647186
10	6	0	-4.537376	-1.170502	-1.838544
11	6	0	-5.486465	-3.699068	-1.152227
12	6	0	-0.327041	-3.215693	0.752450
13	6	0	0.532012	-4.305799	0.638054
14	6	0	-2.831199	2.043341	1.255913
15	6	0	-2.817755	2.387045	2.646587
16	6	0	0.045199	1.966386	1.172481
17	6	0	-3.903939	-1.217664	3.454863
18	6	0	-4.173722	1.669590	0.918735
19	6	0	-4.131766	2.208532	3.157132
20	6	0	-0.206426	-4.648957	-1.629791
21	6	0	-4.967570	1.769245	2.091150
22	6	0	0.902659	0.864152	1.227895
23	6	0	-2.663667	-1.231858	1.498304
24	6	0	0.392488	3.138672	1.853542
25	6	0	-2.583646	-0.797292	3.772277
26	6	0	-3.957157	-1.488973	2.061941
27	6	0	-1.818411	-0.802307	2.575493
28	6	0	-1.387463	3.482758	-0.767574
29	6	0	-2.169519	4.580793	-0.400964
30	6	0	1.572128	3.200639	2.588104
31	6	0	2.076659	0.925036	1.971554
32	6	0	2.416050	2.093466	2.644678
33	6	0	0.586940	-5.028081	-0.549623
34	6	0	-0.394677	4.802787	-2.541504
35	6	0	-0.508747	3.600977	-1.851358
36	6	0	-1.168637	5.896831	-2.161426
37	6	0	-2.058366	5.782403	-1.096032
38	1	0	-0.790471	-0.480526	2.490862
39	1	0	-2.230734	-0.475202	4.742517
40	1	0	-4.737703	-1.272211	4.141372
41	1	0	-4.836078	-1.785021	1.507644

42	1	0	-4.496474	1.306024	-0.047980
43	1	0	-6.013145	1.505410	2.172032
44	1	0	-4.430274	2.335438	4.188901
45	1	0	-1.941955	2.658139	3.219877
46	1	0	-4.139060	-0.202155	-2.130065
47	1	0	-6.326405	-0.984279	-3.014854
48	1	0	-7.180026	-3.230706	-2.396625
49	1	0	-5.849352	-4.689077	-0.892398
50	1	0	-3.687297	-3.896711	0.005597
51	1	0	-0.370606	-2.674428	1.691257
52	1	0	1.166900	-4.586936	1.472676
53	1	0	1.260732	-5.874649	-0.633635
54	1	0	-0.157448	-5.198338	-2.565008
55	1	0	-1.638718	-3.238736	-2.383158
56	1	0	-0.246675	4.015446	1.785104
57	1	0	1.841892	4.119652	3.099791
58	1	0	3.351228	2.148564	3.193715
59	1	0	2.749464	0.075811	1.986560
60	1	0	0.666280	-0.028544	0.652820
61	1	0	0.104119	2.754421	-2.154846
62	1	0	0.299992	4.881346	-3.371894
63	1	0	-1.081278	6.837057	-2.697593
64	1	0	-2.668447	6.631848	-0.803036
65	1	0	-2.867072	4.497923	0.427834
66	45	0	-1.426689	0.310616	-1.474794
67	17	0	-1.138734	-0.712044	-3.585370
68	6	0	3.406385	-1.733164	-0.721870
69	6	0	4.006506	-0.506105	-0.558334
70	16	0	2.018068	-1.612766	-1.742147
71	6	0	3.744309	-3.017466	-0.079684
72	6	0	3.895605	-3.095403	1.308943
73	6	0	3.874802	-4.182724	-0.839374
74	6	0	4.171709	-4.310444	1.923978
75	1	0	3.783597	-2.196612	1.909183
76	6	0	4.149728	-5.399646	-0.223966
77	1	0	3.762532	-4.130244	-1.918289
78	6	0	4.294728	-5.468952	1.158923
79	1	0	4.286939	-4.355382	3.003017
80	1	0	4.253156	-6.296468	-0.827889
81	1	0	4.507571	-6.419490	1.638854
82	6	0	5.225986	-0.332214	0.274264
83	8	0	6.192466	-1.059317	0.257825
84	8	0	5.114940	0.742375	1.075747
85	6	0	6.235230	1.039797	1.915290
86	6	0	6.190392	0.213102	3.189067
87	1	0	6.141809	2.108047	2.122172
88	1	0	7.159699	0.857190	1.361970
89	1	0	7.001720	0.510317	3.861535
90	1	0	5.238969	0.361587	3.711330
91	1	0	6.305461	-0.848736	2.955501
92	6	0	5.064065	2.329601	-1.651225
93	6	0	5.438942	3.668406	-1.685486
94	6	0	4.515486	4.665139	-1.373168
95	6	0	3.216592	4.313160	-1.017864
96	6	0	2.846803	2.972706	-0.974603
97	6	0	3.760007	1.967800	-1.297762
98	1	0	5.783218	1.557247	-1.911889
99	1	0	6.454200	3.934971	-1.965266
100	1	0	4.809718	5.710282	-1.406385
101	1	0	2.485538	5.076132	-0.765459
102	1	0	1.847186	2.696870	-0.659928
103	6	0	3.337269	0.548498	-1.271014
104	6	0	2.257409	0.073197	-1.962960
105	1	0	1.597163	0.619584	-2.623319

Zero-point correction=	0.834583 (Hartree/Particle)
Thermal correction to Energy=	0.889646
Thermal correction to Enthalpy=	0.890590
Thermal correction to Gibbs Free Energy=	0.739542
Sum of electronic and zero-point Energies=	-3969.114845
Sum of electronic and thermal Energies=	-3969.059782
Sum of electronic and thermal Enthalpies=	-3969.058838
Sum of electronic and thermal Free Energies=	-3969.209887

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent =-3972.3157442

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.779585	-0.668721	-0.004658
2	6	0	0.489328	0.673405	-0.145320
3	16	0	-0.682447	-1.583175	0.147256
4	6	0	2.061731	-1.398709	0.060351
5	6	0	2.262752	-2.532342	-0.734203
6	6	0	3.065482	-1.009640	0.953455
7	6	0	3.447444	-3.256236	-0.646232
8	1	0	1.493683	-2.837036	-1.438489
9	6	0	4.246173	-1.734421	1.040161
10	1	0	2.916474	-0.133599	1.573894
11	6	0	4.441750	-2.859149	0.241411
12	1	0	3.592353	-4.129201	-1.275401
13	1	0	5.017186	-1.420363	1.737060

14	1	0	5.367911	-3.421835	0.311094
15	6	0	1.503363	1.731981	-0.367276
16	8	0	2.701132	1.569885	-0.434208
17	8	0	0.912880	2.935489	-0.504581
18	6	0	1.786375	4.050897	-0.732402
19	6	0	2.370317	4.573316	0.568088
20	1	0	1.150048	4.797575	-1.211972
21	1	0	2.575284	3.748871	-1.425259
22	1	0	2.959609	5.475352	0.373543
23	1	0	1.574742	4.826571	1.275128
24	1	0	3.024973	3.824348	1.020262
25	6	0	-5.225486	-1.433854	-0.415903
26	6	0	-3.837435	-1.371460	-0.463480
27	6	0	-3.155502	-0.261624	0.048756
28	6	0	-3.899267	0.783769	0.610209
29	6	0	-5.287147	0.724533	0.646024
30	6	0	-5.955860	-0.385109	0.135522
31	1	0	-5.736984	-2.302230	-0.820005
32	1	0	-3.278842	-2.184897	-0.918860
33	1	0	-3.382194	1.637495	1.038073
34	1	0	-5.847405	1.543968	1.086348
35	1	0	-7.039943	-0.434093	0.171172
36	6	0	-1.687933	-0.173693	0.001614
37	6	0	-0.915000	0.940922	-0.140326
38	1	0	-1.323865	1.933693	-0.277123

Zero-point correction= 0.304627 (Hartree/Particle)
Thermal correction to Energy= 0.323791
Thermal correction to Enthalpy= 0.324735
Thermal correction to Gibbs Free Energy= 0.253623
Sum of electronic and zero-point Energies= -1281.698908
Sum of electronic and thermal Energies= -1281.679744
Sum of electronic and thermal Enthalpies= -1281.678800
Sum of electronic and thermal Free Energies= -1281.749912

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1282.2937664

TS9b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.883194	-1.979156	-1.822271
2	15	0	-0.310557	-1.900759	-0.514071
3	15	0	2.172564	0.591792	0.490501
4	6	0	-2.961057	-2.738885	-0.290326
5	6	0	0.055630	-3.086097	0.841045
6	6	0	1.373440	-3.623475	2.803952
7	6	0	-1.899831	-2.511227	-1.174419
8	6	0	0.857759	-4.916822	2.804311
9	6	0	-0.455213	-4.387714	0.845597
10	6	0	0.969474	-2.720809	1.827684
11	6	0	-0.056792	-5.294790	1.824272
12	6	0	-2.091956	-2.708916	-2.540604
13	6	0	-3.328854	-3.130796	-3.018869
14	6	0	3.309464	-0.442842	-0.506392
15	6	0	3.829291	-0.151512	-1.803927
16	6	0	2.765327	2.300078	0.120443
17	6	0	2.503012	-3.760830	-2.788240
18	6	0	3.901773	-1.677992	-0.078726
19	6	0	4.745719	-1.178707	-2.160680
20	6	0	-4.193092	-3.162664	-0.770877
21	6	0	4.794205	-2.118892	-1.093868
22	6	0	2.541966	2.833660	-1.155414
23	6	0	0.903969	-2.455501	-1.746974
24	6	0	3.400375	3.095895	1.078910
25	6	0	2.200109	-2.666509	-3.645731
26	6	0	1.703775	-3.641659	-1.622702
27	6	0	1.218100	-1.861630	-3.013952
28	6	0	2.901285	0.311800	2.163277
29	6	0	4.291057	0.253797	2.342501
30	6	0	3.839701	4.377800	0.755512
31	6	0	2.989159	4.109733	-1.476297
32	6	0	3.647521	4.883430	-0.525223
33	6	0	-4.380237	-3.355712	-2.138228
34	6	0	2.623973	-0.026948	4.550778
35	6	0	2.079986	0.177186	3.283588
36	6	0	4.003069	-0.089378	4.713471
37	6	0	4.836446	0.055340	3.604742
38	1	0	0.809286	-0.933038	-3.380729
39	1	0	2.676855	-2.448756	-4.591836
40	1	0	3.250652	-4.522298	-2.964481
41	1	0	1.729288	-4.301576	-0.767972
42	1	0	3.697609	-2.188624	0.852249
43	1	0	5.363011	-3.038595	-1.079184
44	1	0	5.271563	-1.254989	-3.102554
45	1	0	3.555510	0.692542	-2.419340
46	1	0	1.364438	-1.715220	1.840149
47	1	0	2.080708	-3.306234	3.565035
48	1	0	1.163380	-5.627310	3.566744
49	1	0	-0.463727	-6.301552	1.818116
50	1	0	-1.159522	-4.700199	0.081734
51	1	0	-1.283554	-2.524204	-3.239042
52	1	0	-3.469521	-3.274872	-4.085692

53	1	0	-5.345536	-3.682126	-2.514269
54	1	0	-5.008562	-3.332867	-0.074044
55	1	0	-2.825101	-2.588786	0.776461
56	1	0	3.561606	2.725069	2.084825
57	1	0	4.334620	4.979216	1.512764
58	1	0	3.989925	5.883306	-0.775490
59	1	0	2.795453	4.507666	-2.467434
60	1	0	1.976142	2.266650	-1.886328
61	1	0	1.003410	0.205757	3.168732
62	1	0	1.963923	-0.141111	5.405331
63	1	0	4.430383	-0.249833	5.698883
64	1	0	5.914952	0.012469	3.723723
65	1	0	4.949513	0.368926	1.486988
66	45	0	-0.335119	0.371405	0.147834
67	17	0	-0.113856	0.996708	-2.185712
68	6	0	-2.785591	0.153502	1.296384
69	6	0	-2.353788	0.445034	0.062640
70	16	0	-1.346728	-0.193566	2.274437
71	6	0	-4.149452	0.097091	1.851329
72	6	0	-5.227328	-0.288287	1.043289
73	6	0	-4.392572	0.416712	3.191209
74	6	0	-6.516703	-0.331978	1.561757
75	1	0	-5.049187	-0.575202	0.011406
76	6	0	-5.682523	0.368841	3.708036
77	1	0	-3.562430	0.713252	3.826345
78	6	0	-6.750338	-0.003524	2.894994
79	1	0	-7.341490	-0.632981	0.921924
80	1	0	-5.854829	0.625963	4.749279
81	1	0	-7.757583	-0.042123	3.299466
82	6	0	-3.215472	0.799966	-1.086566
83	8	0	-3.412835	0.115899	-2.064598
84	8	0	-3.804698	1.998424	-0.890381
85	6	0	-4.751334	2.404387	-1.887113
86	6	0	-4.070031	3.115405	-3.043340
87	1	0	-5.437946	3.068770	-1.358065
88	1	0	-5.296460	1.524035	-2.237150
89	1	0	-4.812984	3.401185	-3.795944
90	1	0	-3.566840	4.021892	-2.693818
91	1	0	-3.334419	2.455717	-3.512099
92	6	0	0.300702	4.832980	0.634590
93	6	0	0.411049	6.035545	-0.049579
94	6	0	-0.198915	6.188711	-1.292657
95	6	0	-0.923586	5.133889	-1.840312
96	6	0	-1.036398	3.927065	-1.158760
97	6	0	-0.419714	3.764721	0.082530
98	1	0	0.796239	4.701784	1.591010
99	1	0	0.984015	6.849586	0.384470
100	1	0	-0.109010	7.127419	-1.832038
101	1	0	-1.400706	5.244681	-2.809963
102	1	0	-1.592490	3.105429	-1.585062
103	6	0	-0.522541	2.530403	0.854394
104	6	0	-0.499347	2.117568	2.034587
105	1	0	-0.387958	2.140274	3.096673

Zero-point correction=	0.830856 (Hartree/Particle)
Thermal correction to Energy=	0.885627
Thermal correction to Enthalpy=	0.886572
Thermal correction to Gibbs Free Energy=	0.741109
Sum of electronic and zero-point Energies=	-3969.007236
Sum of electronic and thermal Energies=	-3968.952465
Sum of electronic and thermal Enthalpies=	-3968.951521
Sum of electronic and thermal Free Energies=	-3969.096983

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.1985543

TS10b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.894421	0.414030	2.262251
2	6	0	-2.612769	1.224119	0.539627
3	6	0	-1.662620	1.205895	-0.440497
4	16	0	-1.854500	0.900556	2.061245
5	6	0	-4.049685	1.524233	0.406249
6	6	0	-4.997580	0.735311	1.065751
7	6	0	-4.485596	2.588877	-0.389687
8	6	0	-6.355707	0.995082	0.915394
9	1	0	-4.658840	-0.089802	1.686142
10	6	0	-5.843223	2.849766	-0.535783
11	1	0	-3.751947	3.220070	-0.883862
12	6	0	-6.782663	2.050353	0.112600
13	1	0	-7.083170	0.371070	1.426381
14	1	0	-6.168327	3.683521	-1.151600
15	1	0	-7.843309	2.254477	-0.001345
16	6	0	-1.926258	1.334144	-1.888892
17	8	0	-1.299546	2.034026	-2.667437
18	8	0	-2.952133	0.565970	-2.287921
19	6	0	-3.326154	0.645097	-3.670476
20	6	0	-4.250574	1.822438	-3.921697
21	1	0	-3.828195	-0.305623	-3.864947
22	1	0	-2.421171	0.704525	-4.279537
23	1	0	-4.592335	1.811662	-4.962135
24	1	0	-5.122576	1.774545	-3.263035

25	1	0	-3.724226	2.763791	-3.741823
26	26	0	2.965253	-2.579128	-0.324204
27	15	0	1.657469	0.459742	-1.149182
28	15	0	-0.284883	-1.787564	0.915640
29	6	0	3.616588	2.425692	-0.772446
30	6	0	0.984852	-0.084725	-2.765280
31	6	0	-0.571307	-1.512754	-3.955375
32	6	0	2.460449	2.074866	-1.474000
33	6	0	0.012440	-1.150584	-5.165780
34	6	0	1.572421	0.267013	-3.984415
35	6	0	-0.086975	-0.976471	-2.767085
36	6	0	1.082903	-0.257995	-5.176484
37	6	0	1.879521	3.005267	-2.343892
38	6	0	2.463662	4.254821	-2.524357
39	6	0	1.119333	-2.904910	0.539612
40	6	0	2.165538	-3.320790	1.419435
41	6	0	-0.727209	-2.212523	2.661561
42	6	0	4.603886	-2.318469	-1.553797
43	6	0	1.271481	-3.650276	-0.679643
44	6	0	2.932364	-4.321886	0.763697
45	6	0	4.198890	3.676430	-0.958315
46	6	0	2.377364	-4.530338	-0.530129
47	6	0	-1.998091	-2.716239	2.963301
48	6	0	3.070341	-0.675839	-1.009939
49	6	0	0.171825	-1.993856	3.710833
50	6	0	4.899687	-1.856533	-0.241362
51	6	0	3.486819	-1.590107	-2.036664
52	6	0	3.964376	-0.847021	0.099474
53	6	0	-1.627253	-2.686772	0.023168
54	6	0	-1.660300	-4.089749	0.010015
55	6	0	-0.180857	-2.303751	5.020307
56	6	0	-2.348893	-3.017886	4.275532
57	6	0	-1.439566	-2.820922	5.308944
58	6	0	3.627260	4.592304	-1.836292
59	6	0	-3.730763	-2.664811	-1.181841
60	6	0	-2.682399	-1.988686	-0.559677
61	6	0	-3.742312	-4.053611	-1.212586
62	6	0	-2.705543	-4.764716	-0.607015
63	1	0	3.872649	-0.349493	1.052832
64	1	0	5.666156	-2.248516	0.413349
65	1	0	5.104754	-3.122471	-2.075848
66	1	0	2.999439	-1.739630	-2.988766
67	1	0	0.650946	-3.555570	-1.559762
68	1	0	2.763476	-5.194699	-1.291095
69	1	0	3.816428	-4.799750	1.163111
70	1	0	2.363809	-2.917349	2.400333
71	1	0	-0.567614	-1.241718	-1.834499
72	1	0	-1.412182	-2.199819	-3.925147
73	1	0	-0.363944	-1.559399	-6.098949
74	1	0	1.543394	0.028049	-6.117394
75	1	0	2.418641	0.946565	-4.005481
76	1	0	0.963660	2.756553	-2.872391
77	1	0	2.005328	4.966598	-3.204518
78	1	0	4.082216	5.567958	-1.979998
79	1	0	5.096954	3.934931	-0.405647
80	1	0	4.063533	1.731456	-0.070310
81	1	0	1.131086	-1.532631	3.514953
82	1	0	0.533937	-2.125130	5.818091
83	1	0	-1.713872	-3.057835	6.332790
84	1	0	-3.341495	-3.405221	4.485705
85	1	0	-2.731525	-2.869643	2.180847
86	1	0	-2.693877	-0.910601	-0.537381
87	1	0	-4.536015	-2.090062	-1.629409
88	1	0	-4.557501	-4.585483	-1.694767
89	1	0	-2.714224	-5.850645	-0.610341
90	1	0	-0.872678	-4.658476	0.493047
91	45	0	0.043608	0.606230	0.602632
92	6	0	-0.351446	2.742854	-0.081228
93	6	0	0.147305	2.808499	1.067087
94	6	0	0.872195	3.487681	2.115530
95	6	0	0.596533	3.282424	3.470043
96	6	0	1.867108	4.399323	1.740074
97	6	0	1.301334	3.989615	4.435275
98	1	0	-0.163774	2.561813	3.748672
99	6	0	2.571193	5.101385	2.711096
100	1	0	2.079685	4.547152	0.686189
101	6	0	2.289461	4.897826	4.059747
102	1	0	1.083814	3.825601	5.486331
103	1	0	3.341352	5.806903	2.412865
104	1	0	2.841206	5.444889	4.818962
105	1	0	-0.495464	3.139807	-1.070210

Zero-point correction= 0.832021 (Hartree/Particle)
Thermal correction to Energy= 0.886479
Thermal correction to Enthalpy= 0.887423
Thermal correction to Gibbs Free Energy= 0.742205
Sum of electronic and zero-point Energies= -3969.019571
Sum of electronic and thermal Energies= -3968.965113
Sum of electronic and thermal Enthalpies= -3968.964169
Sum of electronic and thermal Free Energies= -3969.109387

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2118054

INT14b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.258205	-2.733054	-1.628239
2	15	0	-0.765840	-1.839925	-0.388919
3	15	0	2.196934	0.178933	0.417584
4	6	0	-3.506475	-2.176167	0.046719
5	6	0	-0.574671	-2.881403	1.115231
6	6	0	0.450696	-3.222396	3.289155
7	6	0	-2.477670	-2.241301	-0.898742
8	6	0	-0.125113	-4.485736	3.371164
9	6	0	-1.164234	-4.148549	1.216214
10	6	0	0.216716	-2.427346	2.170025
11	6	0	-0.938504	-4.943660	2.334817
12	6	0	-2.786735	-2.554848	-2.222313
13	6	0	-4.104801	-2.802235	-2.594102
14	6	0	2.994764	-1.274117	-0.363560
15	6	0	3.699505	-1.256507	-1.605558
16	6	0	3.311523	1.539451	-0.133142
17	6	0	1.514918	-4.371203	-2.625487
18	6	0	3.139116	-2.592710	0.187181
19	6	0	4.294394	-2.531533	-1.803911
20	6	0	-4.821050	-2.427702	-0.325817
21	6	0	3.959864	-3.353376	-0.691577
22	6	0	3.086088	2.143514	-1.374904
23	6	0	0.234748	-2.745142	-1.599933
24	6	0	4.377355	1.984810	0.655073
25	6	0	1.488589	-3.230946	-3.476104
26	6	0	0.737528	-4.080955	-1.473792
27	6	0	0.701615	-2.228592	-2.853828
28	6	0	2.720338	-0.011941	2.180937
29	6	0	3.786651	-0.820520	2.593661
30	6	0	5.203538	3.011510	0.206942
31	6	0	3.918458	3.164377	-1.820606
32	6	0	4.978258	3.602042	-1.032177
33	6	0	-5.123085	-2.737723	-1.649733
34	6	0	2.389755	0.648605	4.495845
35	6	0	2.048803	0.741048	3.149680
36	6	0	3.422287	-0.192363	4.898287
37	6	0	4.127859	-0.915018	3.939875
38	1	0	0.527244	-1.224681	-3.211639
39	1	0	2.021916	-3.121762	-4.410642
40	1	0	2.074199	-5.281374	-2.795532
41	1	0	0.605861	-4.728877	-0.618966
42	1	0	2.688612	-2.950774	1.102711
43	1	0	4.219133	-4.395947	-0.566639
44	1	0	4.860047	-2.835363	-2.674109
45	1	0	3.753907	-0.414088	-2.281189
46	1	0	0.655203	-1.439432	2.127238
47	1	0	1.078348	-2.842630	4.090148
48	1	0	0.048251	-5.110191	4.242686
49	1	0	-1.402156	-5.923544	2.399992
50	1	0	-1.805489	-4.511014	0.417900
51	1	0	-2.001616	-2.599855	-2.969967
52	1	0	-4.333507	-3.038650	-3.628891
53	1	0	-6.151477	-2.928478	-1.942459
54	1	0	-5.608689	-2.370543	0.419681
55	1	0	-3.284521	-1.935039	1.082466
56	1	0	4.568608	1.541127	1.625722
57	1	0	6.024249	3.349333	0.833296
58	1	0	5.620263	4.407483	-1.377182
59	1	0	3.716741	3.635000	-2.777645
60	1	0	2.239364	1.836499	-1.979252
61	1	0	1.264113	1.423240	2.846931
62	1	0	1.844884	1.237904	5.227312
63	1	0	3.685174	-0.274298	5.948783
64	1	0	4.953937	-1.554267	4.237435
65	1	0	4.365950	-1.374880	1.865057
66	45	0	-0.276314	0.568444	0.005906
67	17	0	0.029938	0.989819	-2.350276
68	6	0	-2.754929	0.975994	1.096649
69	6	0	-2.260064	0.966175	-0.140321
70	16	0	-1.289584	0.824998	2.179186
71	6	0	-4.100307	1.168494	1.653847
72	6	0	-5.228414	0.805163	0.903923
73	6	0	-4.284480	1.707999	2.931659
74	6	0	-6.504475	0.994195	1.422320
75	1	0	-5.098900	0.359030	-0.076644
76	6	0	-5.562444	1.890677	3.447458
77	1	0	-3.420639	1.993396	3.526493
78	6	0	-6.678333	1.535435	2.693968
79	1	0	-7.368593	0.707344	0.829707
80	1	0	-5.686675	2.315833	4.439111
81	1	0	-7.676534	1.675940	3.097979
82	6	0	-2.997725	1.293876	-1.384379
83	8	0	-3.617410	0.515703	-2.073136
84	8	0	-2.899180	2.607771	-1.634852
85	6	0	-3.528638	3.080649	-2.835421
86	6	0	-2.647951	2.857172	-4.051708
87	1	0	-3.693115	4.143976	-2.649300
88	1	0	-4.493968	2.580769	-2.949925
89	1	0	-3.129434	3.287319	-4.936983

90	1	0	-1.671330	3.330980	-3.917069
91	1	0	-2.488899	1.789738	-4.218082
92	6	0	1.611618	4.334799	0.767680
93	6	0	2.224545	5.447681	0.203781
94	6	0	1.804093	5.921240	-1.036513
95	6	0	0.771748	5.272684	-1.711504
96	6	0	0.167552	4.149290	-1.159397
97	6	0	0.579709	3.673445	0.090083
98	1	0	1.952777	3.948923	1.724405
99	1	0	3.039100	5.938076	0.728734
100	1	0	2.282709	6.790878	-1.478055
101	1	0	0.438164	5.641015	-2.677811
102	1	0	-0.629448	3.628797	-1.677255
103	6	0	-0.063488	2.499377	0.689595
104	6	0	-0.611662	2.478313	1.905782
105	1	0	-0.776556	3.268567	2.633383

Zero-point correction=	0.834078 (Hartree/Particle)
Thermal correction to Energy=	0.888393
Thermal correction to Enthalpy=	0.889337
Thermal correction to Gibbs Free Energy=	0.745904
Sum of electronic and zero-point Energies=	-3969.053133
Sum of electronic and thermal Energies=	-3968.998818
Sum of electronic and thermal Enthalpies=	-3968.997874
Sum of electronic and thermal Free Energies=	-3969.141307

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2457023

INT15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.383564	1.195306	2.398495
2	6	0	1.250855	-2.409896	1.118682
3	6	0	0.140151	-2.541150	0.212359
4	16	0	0.953714	-1.563601	2.563356
5	6	0	2.610399	-2.927334	0.843219
6	6	0	3.748520	-2.227144	1.256984
7	6	0	2.763516	-4.175480	0.227421
8	6	0	5.015741	-2.746829	1.022536
9	1	0	3.630170	-1.266771	1.748594
10	6	0	4.029802	-4.704647	0.014910
11	1	0	1.884928	-4.742559	-0.067286
12	6	0	5.159557	-3.984795	0.401215
13	1	0	5.891974	-2.183807	1.328857
14	1	0	4.135808	-5.679627	-0.451073
15	1	0	6.149850	-4.395461	0.227467
16	6	0	0.297028	-2.911981	-1.222493
17	8	0	-0.547028	-3.533423	-1.838941
18	8	0	1.425072	-2.469207	-1.790873
19	6	0	1.623150	-2.780965	-3.176902
20	6	0	2.199027	-4.174186	-3.351245
21	1	0	2.317256	-2.013879	-3.524582
22	1	0	0.672873	-2.663878	-3.702661
23	1	0	2.396430	-4.361281	-4.411987
24	1	0	3.137547	-4.276330	-2.798017
25	1	0	1.491463	-4.928147	-2.995816
26	26	0	-0.916317	3.603004	-0.706172
27	15	0	-1.719093	0.233813	-0.939444
28	15	0	1.524603	1.357686	0.564894
29	6	0	-4.529933	0.044239	-0.750817
30	6	0	-0.959017	-0.000897	-2.601464
31	6	0	0.987445	0.407916	-3.995125
32	6	0	-3.343982	-0.595284	-1.114713
33	6	0	0.264180	0.044195	-5.127340
34	6	0	-1.680753	-0.357154	-3.745537
35	6	0	0.375539	0.372782	-2.747937
36	6	0	-1.067351	-0.344204	-4.996002
37	6	0	-3.398313	-1.904068	-1.612923
38	6	0	-4.625288	-2.534193	-1.790995
39	6	0	0.917192	3.022469	0.094019
40	6	0	0.264707	3.968258	0.941398
41	6	0	2.447832	1.639102	2.146341
42	6	0	-2.458007	4.100011	-1.977401
43	6	0	1.068022	3.640376	-1.192487
44	6	0	0.052017	5.162693	0.200125
45	6	0	-5.754427	-0.600664	-0.907562
46	6	0	0.550515	4.962272	-1.117438
47	6	0	3.824660	1.401881	2.244906
48	6	0	-2.129273	1.999211	-1.072489
49	6	0	1.752947	2.006297	3.304882
50	6	0	-2.908288	4.125461	-0.627680
51	6	0	-1.983859	2.793706	-2.258860
52	6	0	-2.707385	2.839431	-0.065199
53	6	0	2.950820	1.189028	-0.594182
54	6	0	3.818413	2.253890	-0.878866
55	6	0	2.419541	2.158378	4.515619
56	6	0	4.487150	1.543687	3.461889
57	6	0	3.789550	1.928906	4.600917
58	6	0	-5.807157	-1.883840	-1.440672
59	6	0	4.346717	-0.262852	-1.944962
60	6	0	3.231446	-0.064946	-1.132325
61	6	0	5.191592	0.801923	-2.234652

62	6	0	4.924112	2.062610	-1.698460
63	1	0	-2.892152	2.548833	0.957605
64	1	0	-3.282352	4.991186	-0.098201
65	1	0	-2.428303	4.941157	-2.656780
66	1	0	-1.552422	2.465058	-3.193095
67	1	0	1.499426	3.179276	-2.069814
68	1	0	0.492818	5.667104	-1.935733
69	1	0	-0.451986	6.047923	0.563340
70	1	0	-0.054850	3.787459	1.956673
71	1	0	0.944792	0.650205	-1.875297
72	1	0	2.030316	0.704448	-4.069223
73	1	0	0.733049	0.062616	-6.106789
74	1	0	-1.640397	-0.627477	-5.873921
75	1	0	-2.726876	-0.630920	-3.670716
76	1	0	-2.486433	-2.435890	-1.866742
77	1	0	-4.653199	-3.542370	-2.193618
78	1	0	-6.763887	-2.379999	-1.575140
79	1	0	-6.667802	-0.091734	-0.615561
80	1	0	-4.507643	1.050206	-0.346969
81	1	0	0.677613	2.132645	3.271735
82	1	0	1.857041	2.445027	5.399299
83	1	0	4.306483	2.041706	5.549320
84	1	0	5.555414	1.353520	3.513376
85	1	0	4.397028	1.103127	1.373922
86	1	0	2.566553	-0.895690	-0.938622
87	1	0	4.548903	-1.254466	-2.339725
88	1	0	6.060615	0.655071	-2.869569
89	1	0	5.585894	2.896618	-1.912872
90	1	0	3.635419	3.232504	-0.445929
91	45	0	-0.397358	-0.440819	0.921988
92	6	0	-1.196207	-2.915413	0.796642
93	6	0	-1.749159	-1.887121	1.417885
94	6	0	-2.956770	-1.856053	2.251090
95	6	0	-2.912861	-1.388691	3.570860
96	6	0	-4.161512	-2.371287	1.760841
97	6	0	-4.047763	-1.431680	4.371525
98	1	0	-1.984094	-0.986861	3.957846
99	6	0	-5.299679	-2.402655	2.560149
100	1	0	-4.203422	-2.745426	0.744875
101	6	0	-5.247758	-1.931082	3.868141
102	1	0	-3.995403	-1.066457	5.393251
103	1	0	-6.226769	-2.798311	2.154282
104	1	0	-6.135799	-1.953057	4.493939
105	1	0	-1.550754	-3.943988	0.744069

Zero-point correction=	0.835463 (Hartree/Particle)
Thermal correction to Energy=	0.889444
Thermal correction to Enthalpy=	0.890388
Thermal correction to Gibbs Free Energy=	0.748007
Sum of electronic and zero-point Energies=	-3969.074247
Sum of electronic and thermal Energies=	-3969.020266
Sum of electronic and thermal Enthalpies=	-3969.019322
Sum of electronic and thermal Free Energies=	-3969.161703

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2635856

INT16b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.886847	1.259739	2.841003
2	15	0	-1.290145	1.683474	-0.461431
3	15	0	1.767096	0.158905	0.807496
4	6	0	-2.540650	2.077800	-2.914176
5	6	0	-0.580059	3.379542	-0.375952
6	6	0	1.346093	4.846075	-0.262329
7	6	0	-2.745831	1.991989	-1.533095
8	6	0	0.510238	5.947309	-0.105690
9	6	0	-1.413947	4.497813	-0.253611
10	6	0	0.801406	3.572356	-0.404832
11	6	0	-0.872313	5.771219	-0.110951
12	6	0	-4.036926	2.150136	-1.020121
13	6	0	-5.109879	2.383180	-1.877313
14	6	0	1.075813	0.859700	2.357956
15	6	0	0.685006	0.116833	3.518452
16	6	0	2.571130	-1.353313	1.473683
17	6	0	-2.818253	1.783813	3.328401
18	6	0	0.884310	2.247345	2.669157
19	6	0	0.273251	1.031498	4.523916
20	6	0	-3.613726	2.316175	-3.765853
21	6	0	0.405042	2.346994	4.002333
22	6	0	1.755958	-2.438247	1.801294
23	6	0	-2.028428	1.479608	1.179230
24	6	0	3.952060	-1.471939	1.642193
25	6	0	-2.744763	0.383574	3.080658
26	6	0	-2.384143	2.462662	2.158502
27	6	0	-2.262517	0.192433	1.760217
28	6	0	3.222556	1.219357	0.463832
29	6	0	3.793726	2.069666	1.418053
30	6	0	4.498014	-2.659992	2.123385
31	6	0	2.297052	-3.627648	2.272163
32	6	0	3.676714	-3.741118	2.430095
33	6	0	-4.899404	2.465315	-3.250560

34	6	0	4.999006	1.796223	-1.076278
35	6	0	3.841519	1.082013	-0.783143
36	6	0	5.546379	2.660408	-0.133331
37	6	0	4.943051	2.793230	1.115429
38	1	0	-2.059072	-0.759752	1.291967
39	1	0	-2.971327	-0.397405	3.793778
40	1	0	-3.096575	2.251500	4.263284
41	1	0	-2.265918	3.531607	2.050703
42	1	0	1.054137	3.076494	1.998408
43	1	0	0.129927	3.264754	4.504077
44	1	0	-0.115387	0.766160	5.497660
45	1	0	0.692280	-0.958817	3.614848
46	1	0	1.461975	2.730383	-0.562840
47	1	0	2.425119	4.967260	-0.283265
48	1	0	0.932146	6.942263	0.003187
49	1	0	-1.532332	6.628370	-0.013875
50	1	0	-2.493365	4.375555	-0.279734
51	1	0	-4.209588	2.076550	0.049845
52	1	0	-6.109176	2.502916	-1.468360
53	1	0	-5.735772	2.644196	-3.919980
54	1	0	-3.445149	2.377270	-4.836601
55	1	0	-1.540113	1.950207	-3.319082
56	1	0	4.610235	-0.650377	1.382519
57	1	0	5.573753	-2.742312	2.246514
58	1	0	4.109678	-4.670060	2.788980
59	1	0	1.641488	-4.465785	2.487267
60	1	0	0.683368	-2.339301	1.689722
61	1	0	3.423957	0.421460	-1.531680
62	1	0	5.463960	1.671946	-2.049062
63	1	0	6.445804	3.223437	-0.365619
64	1	0	5.371294	3.455342	1.862306
65	1	0	3.352248	2.164319	2.403644
66	45	0	0.249944	-0.267701	-1.100083
67	17	0	1.144431	1.234935	-2.712485
68	6	0	-1.631528	-2.127412	-1.414196
69	6	0	-0.623798	-2.740193	-0.669091
70	16	0	-1.214389	-1.105622	-2.746065
71	6	0	-3.068240	-2.379116	-1.122186
72	6	0	-3.987140	-1.331355	-1.045743
73	6	0	-3.523874	-3.695252	-0.984686
74	6	0	-5.326819	-1.586365	-0.782754
75	1	0	-3.646907	-0.315184	-1.198191
76	6	0	-4.869548	-3.951377	-0.742133
77	1	0	-2.825799	-4.521782	-1.084996
78	6	0	-5.772541	-2.897703	-0.627411
79	1	0	-6.024018	-0.756339	-0.715172
80	1	0	-5.212343	-4.977327	-0.645309
81	1	0	-6.822407	-3.098276	-0.434785
82	6	0	-0.957149	-3.562896	0.536991
83	8	0	-0.602554	-4.710636	0.689301
84	8	0	-1.626253	-2.861308	1.466214
85	6	0	-2.005107	-3.538590	2.673001
86	6	0	-3.357557	-4.206235	2.514958
87	1	0	-2.029731	-2.747684	3.426182
88	1	0	-1.227739	-4.261057	2.932977
89	1	0	-3.675578	-4.632661	3.472079
90	1	0	-4.107268	-3.483394	2.180391
91	1	0	-3.301217	-5.011420	1.777975
92	6	0	0.743776	-2.943106	-1.193365
93	6	0	1.393123	-1.874444	-1.652399
94	6	0	2.738330	-1.918229	-2.241445
95	6	0	3.771526	-2.563344	-1.546299
96	6	0	3.026951	-1.327648	-3.478888
97	6	0	5.066168	-2.582572	-2.054287
98	1	0	3.553744	-3.039739	-0.596011
99	6	0	4.321059	-1.355733	-3.987327
100	1	0	2.231196	-0.837954	-4.026536
101	6	0	5.347919	-1.970034	-3.272466
102	1	0	5.855349	-3.076249	-1.493948
103	1	0	4.527661	-0.891615	-4.947453
104	1	0	6.359330	-1.979533	-3.669037
105	1	0	1.131563	-3.961143	-1.196858

Zero-point correction= 0.834627 (Hartree/Particle)
Thermal correction to Energy= 0.888220
Thermal correction to Enthalpy= 0.889164
Thermal correction to Gibbs Free Energy= 0.747830
Sum of electronic and zero-point Energies= -3969.072138
Sum of electronic and thermal Energies= -3969.018546
Sum of electronic and thermal Enthalpies= -3969.017602
Sum of electronic and thermal Free Energies= -3969.158936

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2628878

TS11b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.471937	-2.996409	-0.676820
2	15	0	0.534424	-1.938295	0.690750
3	15	0	-2.371083	0.358838	-0.394021
4	6	0	2.110255	-1.526766	2.946559
5	6	0	1.771703	-2.638363	-0.476357

6	6	0	2.383312	-3.263554	-2.741710
7	6	0	1.226481	-2.408231	2.320014
8	6	0	3.698469	-3.480667	-2.337747
9	6	0	3.091421	-2.868812	-0.082021
10	6	0	1.432265	-2.841161	-1.820303
11	6	0	4.045253	-3.286895	-1.006264
12	6	0	0.949715	-3.643814	2.915847
13	6	0	1.547926	-3.988207	4.123598
14	6	0	-2.905115	-1.115541	-1.312753
15	6	0	-4.107246	-1.882615	-1.189674
16	6	0	-3.739981	0.565058	0.807351
17	6	0	-2.267630	-4.877800	0.135565
18	6	0	-2.077212	-1.785012	-2.269871
19	6	0	-4.007325	-3.011099	-2.048479
20	6	0	2.715661	-1.881125	4.149029
21	6	0	-2.754592	-2.948552	-2.720849
22	6	0	-3.502802	0.368602	2.169172
23	6	0	-0.859865	-3.097356	0.569573
24	6	0	-5.034870	0.884825	0.376161
25	6	0	-2.928415	-4.009425	1.049883
26	6	0	-0.991469	-4.323800	-0.155089
27	6	0	-2.065268	-2.915168	1.319488
28	6	0	-2.713101	1.704209	-1.595414
29	6	0	-2.711686	1.496897	-2.976865
30	6	0	-6.076041	0.984059	1.291291
31	6	0	-4.549416	0.468221	3.084792
32	6	0	-5.834792	0.770366	2.648335
33	6	0	2.433422	-3.107796	4.741790
34	6	0	-2.844643	4.093708	-1.980399
35	6	0	-2.797433	3.013086	-1.109085
36	6	0	-2.822550	3.880155	-3.357706
37	6	0	-2.769256	2.579996	-3.852619
38	1	0	-2.287598	-2.068153	1.953716
39	1	0	-3.933422	-4.129717	1.430752
40	1	0	-2.683037	-5.774786	-0.303459
41	1	0	-0.257565	-4.734304	-0.834438
42	1	0	-1.095138	-1.453287	-2.575495
43	1	0	-2.366119	-3.680824	-3.415624
44	1	0	-4.737211	-3.804508	-2.135630
45	1	0	-4.917639	-1.673636	-0.505448
46	1	0	0.410223	-2.684723	-2.144780
47	1	0	2.097978	-3.415181	-3.778812
48	1	0	4.448604	-3.790631	-3.058408
49	1	0	5.069661	-3.441365	-0.682796
50	1	0	3.385014	-2.712956	0.950712
51	1	0	0.268116	-4.341529	2.439040
52	1	0	1.324245	-4.947907	4.580560
53	1	0	2.899630	-3.378665	5.684981
54	1	0	3.400391	-1.184382	4.622993
55	1	0	2.333160	-0.563305	2.502148
56	1	0	-5.224425	1.057892	-0.679724
57	1	0	-7.076219	1.230495	0.946773
58	1	0	-6.648133	0.849962	3.363908
59	1	0	-4.351771	0.317851	4.141812
60	1	0	-2.492359	0.175467	2.515947
61	1	0	-2.801391	3.193423	-0.038889
62	1	0	-2.880729	5.101964	-1.579114
63	1	0	-2.852050	4.723051	-4.041963
64	1	0	-2.768249	2.404285	-4.924608
65	1	0	-2.661971	0.489952	-3.379217
66	45	0	0.128783	0.457155	0.172365
67	17	0	-0.116904	0.929855	2.491975
68	6	0	2.473029	0.684028	-1.123117
69	6	0	2.011434	1.297176	0.003627
70	16	0	1.002316	0.518393	-2.163490
71	6	0	3.779514	0.218929	-1.576278
72	6	0	4.817799	0.010800	-0.651717
73	6	0	4.037859	-0.031242	-2.931905
74	6	0	6.074256	-0.395837	-1.079395
75	1	0	4.628213	0.142999	0.407418
76	6	0	5.290948	-0.461943	-3.351293
77	1	0	3.251641	0.112946	-3.667064
78	6	0	6.318468	-0.639213	-2.429370
79	1	0	6.862729	-0.543838	-0.346935
80	1	0	5.465963	-0.650727	-4.406556
81	1	0	7.299362	-0.969063	-2.758966
82	6	0	2.868900	1.858044	1.084831
83	8	0	3.310275	1.247507	2.034714
84	8	0	3.101729	3.153035	0.860076
85	6	0	3.736454	3.894718	1.914857
86	6	0	2.698226	4.372292	2.913609
87	1	0	4.220637	4.730385	1.405877
88	1	0	4.494805	3.265871	2.386540
89	1	0	3.184795	4.948208	3.708333
90	1	0	1.955469	5.006256	2.420999
91	1	0	2.183948	3.519083	3.365388
92	6	0	0.405740	2.167510	-1.840670
93	6	0	0.554754	2.420062	-0.519774
94	6	0	0.296240	3.758049	0.043445
95	6	0	-0.538492	3.968926	1.144620
96	6	0	0.877118	4.868772	-0.583870
97	6	0	-0.809535	5.260531	1.586252
98	1	0	-0.965758	3.113622	1.654680

99	6	0	0.611735	6.157784	-0.136998
100	1	0	1.558032	4.707334	-1.414364
101	6	0	-0.239036	6.359437	0.948555
102	1	0	-1.465563	5.405144	2.439860
103	1	0	1.073011	7.006678	-0.633798
104	1	0	-0.445334	7.365829	1.301636
105	1	0	-0.088169	2.737642	-2.617989

Zero-point correction= 0.832209 (Hartree/Particle)
Thermal correction to Energy= 0.886537
Thermal correction to Enthalpy= 0.887481
Thermal correction to Gibbs Free Energy= 0.741591
Sum of electronic and zero-point Energies= -3969.016786
Sum of electronic and thermal Energies= -3968.962458
Sum of electronic and thermal Enthalpies= -3968.961514
Sum of electronic and thermal Free Energies= -3969.107404

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2020532

TS12b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.295711	1.935696	2.749279
2	15	0	-1.103769	1.759834	-0.538652
3	15	0	1.916482	0.205611	0.813815
4	6	0	-2.604961	1.559395	-2.848742
5	6	0	-0.572442	3.479546	-0.869508
6	6	0	1.185401	5.089830	-1.275555
7	6	0	-2.679783	1.642779	-1.452761
8	6	0	0.248339	6.119176	-1.282483
9	6	0	-1.511938	4.515848	-0.903150
10	6	0	0.777444	3.773347	-1.075296
11	6	0	-1.102705	5.830584	-1.101103
12	6	0	-3.922746	1.565948	-0.824506
13	6	0	-5.081015	1.408521	-1.582047
14	6	0	1.578873	1.334912	2.212826
15	6	0	1.332768	1.005687	3.584091
16	6	0	2.343464	-1.342443	1.701000
17	6	0	-2.203517	2.434038	3.346117
18	6	0	1.453872	2.758062	2.096113
19	6	0	1.043045	2.205099	4.289328
20	6	0	-3.763557	1.410125	-3.600656
21	6	0	1.125507	3.287645	3.371167
22	6	0	1.320631	-2.023436	2.370311
23	6	0	-1.609265	1.802622	1.202725
24	6	0	3.618944	-1.908678	1.664790
25	6	0	-2.039717	1.019589	3.337772
26	6	0	-1.942863	2.918634	2.035734
27	6	0	-1.670774	0.629655	2.023387
28	6	0	3.548718	0.802558	0.234665
29	6	0	4.399090	1.552448	1.056862
30	6	0	3.862609	-3.134000	2.283069
31	6	0	1.566067	-3.239353	2.996528
32	6	0	2.838911	-3.803140	2.946274
33	6	0	-5.002681	1.328783	-2.967981
34	6	0	5.255465	0.790319	-1.480633
35	6	0	3.986544	0.425926	-1.038694
36	6	0	6.091051	1.544502	-0.663144
37	6	0	5.660432	1.926710	0.606333
38	1	0	-1.424577	-0.372811	1.701424
39	1	0	-2.119899	0.363831	4.194174
40	1	0	-2.429560	3.042154	4.211621
41	1	0	-1.930240	3.955834	1.730663
42	1	0	1.554782	3.331094	1.186819
43	1	0	0.922285	4.327686	3.586737
44	1	0	0.770417	2.273347	5.333717
45	1	0	1.330113	0.010374	4.004490
46	1	0	1.505695	2.969230	-1.107574
47	1	0	2.236863	5.304563	-1.440469
48	1	0	0.567284	7.144767	-1.444274
49	1	0	-1.839925	6.627651	-1.123367
50	1	0	-2.568585	4.291678	-0.782612
51	1	0	-3.990345	1.613784	0.258274
52	1	0	-6.042311	1.330333	-1.083911
53	1	0	-5.906629	1.195944	-3.555295
54	1	0	-3.696144	1.340531	-4.682195
55	1	0	-1.635427	1.597086	-3.339103
56	1	0	4.424414	-1.402960	1.142080
57	1	0	4.857728	-3.566941	2.240208
58	1	0	3.028858	-4.761574	3.419711
59	1	0	0.758486	-3.758638	3.503434
60	1	0	0.319949	-1.603462	2.397149
61	1	0	3.339054	-0.145344	-1.691550
62	1	0	5.578884	0.484094	-2.470615
63	1	0	7.077610	1.835779	-1.012568
64	1	0	6.309251	2.513976	1.249603
65	1	0	4.078444	1.840502	2.053353
66	45	0	0.247187	-0.190888	-0.975486
67	17	0	1.189679	0.967841	-2.838397
68	6	0	-1.698987	-2.031949	-0.910756
69	6	0	-0.830833	-2.805843	-0.089369
70	16	0	-1.017958	-1.472718	-2.403046

71	6	0	-3.183034	-1.967276	-0.787545
72	6	0	-3.853329	-1.525802	0.358097
73	6	0	-3.958781	-2.364034	-1.888065
74	6	0	-5.243870	-1.506027	0.411221
75	1	0	-3.291695	-1.184042	1.214243
76	6	0	-5.345977	-2.338173	-1.836982
77	1	0	-3.465878	-2.708150	-2.792472
78	6	0	-5.998627	-1.913679	-0.682281
79	1	0	-5.734849	-1.151300	1.313504
80	1	0	-5.918109	-2.657211	-2.703057
81	1	0	-7.083718	-1.895356	-0.639562
82	6	0	-1.272293	-3.599391	1.093537
83	8	0	-1.075650	-4.785218	1.218111
84	8	0	-1.843565	-2.836617	2.043625
85	6	0	-2.346118	-3.519888	3.203680
86	6	0	-3.703192	-4.144779	2.935727
87	1	0	-2.404297	-2.741166	3.967140
88	1	0	-1.618962	-4.275486	3.511646
89	1	0	-4.090599	-4.594537	3.855813
90	1	0	-4.415136	-3.392779	2.584709
91	1	0	-3.619491	-4.926902	2.177187
92	6	0	0.472274	-3.031504	-0.553958
93	6	0	0.956490	-2.100304	-1.464665
94	6	0	2.162901	-2.375418	-2.267533
95	6	0	3.264825	-2.975878	-1.638162
96	6	0	2.281784	-2.011565	-3.613891
97	6	0	4.456882	-3.174456	-2.324695
98	1	0	3.195147	-3.254677	-0.591952
99	6	0	3.472410	-2.221685	-4.300517
100	1	0	1.441262	-1.549673	-4.117692
101	6	0	4.568461	-2.793873	-3.659173
102	1	0	5.301514	-3.626048	-1.812076
103	1	0	3.544031	-1.929477	-5.344060
104	1	0	5.500151	-2.946468	-4.196150
105	1	0	0.993848	-3.942480	-0.276402

Zero-point correction= 0.832715 (Hartree/Particle)
Thermal correction to Energy= 0.886834
Thermal correction to Enthalpy= 0.887778
Thermal correction to Gibbs Free Energy= 0.743184
Sum of electronic and zero-point Energies= -3969.053204
Sum of electronic and thermal Energies= -3968.999086
Sum of electronic and thermal Enthalpies= -3968.998141
Sum of electronic and thermal Free Energies= -3969.142736

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2432883

INT17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.910217	2.222566	-0.930254
2	15	0	-2.435324	-0.914944	0.467542
3	15	0	0.359197	2.450834	-0.002602
4	6	0	-2.166307	-2.193410	2.905196
5	6	0	-3.023167	-1.982567	-0.904387
6	6	0	-2.918191	-2.434648	-3.282622
7	6	0	-3.085275	-1.651656	2.001477
8	6	0	-3.957390	-3.352387	-3.159261
9	6	0	-4.054430	-2.916895	-0.786087
10	6	0	-2.450624	-1.760757	-2.159367
11	6	0	-4.517983	-3.597190	-1.908334
12	6	0	-4.450453	-1.664368	2.310566
13	6	0	-4.894449	-2.244606	3.493946
14	6	0	-0.932674	2.884690	-1.197160
15	6	0	-1.855361	3.971006	-1.214675
16	6	0	0.204095	3.698855	1.318132
17	6	0	-4.937079	2.121066	-0.664714
18	6	0	-1.311735	1.982497	-2.254267
19	6	0	-2.773186	3.754537	-2.278669
20	6	0	-2.615923	-2.775707	4.088199
21	6	0	-2.438924	2.526291	-2.918493
22	6	0	-0.238747	3.283600	2.576395
23	6	0	-3.485906	0.552039	0.204424
24	6	0	0.486486	5.050063	1.091321
25	6	0	-4.325428	2.686998	0.492155
26	6	0	-4.419485	0.811105	-0.845626
27	6	0	-3.425623	1.732505	1.022264
28	6	0	1.933484	2.868109	-0.817975
29	6	0	2.009310	3.387932	-2.112171
30	6	0	0.297715	5.982006	2.105896
31	6	0	-0.419437	4.219176	3.592811
32	6	0	-0.159376	5.566035	3.356192
33	6	0	-3.976832	-2.807672	4.379579
34	6	0	4.347361	2.838960	-0.693715
35	6	0	3.109507	2.590890	-0.114104
36	6	0	4.420365	3.349545	-1.988527
37	6	0	3.252623	3.622808	-2.696582
38	1	0	-2.778998	1.865537	1.878306
39	1	0	-4.476835	3.689950	0.867508
40	1	0	-5.641602	2.618528	-1.317665
41	1	0	-4.660800	0.130682	-1.650665
42	1	0	-0.795748	1.064805	-2.503995

43	1	0	-2.973676	2.067479	-3.738725
44	1	0	-3.609309	4.392782	-2.530617
45	1	0	-1.869204	4.791541	-0.510367
46	1	0	-1.629655	-1.055238	-2.248360
47	1	0	-2.457058	-2.255250	-4.249408
48	1	0	-4.322461	-3.883706	-4.033405
49	1	0	-5.317838	-4.324538	-1.803372
50	1	0	-4.494270	-3.122897	0.184364
51	1	0	-5.165719	-1.214614	1.626175
52	1	0	-5.955127	-2.253357	3.727568
53	1	0	-4.324539	-3.259746	5.304005
54	1	0	-1.897094	-3.191728	4.787594
55	1	0	-1.102038	-2.124691	2.696356
56	1	0	0.859909	5.369857	0.121423
57	1	0	0.512582	7.031191	1.925642
58	1	0	-0.301348	6.294585	4.149302
59	1	0	-0.756952	3.892004	4.571795
60	1	0	-0.417545	2.225199	2.751986
61	1	0	3.056569	2.152851	0.879017
62	1	0	5.253621	2.604208	-0.144502
63	1	0	5.388768	3.527006	-2.446879
64	1	0	3.307113	4.024518	-3.704408
65	1	0	1.100848	3.606058	-2.666614
66	45	0	-0.586186	0.426905	0.311305
67	17	0	0.916359	-0.408429	1.936008
68	6	0	1.553462	-2.348470	-1.209231
69	6	0	2.744218	-2.165941	-0.552044
70	16	0	1.324284	-1.103253	-2.393807
71	6	0	0.515201	-3.381433	-1.038320
72	6	0	-0.051320	-3.598562	0.223780
73	6	0	0.044667	-4.109229	-2.134486
74	6	0	-1.064498	-4.536443	0.378981
75	1	0	0.314167	-3.020713	1.063965
76	6	0	-0.972284	-5.045409	-1.974375
77	1	0	0.483490	-3.945034	-3.115225
78	6	0	-1.528732	-5.259757	-0.717814
79	1	0	-1.506096	-4.688040	1.359867
80	1	0	-1.334929	-5.600052	-2.834550
81	1	0	-2.328982	-5.983651	-0.594436
82	6	0	3.300309	-3.152651	0.413154
83	8	0	2.681651	-3.763145	1.254020
84	8	0	4.619545	-3.313032	0.201296
85	6	0	5.316987	-4.164187	1.118464
86	6	0	5.699245	-3.409909	2.379988
87	1	0	6.201642	-4.490114	0.567160
88	1	0	4.692499	-5.031102	1.348324
89	1	0	6.286403	-4.059102	3.038552
90	1	0	6.294697	-2.526446	2.132166
91	1	0	4.802463	-3.090151	2.917903
92	6	0	2.807900	-0.334575	-1.984540
93	6	0	3.461910	-0.994982	-0.988051
94	6	0	4.704445	-0.483431	-0.367941
95	6	0	4.729955	-0.215468	1.004922
96	6	0	5.838896	-0.218332	-1.135846
97	6	0	5.874114	0.310694	1.594926
98	1	0	3.835000	-0.399661	1.595499
99	6	0	6.986146	0.303193	-0.543645
100	1	0	5.819848	-0.431591	-2.200798
101	6	0	7.007757	0.568884	0.823647
102	1	0	5.880839	0.519600	2.660974
103	1	0	7.865923	0.499490	-1.150080
104	1	0	7.902257	0.975668	1.286624
105	1	0	3.096834	0.599793	-2.448310

Zero-point correction=	0.833864 (Hartree/Particle)
Thermal correction to Energy=	0.889240
Thermal correction to Enthalpy=	0.890184
Thermal correction to Gibbs Free Energy=	0.738023
Sum of electronic and zero-point Energies=	-3969.090245
Sum of electronic and thermal Energies=	-3969.034870
Sum of electronic and thermal Enthalpies=	-3969.033926
Sum of electronic and thermal Free Energies=	-3969.186087

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.2815218

INT18b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.646347	-0.130390	2.775511
2	15	0	-2.496724	-0.654022	-0.615094
3	15	0	0.023690	1.114093	1.064082
4	6	0	-1.964780	-2.592095	-2.616294
5	6	0	-3.951219	0.308513	-1.169646
6	6	0	-4.909510	2.473651	-1.660436
7	6	0	-2.648590	-2.309487	-1.429713
8	6	0	-6.147957	1.878142	-1.882549
9	6	0	-5.193640	-0.285749	-1.407531
10	6	0	-3.812706	1.690911	-1.311481
11	6	0	-6.288173	0.497023	-1.761029
12	6	0	-3.424426	-3.321095	-0.843998
13	6	0	-3.512837	-4.579869	-1.431034
14	6	0	-1.165397	1.198353	2.441721

15	6	0	-1.053947	0.685010	3.772135
16	6	0	1.532487	0.513057	1.921240
17	6	0	-4.176164	-1.486947	3.027836
18	6	0	-2.440967	1.839884	2.334965
19	6	0	-2.257718	0.987574	4.465733
20	6	0	-2.056545	-3.852196	-3.200706
21	6	0	-3.111569	1.702096	3.579331
22	6	0	1.539798	-0.814278	2.367280
23	6	0	-2.998079	-1.138960	1.068040
24	6	0	2.673248	1.293392	2.115668
25	6	0	-2.918028	-2.139905	3.153000
26	6	0	-4.233940	-0.879459	1.743219
27	6	0	-2.194699	-1.932725	1.947934
28	6	0	0.282303	2.923174	0.847203
29	6	0	0.573549	3.740034	1.947521
30	6	0	3.784367	0.766799	2.771632
31	6	0	2.642392	-1.336230	3.030637
32	6	0	3.767130	-0.541509	3.241356
33	6	0	-2.825065	-4.850152	-2.611224
34	6	0	0.182663	4.893617	-0.553595
35	6	0	0.081332	3.512576	-0.402594
36	6	0	0.496688	5.694042	0.538311
37	6	0	0.692279	5.115372	1.791720
38	1	0	-1.203873	-2.304331	1.725179
39	1	0	-2.553795	-2.658382	4.029407
40	1	0	-4.933830	-1.413697	3.796022
41	1	0	-5.041101	-0.270971	1.359568
42	1	0	-2.842084	2.299343	1.440963
43	1	0	-4.117325	2.036221	3.794607
44	1	0	-2.497303	0.685483	5.476193
45	1	0	-0.217041	0.123734	4.163125
46	1	0	-2.834850	2.143771	-1.170599
47	1	0	-4.790444	3.546789	-1.774895
48	1	0	-7.002238	2.487642	-2.162923
49	1	0	-7.249571	0.027631	-1.947455
50	1	0	-5.307060	-1.362727	-1.321000
51	1	0	-3.959534	-3.137346	0.081783
52	1	0	-4.118345	-5.349352	-0.960722
53	1	0	-2.889159	-5.833906	-3.067404
54	1	0	-1.512205	-4.051307	-4.118702
55	1	0	-1.359440	-1.824121	-3.083841
56	1	0	2.705697	2.311802	1.743560
57	1	0	4.671890	1.378140	2.902141
58	1	0	4.637809	-0.949163	3.746182
59	1	0	2.630797	-2.369296	3.364112
60	1	0	0.673305	-1.443878	2.195072
61	1	0	-0.163634	2.893287	-1.263199
62	1	0	0.029890	5.335926	-1.532032
63	1	0	0.585408	6.769664	0.416472
64	1	0	0.926075	5.737676	2.650674
65	1	0	0.699790	3.296362	2.931719
66	45	0	-0.474014	0.298439	-0.994575
67	17	0	-0.997592	0.544936	-3.346488
68	6	0	2.749060	-1.177620	-0.899741
69	6	0	3.935992	-0.675337	-0.427690
70	16	0	1.881006	0.079015	-1.749968
71	6	0	2.216162	-2.555700	-0.931193
72	6	0	0.908885	-2.830449	-0.522226
73	6	0	2.998134	-3.600383	-1.439638
74	6	0	0.390685	-4.118871	-0.611030
75	1	0	0.287545	-2.011968	-0.165946
76	6	0	2.485307	-4.888812	-1.517288
77	1	0	4.006706	-3.393925	-1.783445
78	6	0	1.179799	-5.152363	-1.103424
79	1	0	-0.639545	-4.303872	-0.319102
80	1	0	3.101767	-5.687967	-1.918859
81	1	0	0.774049	-6.156645	-1.182835
82	6	0	4.975477	-1.383539	0.358470
83	8	0	6.063916	-0.904082	0.597184
84	8	0	4.573224	-2.579772	0.801085
85	6	0	5.512664	-3.341123	1.565492
86	6	0	6.402269	-4.169568	0.655852
87	1	0	4.893303	-3.976399	2.202578
88	1	0	6.102924	-2.664284	2.188170
89	1	0	7.064277	-4.804110	1.254162
90	1	0	5.793933	-4.811259	0.011087
91	1	0	7.019924	-3.518060	0.031477
92	6	0	4.130362	0.712717	-0.726852
93	6	0	3.101286	1.282088	-1.407448
94	6	0	2.959634	2.664215	-1.882039
95	6	0	3.603705	3.703996	-1.200516
96	6	0	2.196166	2.967230	-3.016873
97	6	0	3.511228	5.012099	-1.658909
98	1	0	4.166320	3.485230	-0.297428
99	6	0	2.103451	4.278343	-3.469657
100	1	0	1.668688	2.179192	-3.549217
101	6	0	2.766483	5.303423	-2.799309
102	1	0	4.014221	5.808077	-1.117952
103	1	0	1.512208	4.495409	-4.354193
104	1	0	2.694255	6.326046	-3.158018
105	1	0	5.034403	1.234096	-0.436881

Zero-point correction= 0.835117 (Hartree/Particle)

Thermal correction to Energy= 0.889595
Thermal correction to Enthalpy= 0.890540
Thermal correction to Gibbs Free Energy= 0.744421
Sum of electronic and zero-point Energies= -3969.128406
Sum of electronic and thermal Energies= -3969.073927
Sum of electronic and thermal Enthalpies= -3969.072983
Sum of electronic and thermal Free Energies= -3969.219102

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3972.3208271

2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.042089	-0.000028	-0.000003
2	7	0	3.201202	0.000015	0.000006
3	6	0	0.604388	-0.000006	-0.000005
4	6	0	-0.091090	-1.213958	-0.000003
5	6	0	-0.091064	1.213944	-0.000002
6	6	0	-1.480331	-1.207730	0.000002
7	1	0	0.459301	-2.148836	-0.000002
8	6	0	-1.480319	1.207739	0.000000
9	1	0	0.459326	2.148823	0.000000
10	6	0	-2.174225	0.000017	0.000002
11	1	0	-2.021907	-2.148208	0.000004
12	1	0	-2.021862	2.148236	0.000002
13	1	0	-3.259964	0.000015	0.000005

Zero-point correction= 0.100597 (Hartree/Particle)
Thermal correction to Energy= 0.106664
Thermal correction to Enthalpy= 0.107608
Thermal correction to Gibbs Free Energy= 0.070334
Sum of electronic and zero-point Energies= -324.272361
Sum of electronic and thermal Energies= -324.266294
Sum of electronic and thermal Enthalpies= -324.265350
Sum of electronic and thermal Free Energies= -324.302624

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -324.4727366

INT8c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.888894	-1.180136	-3.034880
2	6	0	-1.519962	2.209905	-0.591230
3	6	0	-1.182545	1.183332	0.206179
4	16	0	-0.634942	2.064368	-2.116117
5	6	0	-2.528091	3.267771	-0.379028
6	6	0	-2.259980	4.585580	-0.763813
7	6	0	-3.770790	2.975155	0.192080
8	6	0	-3.195568	5.591222	-0.547732
9	1	0	-1.309214	4.815675	-1.236091
10	6	0	-4.707637	3.979902	0.407964
11	1	0	-4.008270	1.947299	0.450502
12	6	0	-4.420480	5.293631	0.045527
13	1	0	-2.969599	6.611254	-0.845407
14	1	0	-5.667964	3.734194	0.852761
15	1	0	-5.152764	6.078477	0.211377
16	6	0	-1.878270	0.829464	1.446170
17	8	0	-2.523583	-0.193180	1.628911
18	8	0	-1.727041	1.764650	2.398214
19	6	0	-2.402281	1.541565	3.641863
20	6	0	-3.857908	1.969006	3.577472
21	1	0	-1.844787	2.149384	4.358389
22	1	0	-2.308554	0.486854	3.913330
23	1	0	-4.311385	1.894068	4.571761
24	1	0	-3.942080	3.001847	3.227617
25	1	0	-4.416665	1.321707	2.896138
26	26	0	3.694327	-1.857234	0.414456
27	15	0	0.335491	-1.965576	0.305867
28	15	0	1.969169	1.124462	-0.368418
29	6	0	-0.607017	-4.139306	-1.183253
30	6	0	0.181393	-1.825960	2.126788
31	6	0	0.390303	-0.458612	4.116573
32	6	0	-0.884671	-3.251430	-0.141741
33	6	0	0.123111	-1.566579	4.915318
34	6	0	-0.094250	-2.933656	2.935732
35	6	0	0.411488	-0.593025	2.732156
36	6	0	-0.124017	-2.802745	4.320840
37	6	0	-2.145250	-3.270583	0.465473
38	6	0	-3.104808	-4.187453	0.048526
39	6	0	3.364785	0.167566	0.350148
40	6	0	4.520662	-0.178027	-0.424743
41	6	0	2.873343	1.988742	-1.715032
42	6	0	3.904463	-3.881770	0.745449
43	6	0	3.614375	-0.294971	1.689499
44	6	0	5.465150	-0.812964	0.422326
45	6	0	-1.573802	-5.049955	-1.599799
46	6	0	4.910193	-0.878736	1.728954
47	6	0	3.883075	2.891228	-1.353925
48	6	0	1.935919	-2.817374	0.164992
49	6	0	2.620884	1.741975	-3.062771

50	6	0	3.944993	-3.609105	-0.649926
51	6	0	2.667545	-3.405140	1.251690
52	6	0	2.739533	-2.959289	-1.015692
53	6	0	1.688040	2.518639	0.809963
54	6	0	1.923438	2.448439	2.184511
55	6	0	3.370665	2.395559	-4.039913
56	6	0	4.623300	3.543057	-2.331286
57	6	0	4.366664	3.295599	-3.679327
58	6	0	-2.821560	-5.078797	-0.983487
59	6	0	0.827516	4.764675	1.122841
60	6	0	1.157898	3.705578	0.287556
61	6	0	1.035053	4.669688	2.496026
62	6	0	1.596626	3.513078	3.021226
63	1	0	2.479661	-2.566947	-1.988782
64	1	0	4.775157	-3.809416	-1.313660
65	1	0	4.697739	-4.323106	1.333668
66	1	0	2.363709	-3.420941	2.288237
67	1	0	2.927026	-0.284368	2.521145
68	1	0	5.360447	-1.348584	2.592728
69	1	0	6.416006	-1.222455	0.110323
70	1	0	4.634086	-0.003806	-1.485204
71	1	0	0.580183	0.283378	2.117849
72	1	0	0.563697	0.517555	4.560901
73	1	0	0.097235	-1.467497	5.996558
74	1	0	-0.342031	-3.669667	4.937478
75	1	0	-0.285426	-3.901547	2.481876
76	1	0	-2.385954	-2.545415	1.237284
77	1	0	-4.083928	-4.189086	0.518484
78	1	0	-3.574999	-5.788960	-1.311589
79	1	0	-1.349066	-5.735140	-2.411597
80	1	0	0.353988	-4.107706	-1.685630
81	1	0	1.858181	1.026713	-3.350543
82	1	0	3.166526	2.195352	-5.087208
83	1	0	4.944369	3.805888	-4.444836
84	1	0	5.398932	4.245302	-2.040655
85	1	0	4.089628	3.086287	-0.305525
86	1	0	0.990799	3.792034	-0.780276
87	1	0	0.399236	5.666540	0.696541
88	1	0	0.771232	5.496658	3.148572
89	1	0	1.791456	3.431916	4.086858
90	1	0	2.379594	1.574703	2.626112
91	45	0	0.001832	0.014617	-1.001160
92	6	0	-4.974878	-1.984877	-2.729103
93	6	0	-6.306937	-2.366173	-2.620680
94	6	0	-6.987205	-2.196358	-1.416228
95	6	0	-6.341379	-1.644689	-0.310538
96	6	0	-5.010091	-1.259836	-0.400801
97	6	0	-4.336406	-1.432865	-1.616530
98	1	0	-4.430120	-2.113461	-3.658148
99	1	0	-6.814057	-2.797195	-3.477740
100	1	0	-8.028118	-2.495696	-1.338373
101	1	0	-6.874988	-1.516536	0.625870
102	1	0	-4.472979	-0.845902	0.448295
103	6	0	-2.958997	-1.051340	-1.660724
104	7	0	-1.855965	-0.733487	-1.574310

Zero-point correction= 0.822862 (Hartree/Particle)
Thermal correction to Energy= 0.876892
Thermal correction to Enthalpy= 0.877836
Thermal correction to Gibbs Free Energy= 0.734012
Sum of electronic and zero-point Energies= -3985.141067
Sum of electronic and thermal Energies= -3985.087037
Sum of electronic and thermal Enthalpies= -3985.086093
Sum of electronic and thermal Free Energies= -3985.229917

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3385217

TS5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.527422	1.605662	-2.658080
2	6	0	2.529361	-0.764331	0.230940
3	6	0	1.410654	-0.393183	0.865151
4	16	0	2.376486	-0.355717	-1.500960
5	6	0	3.767729	-1.359133	0.767774
6	6	0	4.411378	-2.401045	0.088686
7	6	0	4.319318	-0.893052	1.967174
8	6	0	5.560799	-2.983076	0.612316
9	1	0	4.001343	-2.757795	-0.852811
10	6	0	5.467787	-1.478370	2.490416
11	1	0	3.848167	-0.061655	2.482424
12	6	0	6.089746	-2.527225	1.818318
13	1	0	6.044660	-3.795882	0.078213
14	1	0	5.883645	-1.104765	3.421703
15	1	0	6.987832	-2.981337	2.226552
16	6	0	1.244528	-0.569917	2.323991
17	8	0	1.288673	0.323627	3.146682
18	8	0	1.058195	-1.858054	2.637638
19	6	0	0.979664	-2.192365	4.028555
20	6	0	2.366226	-2.362132	4.622816
21	1	0	0.420780	-3.130972	4.042880
22	1	0	0.409600	-1.420829	4.551719

23	1	0	2.289570	-2.753228	5.643032
24	1	0	2.959182	-3.057016	4.020767
25	1	0	2.886796	-1.401690	4.657792
26	26	0	-4.061821	0.342216	-0.745221
27	15	0	-1.315179	1.576732	0.798533
28	15	0	-1.024291	-1.440118	-1.070471
29	6	0	-1.402506	4.393898	0.791657
30	6	0	-1.716787	0.806491	2.411677
31	6	0	-2.232416	-1.201323	3.664355
32	6	0	-0.752365	3.248428	1.249585
33	6	0	-2.584837	-0.430052	4.768388
34	6	0	-2.061208	1.575530	3.526489
35	6	0	-1.795299	-0.581344	2.499530
36	6	0	-2.489086	0.958141	4.698127
37	6	0	0.384082	3.365606	2.058974
38	6	0	0.848438	4.624365	2.417487
39	6	0	-2.850717	-1.294864	-1.071282
40	6	0	-3.544206	-0.933484	-2.271276
41	6	0	-0.767906	-2.158443	-2.747351
42	6	0	-5.294684	1.812633	0.004389
43	6	0	-3.852095	-1.557904	-0.072829
44	6	0	-4.939681	-1.002430	-2.026154
45	6	0	-0.923810	5.653593	1.146362
46	6	0	-5.131699	-1.395247	-0.672996
47	6	0	-1.345603	-3.409659	-3.005805
48	6	0	-2.990088	1.808601	0.145633
49	6	0	-0.044223	-1.518304	-3.750825
50	6	0	-4.773262	2.209844	-1.259048
51	6	0	-4.202773	1.574703	0.877788
52	6	0	-3.358204	2.214599	-1.179254
53	6	0	-0.579484	-2.920948	-0.065589
54	6	0	-1.404638	-3.578541	0.846697
55	6	0	0.103692	-2.125567	-4.998023
56	6	0	-1.199161	-4.008299	-4.249115
57	6	0	-0.469552	-3.365895	-5.249462
58	6	0	0.198258	5.769606	1.959916
59	6	0	1.218965	-4.437635	0.526875
60	6	0	0.731176	-3.386952	-0.235948
61	6	0	0.397592	-5.063504	1.461676
62	6	0	-0.918214	-4.641139	1.607372
63	1	0	-2.660309	2.409157	-1.980374
64	1	0	-5.351268	2.415765	-2.149733
65	1	0	-6.338673	1.663107	0.244698
66	1	0	-4.270232	1.223956	1.897699
67	1	0	-3.690036	-1.772553	0.972261
68	1	0	-6.081136	-1.492595	-0.164453
69	1	0	-5.716791	-0.747437	-2.733278
70	1	0	-3.067077	-0.629685	-3.192853
71	1	0	-1.478595	-1.191581	1.664505
72	1	0	-2.273798	-2.286292	3.709381
73	1	0	-2.922617	-0.907146	5.683653
74	1	0	-2.750497	1.565378	5.559576
75	1	0	-1.996784	2.657900	3.479740
76	1	0	0.896058	2.472571	2.408472
77	1	0	1.727965	4.710877	3.048402
78	1	0	0.569992	6.752322	2.236043
79	1	0	-1.431817	6.542653	0.784846
80	1	0	-2.280277	4.310455	0.159011
81	1	0	0.377062	-0.537121	-3.573323
82	1	0	0.667678	-1.615303	-5.772828
83	1	0	-0.351654	-3.834762	-6.222177
84	1	0	-1.652734	-4.976818	-4.437346
85	1	0	-1.909862	-3.919063	-2.229449
86	1	0	1.376298	-2.919767	-0.972719
87	1	0	2.246845	-4.760982	0.394277
88	1	0	0.778101	-5.885778	2.060443
89	1	0	-1.580118	-5.142604	2.307877
90	1	0	-2.439368	-3.288127	0.967066
91	45	0	0.261651	0.485504	-0.565044
92	6	0	3.601015	3.685177	-2.277212
93	6	0	4.707264	4.292628	-2.859676
94	6	0	5.937877	3.639921	-2.869224
95	6	0	6.064750	2.374101	-2.299342
96	6	0	4.962182	1.753770	-1.724513
97	6	0	3.732440	2.413430	-1.709514
98	1	0	2.632759	4.174184	-2.258814
99	1	0	4.606280	5.275370	-3.309772
100	1	0	6.800572	4.116467	-3.325484
101	1	0	7.024557	1.867035	-2.306292
102	1	0	5.047713	0.764760	-1.284866
103	6	0	2.553263	1.837844	-1.073987
104	7	0	1.581522	2.123096	-0.427232

Zero-point correction= 0.821783 (Hartree/Particle)
Thermal correction to Energy= 0.875854
Thermal correction to Enthalpy= 0.876798
Thermal correction to Gibbs Free Energy= 0.732535
Sum of electronic and zero-point Energies= -3985.118089
Sum of electronic and thermal Energies= -3985.064018
Sum of electronic and thermal Enthalpies= -3985.063074
Sum of electronic and thermal Free Energies= -3985.207337

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3097041

TS6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.595228	-0.135000	-3.107560
2	6	0	-2.362051	1.077877	-0.716954
3	6	0	-1.730748	0.020908	-0.085617
4	16	0	-1.435183	1.542074	-2.093969
5	6	0	-3.645609	1.715399	-0.370589
6	6	0	-3.889740	3.050767	-0.713786
7	6	0	-4.653137	0.993045	0.280469
8	6	0	-5.096402	3.657461	-0.386421
9	1	0	-3.123330	3.613808	-1.238816
10	6	0	-5.864606	1.596511	0.594712
11	1	0	-4.503623	-0.055266	0.517054
12	6	0	-6.088037	2.932466	0.271389
13	1	0	-5.265423	4.697132	-0.650574
14	1	0	-6.638091	1.016020	1.088966
15	1	0	-7.034221	3.404043	0.519919
16	6	0	-2.034014	-0.497891	1.256672
17	8	0	-2.071235	-1.677364	1.562044
18	8	0	-2.228428	0.486669	2.148699
19	6	0	-2.594599	0.096210	3.477722
20	6	0	-4.088923	-0.152271	3.582354
21	1	0	-2.284247	0.940878	4.096758
22	1	0	-2.024427	-0.791850	3.759669
23	1	0	-4.357011	-0.373783	4.620910
24	1	0	-4.649689	0.727886	3.254363
25	1	0	-4.377318	-1.006903	2.962820
26	26	0	4.199020	-0.294609	0.268666
27	15	0	1.237225	-1.859014	-0.047556
28	15	0	1.283201	1.697504	-0.110231
29	6	0	1.356746	-4.063498	-1.776319
30	6	0	1.032315	-2.028029	1.766919
31	6	0	0.703235	-0.966468	3.919384
32	6	0	0.702088	-3.480461	-0.691415
33	6	0	0.938921	-2.177370	4.562664
34	6	0	1.261729	-3.243842	2.419901
35	6	0	0.740446	-0.901981	2.530229
36	6	0	1.210756	-3.317409	3.808286
37	6	0	-0.446548	-4.083620	-0.168231
38	6	0	-0.920412	-5.269896	-0.714839
39	6	0	2.996451	1.370968	0.464671
40	6	0	4.115316	1.653383	-0.383951
41	6	0	1.616934	3.184766	-1.147669
42	6	0	5.272687	-2.041298	0.459728
43	6	0	3.531093	0.938254	1.727726
44	6	0	5.309524	1.431772	0.348978
45	6	0	0.875808	-5.250830	-2.321755
46	6	0	4.950747	1.000179	1.655681
47	6	0	2.079862	4.340232	-0.503119
48	6	0	3.050368	-1.899397	-0.159363
49	6	0	1.465189	3.188957	-2.532873
50	6	0	5.219185	-1.652441	-0.907354
51	6	0	3.942734	-2.206495	0.924255
52	6	0	3.859359	-1.568862	-1.296490
53	6	0	0.393724	2.508424	1.290812
54	6	0	0.749122	2.432115	2.639638
55	6	0	1.761766	4.340047	-3.262392
56	6	0	2.372809	5.484116	-1.233204
57	6	0	2.210510	5.486688	-2.618277
58	6	0	-0.259602	-5.856282	-1.792075
59	6	0	-1.564104	3.796054	1.929692
60	6	0	-0.759291	3.227195	0.951716
61	6	0	-1.219632	3.680308	3.272895
62	6	0	-0.051638	3.011043	3.621821
63	1	0	3.477226	-1.235599	-2.250027
64	1	0	6.066386	-1.402672	-1.531652
65	1	0	6.166337	-2.140650	1.061070
66	1	0	3.657358	-2.449803	1.936903
67	1	0	2.977932	0.555255	2.571712
68	1	0	5.632959	0.700306	2.439423
69	1	0	6.314051	1.528887	-0.039219
70	1	0	4.046291	1.959894	-1.418361
71	1	0	0.509137	0.034095	2.038601
72	1	0	0.470200	-0.070282	4.488142
73	1	0	0.902503	-2.238304	5.646430
74	1	0	1.387036	-4.268218	4.302183
75	1	0	1.487370	-4.135662	1.843347
76	1	0	-0.975306	-3.611933	0.655374
77	1	0	-1.813256	-5.732614	-0.304209
78	1	0	-0.634582	-6.779905	-2.223234
79	1	0	1.387778	-5.698036	-3.168314
80	1	0	2.231770	-3.587738	-2.207310
81	1	0	1.148819	2.288648	-3.047025
82	1	0	1.639208	4.329456	-4.341132
83	1	0	2.437508	6.381947	-3.190142
84	1	0	2.726810	6.374214	-0.721622
85	1	0	2.209034	4.347032	0.575513
86	1	0	-1.025290	3.347607	-0.091945
87	1	0	-2.467162	4.322125	1.635960
88	1	0	-1.848577	4.122129	4.040242

89	1	0	0.249710	2.941960	4.663499
90	1	0	1.659908	1.937020	2.944769
91	45	0	0.080096	-0.085836	-1.144074
92	6	0	-4.431437	-1.192110	-2.237580
93	6	0	-5.793436	-1.461658	-2.172044
94	6	0	-6.282911	-2.360152	-1.227228
95	6	0	-5.407261	-2.997996	-0.350349
96	6	0	-4.042794	-2.735993	-0.405412
97	6	0	-3.556733	-1.826617	-1.348209
98	1	0	-4.036854	-0.485288	-2.960360
99	1	0	-6.472348	-0.963564	-2.856762
100	1	0	-7.348121	-2.564854	-1.174165
101	1	0	-5.787288	-3.704140	0.381730
102	1	0	-3.356308	-3.205247	0.286779
103	6	0	-2.145523	-1.471395	-1.424419
104	7	0	-1.121166	-1.577264	-2.038378

Zero-point correction= 0.822165 (Hartree/Particle)
Thermal correction to Energy= 0.875824
Thermal correction to Enthalpy= 0.876768
Thermal correction to Gibbs Free Energy= 0.735506
Sum of electronic and zero-point Energies= -3985.112356
Sum of electronic and thermal Energies= -3985.058697
Sum of electronic and thermal Enthalpies= -3985.057753
Sum of electronic and thermal Free Energies= -3985.199015

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3013302

INT9c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.635315	1.394346	-2.765991
2	6	0	2.501505	-0.854088	0.157968
3	6	0	1.409551	-0.412176	0.789856
4	16	0	2.347773	-0.452001	-1.593926
5	6	0	3.725017	-1.490313	0.679078
6	6	0	4.277555	-2.611041	0.047430
7	6	0	4.351000	-0.981247	1.823089
8	6	0	5.414017	-3.224379	0.563528
9	1	0	3.809240	-3.004864	-0.851407
10	6	0	5.485240	-1.599324	2.339589
11	1	0	3.948104	-0.093137	2.299381
12	6	0	6.018058	-2.723541	1.715157
13	1	0	5.828940	-4.096380	0.066362
14	1	0	5.960179	-1.191929	3.227313
15	1	0	6.906066	-3.202121	2.117228
16	6	0	1.294082	-0.521275	2.262571
17	8	0	1.497710	0.392484	3.036317
18	8	0	0.968186	-1.761845	2.636628
19	6	0	0.951295	-2.044883	4.041586
20	6	0	2.323903	-2.505568	4.495592
21	1	0	0.207227	-2.837291	4.147904
22	1	0	0.619871	-1.156792	4.584002
23	1	0	2.287958	-2.816399	5.545163
24	1	0	2.663183	-3.349433	3.887351
25	1	0	3.052281	-1.696129	4.397776
26	26	0	-4.082674	0.531903	-0.605223
27	15	0	-1.169838	1.695191	0.709564
28	15	0	-1.203848	-1.476580	-0.959052
29	6	0	-1.083489	4.502466	0.500188
30	6	0	-1.509970	1.054822	2.391520
31	6	0	-2.147032	-0.817376	3.789602
32	6	0	-0.476027	3.350491	0.998137
33	6	0	-2.324031	0.042019	4.870437
34	6	0	-1.681756	1.911984	3.481530
35	6	0	-1.735143	-0.309420	2.563044
36	6	0	-2.081950	1.404937	4.714402
37	6	0	0.731969	3.444368	1.700049
38	6	0	1.310371	4.688599	1.913827
39	6	0	-3.014549	-1.213197	-0.906432
40	6	0	-3.721215	-0.841781	-2.094906
41	6	0	-1.049194	-2.325414	-2.587239
42	6	0	-5.175898	2.101015	0.156880
43	6	0	-3.993309	-1.353253	0.136539
44	6	0	-5.107803	-0.787314	-1.798128
45	6	0	-0.491535	5.746285	0.708934
46	6	0	-5.278631	-1.111056	-0.423929
47	6	0	-1.726127	-3.540849	-2.762854
48	6	0	-2.870050	1.973177	0.147505
49	6	0	-0.280206	-1.815182	-3.631073
50	6	0	-4.720292	2.415542	-1.154433
51	6	0	-4.041956	1.837627	0.966859
52	6	0	-3.304747	2.342652	-1.167570
53	6	0	-0.799241	-2.911304	0.126103
54	6	0	-1.615905	-3.460596	1.114095
55	6	0	-0.186663	-2.513514	-4.834989
56	6	0	-1.633602	-4.230912	-3.963352
57	6	0	-0.858300	-3.717716	-5.003569
58	6	0	0.702833	5.840137	1.415538
59	6	0	0.952886	-4.464589	0.765145
60	6	0	0.482772	-3.448307	-0.053532
61	6	0	0.140750	-4.981756	1.772270

62	6	0	-1.147760	-4.486839	1.933951
63	1	0	-2.653462	2.462472	-2.020879
64	1	0	-5.345689	2.617083	-2.013547
65	1	0	-6.207537	2.022359	0.472458
66	1	0	-4.060272	1.539341	2.005170
67	1	0	-3.809809	-1.541274	1.183202
68	1	0	-6.212184	-1.108894	0.122055
69	1	0	-5.888724	-0.496443	-2.487027
70	1	0	-3.255851	-0.612365	-3.043692
71	1	0	-1.555929	-0.991727	1.743290
72	1	0	-2.306229	-1.886569	3.899653
73	1	0	-2.640778	-0.348782	5.832982
74	1	0	-2.207238	2.080192	5.555433
75	1	0	-1.506709	2.976660	3.367512
76	1	0	1.211983	2.546346	2.080682
77	1	0	2.246841	4.757750	2.458945
78	1	0	1.164041	6.810459	1.576221
79	1	0	-0.967082	6.640160	0.316579
80	1	0	-2.015707	4.435802	-0.051132
81	1	0	0.215711	-0.859384	-3.520882
82	1	0	0.411973	-2.102581	-5.642184
83	1	0	-0.783587	-4.256978	-5.943500
84	1	0	-2.162549	-5.171136	-4.087780
85	1	0	-2.326434	-3.949628	-1.954458
86	1	0	1.120968	-3.063884	-0.842898
87	1	0	1.958991	-4.846368	0.620634
88	1	0	0.507178	-5.774875	2.417378
89	1	0	-1.802790	-4.902500	2.694647
90	1	0	-2.630323	-3.110324	1.249785
91	45	0	0.241260	0.429080	-0.648637
92	6	0	3.810319	3.468646	-2.047358
93	6	0	4.957281	4.104983	-2.502732
94	6	0	6.116775	3.370115	-2.747897
95	6	0	6.125438	1.994750	-2.533405
96	6	0	4.977489	1.350571	-2.081787
97	6	0	3.816997	2.084613	-1.837140
98	1	0	2.897292	4.021061	-1.850351
99	1	0	4.946135	5.177663	-2.671960
100	1	0	7.011726	3.869370	-3.107680
101	1	0	7.028124	1.420095	-2.717752
102	1	0	4.988893	0.278093	-1.909568
103	6	0	2.582409	1.461681	-1.325270
104	7	0	1.619160	1.959921	-0.727282

Zero-point correction=	0.822300 (Hartree/Particle)
Thermal correction to Energy=	0.876772
Thermal correction to Enthalpy=	0.877716
Thermal correction to Gibbs Free Energy=	0.732108
Sum of electronic and zero-point Energies=	-3985.119709
Sum of electronic and thermal Energies=	-3985.065237
Sum of electronic and thermal Enthalpies=	-3985.064293
Sum of electronic and thermal Free Energies=	-3985.209900

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3128575

INT10c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.262556	-0.811342	-3.048015
2	6	0	-2.255892	1.479684	-0.904925
3	6	0	-2.044720	0.237123	-0.163343
4	16	0	-1.306912	1.572002	-2.275899
5	6	0	-3.187979	2.542794	-0.499031
6	6	0	-2.948100	3.885293	-0.819944
7	6	0	-4.361286	2.204265	0.187805
8	6	0	-3.844891	4.870965	-0.427928
9	1	0	-2.047836	4.153322	-1.364834
10	6	0	-5.267044	3.189049	0.558427
11	1	0	-4.576695	1.162318	0.401573
12	6	0	-5.004250	4.525213	0.264335
13	1	0	-3.641727	5.910413	-0.666212
14	1	0	-6.178580	2.913562	1.079433
15	1	0	-5.707215	5.295856	0.566079
16	6	0	-2.183809	0.210958	1.307973
17	8	0	-2.507042	-0.758743	1.969612
18	8	0	-1.845169	1.389317	1.851789
19	6	0	-1.995322	1.550545	3.265965
20	6	0	-3.334217	2.193605	3.575027
21	1	0	-1.164605	2.197388	3.558666
22	1	0	-1.889741	0.578341	3.750120
23	1	0	-3.422365	2.377900	4.650926
24	1	0	-3.438313	3.144728	3.044300
25	1	0	-4.154166	1.535342	3.271286
26	26	0	3.931077	-1.323892	0.197607
27	15	0	0.600938	-2.007780	0.236827
28	15	0	1.711892	1.381941	-0.350087
29	6	0	0.099732	-4.474259	-0.989430
30	6	0	0.489830	-1.774818	2.051625
31	6	0	0.747946	-0.317013	3.969278
32	6	0	-0.365579	-3.522259	-0.082190
33	6	0	0.643548	-1.409674	4.824599
34	6	0	0.374615	-2.867186	2.917926

35	6	0	0.657451	-0.502047	2.593406
36	6	0	0.445304	-2.683303	4.295024
37	6	0	-1.636451	-3.669127	0.485482
38	6	0	-2.425105	-4.763206	0.152063
39	6	0	3.313040	0.647047	0.151498
40	6	0	4.376440	0.433538	-0.780774
41	6	0	2.311134	2.591257	-1.610863
42	6	0	4.448967	-3.261800	0.654002
43	6	0	3.804153	0.262410	1.446246
44	6	0	5.510986	-0.040337	-0.070781
45	6	0	-0.693924	-5.569697	-1.317934
46	6	0	5.163542	-0.136268	1.305319
47	6	0	3.154861	3.635798	-1.208536
48	6	0	2.325611	-2.548853	0.092006
49	6	0	1.960814	2.481954	-2.956317
50	6	0	4.399360	-3.091075	-0.757595
51	6	0	3.173361	-2.937956	1.183813
52	6	0	3.096853	-2.660178	-1.110981
53	6	0	1.302167	2.583961	0.996619
54	6	0	2.065429	2.855951	2.136267
55	6	0	2.440129	3.407706	-3.883193
56	6	0	3.631863	4.554522	-2.133665
57	6	0	3.271867	4.443541	-3.476600
58	6	0	-1.955401	-5.715596	-0.749524
59	6	0	-0.295971	4.267290	1.717455
60	6	0	0.127556	3.314794	0.800906
61	6	0	0.456419	4.509288	2.863731
62	6	0	1.639897	3.804885	3.065442
63	1	0	2.749471	-2.381073	-2.094910
64	1	0	5.226322	-3.212820	-1.443940
65	1	0	5.320889	-3.533844	1.233576
66	1	0	2.908040	-2.926463	2.231007
67	1	0	3.236629	0.228341	2.364946
68	1	0	5.796073	-0.510999	2.098646
69	1	0	6.455880	-0.327007	-0.511525
70	1	0	4.302136	0.584386	-1.848999
71	1	0	0.694984	0.362257	1.942313
72	1	0	0.888613	0.685570	4.363969
73	1	0	0.709545	-1.270667	5.899660
74	1	0	0.351942	-3.539307	4.956589
75	1	0	0.236820	-3.865097	2.513668
76	1	0	-2.021661	-2.915290	1.167240
77	1	0	-3.415832	-4.859140	0.585870
78	1	0	-2.576669	-6.566069	-1.015338
79	1	0	-0.326229	-6.304849	-2.027447
80	1	0	1.074389	-4.360284	-1.451956
81	1	0	1.350932	1.650946	-3.291576
82	1	0	2.163282	3.304653	-4.928021
83	1	0	3.643369	5.162637	-4.201078
84	1	0	4.285188	5.358231	-1.806878
85	1	0	3.437992	3.735941	-0.164722
86	1	0	-0.463056	3.136189	-0.087077
87	1	0	-1.223172	4.803828	1.537337
88	1	0	0.128671	5.247438	3.589807
89	1	0	2.247903	4.000547	3.944084
90	1	0	3.008801	2.350862	2.300055
91	45	0	-0.110464	-0.196261	-1.101237
92	6	0	-4.317224	-2.047281	-2.286700
93	6	0	-5.600828	-2.558971	-2.427806
94	6	0	-6.489984	-2.525817	-1.354933
95	6	0	-6.081393	-1.985338	-0.139608
96	6	0	-4.794594	-1.473152	0.007309
97	6	0	-3.902686	-1.492996	-1.069052
98	1	0	-3.612965	-2.071221	-3.111909
99	1	0	-5.909869	-2.981989	-3.379170
100	1	0	-7.494233	-2.924875	-1.465602
101	1	0	-6.762932	-1.971796	0.706398
102	1	0	-4.468549	-1.102511	0.972242
103	6	0	-2.505893	-0.987122	-0.991306
104	7	0	-1.575460	-1.432515	-1.718850

Zero-point correction=	0.822834 (Hartree/Particle)
Thermal correction to Energy=	0.875186
Thermal correction to Enthalpy=	0.876130
Thermal correction to Gibbs Free Energy=	0.737413
Sum of electronic and zero-point Energies=	-3985.131505
Sum of electronic and thermal Energies=	-3985.079153
Sum of electronic and thermal Enthalpies=	-3985.078209
Sum of electronic and thermal Free Energies=	-3985.216927

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3201916

INT11c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	3.374461	0.049944	-2.366380
2	15	0	2.614142	0.813617	0.873619
3	15	0	0.468113	-1.244190	-1.186217
4	6	0	3.105960	0.809523	3.627303
5	6	0	2.901235	2.611500	1.053224
6	6	0	2.096462	4.886956	0.969149
7	6	0	3.363149	0.145559	2.421258

8	6	0	3.365872	5.354910	1.288127
9	6	0	4.175895	3.087486	1.390066
10	6	0	1.860275	3.517503	0.856078
11	6	0	4.407358	4.451737	1.503887
12	6	0	4.110313	-1.035769	2.450081
13	6	0	4.589315	-1.544202	3.654760
14	6	0	1.451038	-0.533781	-2.530007
15	6	0	2.257201	-1.229288	-3.490719
16	6	0	1.214014	-2.872870	-0.829953
17	6	0	5.352295	0.589725	-2.160550
18	6	0	1.565336	0.868720	-2.815068
19	6	0	2.866255	-0.266240	-4.337486
20	6	0	3.587548	0.300244	4.827865
21	6	0	2.436504	1.025201	-3.923188
22	6	0	1.801067	-3.090988	0.419542
23	6	0	3.848356	0.382715	-0.409402
24	6	0	1.211158	-3.907298	-1.772368
25	6	0	5.181628	-0.796005	-1.896469
26	6	0	4.538771	1.314845	-1.249215
27	6	0	4.250227	-0.930454	-0.831313
28	6	0	-1.116180	-1.643411	-1.996931
29	6	0	-1.578110	-0.858513	-3.056355
30	6	0	1.825439	-5.121192	-1.483568
31	6	0	2.415217	-4.306492	0.708882
32	6	0	2.435404	-5.318927	-0.245775
33	6	0	4.328215	-0.878657	4.847548
34	6	0	-3.146367	-2.949249	-2.098614
35	6	0	-1.910056	-2.690282	-1.517468
36	6	0	-3.607904	-2.158301	-3.147202
37	6	0	-2.819569	-1.117657	-3.628446
38	1	0	3.866041	-1.870334	-0.462763
39	1	0	5.631435	-1.612455	-2.444780
40	1	0	5.957274	1.019637	-2.947062
41	1	0	4.419389	2.388543	-1.220150
42	1	0	1.094589	1.664742	-2.256925
43	1	0	2.760186	1.968261	-4.341432
44	1	0	3.579184	-0.479033	-5.122399
45	1	0	2.431605	-2.295293	-3.519966
46	1	0	0.859352	3.156878	0.646598
47	1	0	1.278556	5.584662	0.817780
48	1	0	3.545551	6.422045	1.381305
49	1	0	5.397849	4.812337	1.765198
50	1	0	4.985837	2.384144	1.564143
51	1	0	4.344918	-1.564601	1.534982
52	1	0	5.173875	-2.459856	3.654686
53	1	0	4.701962	-1.274817	5.787150
54	1	0	3.376256	0.827521	5.753069
55	1	0	2.515265	1.718388	3.629071
56	1	0	0.711885	-3.768362	-2.727345
57	1	0	1.820891	-5.916692	-2.222376
58	1	0	2.912360	-6.268438	-0.022228
59	1	0	2.868824	-4.458131	1.683509
60	1	0	1.780875	-2.314144	1.179330
61	1	0	-1.572774	-3.293222	-0.679878
62	1	0	-3.755837	-3.763131	-1.718373
63	1	0	-4.581589	-2.351472	-3.586184
64	1	0	-3.170810	-0.499809	-4.449663
65	1	0	-0.975342	-0.038452	-3.432243
66	17	0	-0.115659	1.278775	2.767459
67	45	0	0.283026	0.017982	0.745503
68	6	0	-2.571612	1.241364	-0.271004
69	6	0	-3.188584	0.215205	0.360288
70	16	0	-0.878410	1.582786	-0.465285
71	6	0	-4.693465	0.250219	0.365496
72	8	0	-5.406783	-0.272029	-0.463825
73	8	0	-5.147793	0.961085	1.400836
74	6	0	-6.566883	1.169988	1.461578
75	1	0	-6.764544	1.380108	2.514396
76	1	0	-7.075709	0.246857	1.173772
77	6	0	-2.514414	-0.878724	1.091088
78	6	0	-3.384423	2.316347	-0.924255
79	6	0	-3.437265	3.592769	-0.356908
80	6	0	-4.106303	2.048562	-2.089702
81	6	0	-4.215900	4.585331	-0.943233
82	1	0	-2.879131	3.790819	0.553414
83	6	0	-4.878345	3.046490	-2.676836
84	1	0	-4.074337	1.049997	-2.512290
85	6	0	-4.936628	4.314736	-2.104668
86	1	0	-4.263325	5.570797	-0.489278
87	1	0	-5.439264	2.829981	-3.581420
88	1	0	-5.544089	5.090759	-2.561353
89	6	0	-6.971981	2.332146	0.571529
90	1	0	-8.043427	2.530732	0.682566
91	1	0	-6.417023	3.235020	0.842427
92	1	0	-6.765490	2.103636	-0.477469
93	7	0	-1.259490	-1.036153	1.202808
94	6	0	-3.343092	-1.889259	1.833326
95	6	0	-3.039867	-2.123508	3.178089
96	6	0	-4.360026	-2.624899	1.219716
97	6	0	-3.752084	-3.073777	3.901286
98	1	0	-2.245746	-1.546287	3.641989
99	6	0	-5.065768	-3.580263	1.946167
100	1	0	-4.604112	-2.443465	0.179605

101	6	0	-4.766422	-3.805412	3.286724
102	1	0	-3.516976	-3.241634	4.948337
103	1	0	-5.854752	-4.147835	1.460683
104	1	0	-5.323414	-4.546841	3.852689

Zero-point correction= 0.822880 (Hartree/Particle)
Thermal correction to Energy= 0.877435
Thermal correction to Enthalpy= 0.878379
Thermal correction to Gibbs Free Energy= 0.730901
Sum of electronic and zero-point Energies= -3985.136035
Sum of electronic and thermal Energies= -3985.081480
Sum of electronic and thermal Enthalpies= -3985.080535
Sum of electronic and thermal Free Energies= -3985.228014

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3378112

TS7c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.862806	-0.027407	-0.164966
2	6	0	1.827721	0.288388	0.706324
3	16	0	2.283607	0.563969	-1.682139
4	6	0	4.311620	-0.166855	0.096388
5	6	0	4.818572	-1.209143	0.883777
6	6	0	5.220572	0.742655	-0.463222
7	6	0	6.185261	-1.327832	1.113557
8	1	0	4.126033	-1.927339	1.304126
9	6	0	6.587640	0.617467	-0.240064
10	1	0	4.848697	1.563796	-1.070408
11	6	0	7.077312	-0.416970	0.553109
12	1	0	6.556246	-2.144793	1.727358
13	1	0	7.272036	1.337916	-0.679250
14	1	0	8.144509	-0.514689	0.729744
15	6	0	1.834083	0.040130	2.173457
16	8	0	1.531097	0.833100	3.036435
17	8	0	2.204819	-1.225308	2.438286
18	6	0	2.359593	-1.568987	3.822337
19	6	0	3.703097	-1.108508	4.360474
20	1	0	2.270498	-2.658037	3.836003
21	1	0	1.537098	-1.129106	4.390694
22	1	0	3.811835	-1.425089	5.403396
23	1	0	4.526746	-1.531245	3.778623
24	1	0	3.774421	-0.018626	4.321605
25	6	0	2.024891	3.771901	-2.680924
26	6	0	1.830043	4.959098	-3.377864
27	6	0	1.032389	5.963535	-2.835584
28	6	0	0.431889	5.783109	-1.590672
29	6	0	0.627876	4.602540	-0.889402
30	6	0	1.426579	3.591059	-1.433475
31	1	0	2.641326	2.983470	-3.100981
32	1	0	2.298377	5.098063	-4.347413
33	1	0	0.877146	6.888146	-3.384155
34	1	0	-0.197513	6.559329	-1.165894
35	1	0	0.163371	4.446987	0.076093
36	6	0	1.614831	2.359677	-0.672439
37	7	0	1.470599	2.060420	0.526346
38	17	0	-1.168105	1.667038	-2.318215
39	26	0	-3.790873	-1.293392	-0.295872
40	15	0	-1.582856	0.942658	0.965204
41	15	0	-0.390216	-1.698721	-1.062910
42	6	0	-2.542028	3.569985	0.709924
43	6	0	-1.520392	0.114241	2.594836
44	6	0	-1.006996	-1.880307	3.867291
45	6	0	-1.650575	2.719552	1.366982
46	6	0	-1.639396	-1.339355	4.982857
47	6	0	-2.143847	0.657825	3.721985
48	6	0	-0.941091	-1.148689	2.686255
49	6	0	-2.197769	-0.064662	4.909690
50	6	0	-0.744718	3.241388	2.299631
51	6	0	-0.763909	4.601114	2.592446
52	6	0	-2.088227	-2.332151	-0.793182
53	6	0	-3.043113	-2.394563	-1.859767
54	6	0	-0.170304	-2.127367	-2.837294
55	6	0	-5.417218	-0.348735	0.542913
56	6	0	-2.729697	-2.881462	0.371167
57	6	0	-4.233984	-2.990045	-1.368977
58	6	0	-2.546012	4.931808	1.000135
59	6	0	-4.038175	-3.299690	0.004552
60	6	0	-0.206683	-3.481266	-3.202069
61	6	0	-3.274351	0.513333	0.458073
62	6	0	0.014062	-1.156714	-3.819445
63	6	0	-5.190980	0.143148	-0.772583
64	6	0	-4.245879	-0.115627	1.307753
65	6	0	-3.879145	0.676350	-0.833303
66	6	0	0.750234	-2.918028	-0.294234
67	6	0	0.438185	-3.732087	0.797549
68	6	0	0.166895	-1.536674	-5.153188
69	6	0	-0.052508	-3.854072	-4.529830
70	6	0	0.137562	-2.879066	-5.509691
71	6	0	-1.663279	5.447261	1.945502
72	6	0	3.000601	-3.825966	-0.271264
73	6	0	2.045489	-2.981644	-0.825415

74	6	0	2.683721	-4.615839	0.829771
75	6	0	1.397721	-4.571026	1.357610
76	1	0	-3.379913	1.079579	-1.702121
77	1	0	-5.878890	0.072379	-1.604269
78	1	0	-6.305090	-0.859317	0.890623
79	1	0	-4.091733	-0.416760	2.333592
80	1	0	-2.337056	-2.919199	1.375342
81	1	0	-4.774139	-3.717954	0.677542
82	1	0	-5.145970	-3.134532	-1.931508
83	1	0	-2.882804	-2.018850	-2.860535
84	1	0	-0.399716	-1.551815	1.838706
85	1	0	-0.542698	-2.861412	3.916346
86	1	0	-1.687567	-1.901389	5.910825
87	1	0	-2.680334	0.368712	5.780409
88	1	0	-2.594914	1.643851	3.669814
89	1	0	-0.016324	2.591143	2.775760
90	1	0	-0.060769	5.000735	3.316712
91	1	0	-1.669615	6.509685	2.172012
92	1	0	-3.239268	5.588060	0.482953
93	1	0	-3.226887	3.176023	-0.033215
94	1	0	0.010677	-0.106094	-3.551741
95	1	0	0.307277	-0.771434	-5.910413
96	1	0	0.261654	-3.170052	-6.548809
97	1	0	-0.078132	-4.905371	-4.800677
98	1	0	-0.350568	-4.244909	-2.442863
99	1	0	2.307489	-2.383443	-1.690286
100	1	0	3.997799	-3.853427	-0.698628
101	1	0	3.430859	-5.274155	1.263310
102	1	0	1.128363	-5.203695	2.198750
103	1	0	-0.560447	-3.745597	1.211619
104	45	0	0.182654	0.524271	-0.526306

Zero-point correction=	0.820554 (Hartree/Particle)
Thermal correction to Energy=	0.874486
Thermal correction to Enthalpy=	0.875430
Thermal correction to Gibbs Free Energy=	0.732229
Sum of electronic and zero-point Energies=	-3985.083821
Sum of electronic and thermal Energies=	-3985.029889
Sum of electronic and thermal Enthalpies=	-3985.028945
Sum of electronic and thermal Free Energies=	-3985.172146

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.2698208

TS8c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-3.759741	-0.483088	-1.817327
2	15	0	-1.897708	-1.399255	0.886200
3	15	0	-1.250717	1.568547	-0.907701
4	6	0	-1.659996	-2.273298	3.552375
5	6	0	-1.463420	-3.134502	0.486225
6	6	0	-0.106694	-4.703141	-0.757486
7	6	0	-2.377496	-1.463444	2.664076
8	6	0	-0.861077	-5.760385	-0.258923
9	6	0	-2.218972	-4.201859	0.984910
10	6	0	-0.403932	-3.394958	-0.382856
11	6	0	-1.917059	-5.508015	0.616005
12	6	0	-3.395811	-0.649349	3.170244
13	6	0	-3.691736	-0.642378	4.530519
14	6	0	-2.273476	0.824843	-2.198989
15	6	0	-3.494639	1.292424	-2.785175
16	6	0	-2.348673	2.666562	0.059504
17	6	0	-5.303636	-1.768458	-1.354409
18	6	0	-1.972365	-0.445901	-2.794682
19	6	0	-3.942927	0.312912	-3.711332
20	6	0	-1.961275	-2.268246	4.910137
21	6	0	-3.003197	-0.756003	-3.719058
22	6	0	-2.543819	2.415998	1.420097
23	6	0	-3.520316	-1.275053	0.041562
24	6	0	-2.976586	3.769735	-0.529088
25	6	0	-5.538145	-0.487483	-0.786223
26	6	0	-4.071604	-2.257595	-0.844224
27	6	0	-4.443362	-0.174961	0.063569
28	6	0	-0.210373	2.758487	-1.826165
29	6	0	-0.045990	2.663298	-3.208023
30	6	0	-3.825084	4.576167	0.221601
31	6	0	-3.390957	3.225713	2.172798
32	6	0	-4.039680	4.300303	1.571318
33	6	0	-2.974006	-1.451648	5.405057
34	6	0	1.348972	4.604446	-1.777089
35	6	0	0.493119	3.736144	-1.112821
36	6	0	1.512079	4.504497	-3.158363
37	6	0	0.813101	3.536948	-3.871823
38	1	0	-4.309571	0.767271	0.574253
39	1	0	-6.368447	0.168876	-1.008710
40	1	0	-5.928226	-2.268204	-2.082209
41	1	0	-3.600653	-3.190879	-1.116974
42	1	0	-1.133794	-1.078151	-2.533773
43	1	0	-3.086384	-1.672852	-4.286113
44	1	0	-4.867712	0.351030	-4.270901
45	1	0	-4.021548	2.196636	-2.515257
46	1	0	0.202468	-2.575373	-0.754617

47	1	0	0.722843	-4.888574	-1.434156
48	1	0	-0.626844	-6.781679	-0.545160
49	1	0	-2.505813	-6.329990	1.012292
50	1	0	-3.044737	-4.010243	1.664510
51	1	0	-3.977553	-0.017489	2.510376
52	1	0	-4.489214	-0.005199	4.902037
53	1	0	-3.202424	-1.446945	6.466874
54	1	0	-1.391519	-2.901538	5.583236
55	1	0	-0.855299	-2.898708	3.185230
56	1	0	-2.784382	4.008264	-1.571615
57	1	0	-4.310838	5.428650	-0.243608
58	1	0	-4.698913	4.934290	2.156728
59	1	0	-3.535289	3.016231	3.228427
60	1	0	-2.031084	1.583184	1.895069
61	1	0	0.390183	3.802730	-0.034779
62	1	0	1.901677	5.348190	-1.211269
63	1	0	2.187129	5.179539	-3.676370
64	1	0	0.939082	3.452557	-4.947034
65	1	0	-0.579255	1.903325	-3.771051
66	17	0	1.091249	-1.242338	2.052752
67	45	0	-0.119868	0.085723	0.437162
68	6	0	3.039120	-0.587285	-0.804328
69	6	0	3.587376	0.234037	0.130845
70	16	0	1.426955	-0.305527	-1.341335
71	6	0	4.987135	0.057152	0.605956
72	8	0	5.852517	0.903797	0.555841
73	8	0	5.167197	-1.176956	1.089681
74	6	0	6.507246	-1.550644	1.435589
75	1	0	6.385918	-2.325629	2.194862
76	1	0	7.017556	-0.689621	1.873379
77	6	0	2.718659	1.300737	0.585237
78	6	0	3.744494	-1.727014	-1.443161
79	6	0	3.403703	-3.034636	-1.083847
80	6	0	4.747111	-1.504957	-2.387339
81	6	0	4.068711	-4.107795	-1.664913
82	1	0	2.640356	-3.191364	-0.326455
83	6	0	5.403747	-2.583912	-2.974506
84	1	0	5.008394	-0.485724	-2.657221
85	6	0	5.066210	-3.885362	-2.614984
86	1	0	3.812956	-5.122338	-1.372393
87	1	0	6.181038	-2.405578	-3.711619
88	1	0	5.579450	-4.726745	-3.071392
89	6	0	7.242765	-2.076390	0.216080
90	1	0	8.238025	-2.432239	0.503549
91	1	0	6.689168	-2.903313	-0.238938
92	1	0	7.359867	-1.285296	-0.529948
93	7	0	1.467363	1.325835	0.296001
94	6	0	3.173842	2.477030	1.387466
95	6	0	2.522677	2.739524	2.595695
96	6	0	4.159478	3.349395	0.921984
97	6	0	2.862973	3.864868	3.339369
98	1	0	1.761838	2.046670	2.943182
99	6	0	4.484866	4.481362	1.662334
100	1	0	4.671097	3.135152	-0.008880
101	6	0	3.840007	4.739681	2.870279
102	1	0	2.363751	4.058585	4.284219
103	1	0	5.249154	5.161261	1.297455
104	1	0	4.102930	5.621641	3.447702

Zero-point correction=	0.822346 (Hartree/Particle)
Thermal correction to Energy=	0.876351
Thermal correction to Enthalpy=	0.877295
Thermal correction to Gibbs Free Energy=	0.730442
Sum of electronic and zero-point Energies=	-3985.116528
Sum of electronic and thermal Energies=	-3985.062524
Sum of electronic and thermal Enthalpies=	-3985.061579
Sum of electronic and thermal Free Energies=	-3985.208433

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.311932

INT12c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.406484	2.608901	0.050566
2	6	0	-2.591381	1.674060	1.045891
3	16	0	-3.716950	2.491319	-1.063767
4	6	0	-1.272755	3.495794	-0.294682
5	6	0	-0.923742	4.609904	0.473411
6	6	0	-0.552925	3.219183	-1.465273
7	6	0	0.137459	5.420757	0.083983
8	1	0	-1.483078	4.829331	1.376277
9	6	0	0.515534	4.027095	-1.846157
10	1	0	-0.849506	2.372693	-2.084240
11	6	0	0.863666	5.127848	-1.070008
12	1	0	0.399473	6.287509	0.684606
13	1	0	1.072011	3.790082	-2.747708
14	1	0	1.698095	5.757783	-1.363081
15	6	0	-1.762076	1.441703	2.257417
16	8	0	-1.930464	0.519639	3.022268
17	8	0	-0.843258	2.404164	2.446797
18	6	0	-0.120225	2.399868	3.685687
19	6	0	-0.278804	3.763013	4.330557

20	1	0	0.926275	2.199147	3.444179
21	1	0	-0.499574	1.595251	4.317436
22	1	0	0.306142	3.811941	5.254828
23	1	0	0.070453	4.552512	3.657489
24	1	0	-1.328300	3.955655	4.573337
25	6	0	-6.775221	1.079174	-0.896659
26	6	0	-7.868873	0.338973	-1.336416
27	6	0	-7.759719	-1.040964	-1.491521
28	6	0	-6.553178	-1.679853	-1.212315
29	6	0	-5.457710	-0.945880	-0.773640
30	6	0	-5.570658	0.436565	-0.604619
31	1	0	-6.862295	2.154188	-0.761962
32	1	0	-8.807761	0.839848	-1.553078
33	1	0	-8.614019	-1.616668	-1.836248
34	1	0	-6.455280	-2.753166	-1.346082
35	1	0	-4.503496	-1.423934	-0.584278
36	6	0	-4.385084	1.179596	-0.138541
37	7	0	-3.699272	0.874475	0.918867
38	17	0	-1.924034	-0.396760	-2.063864
39	26	0	2.945095	-2.874614	-0.809134
40	15	0	-0.060660	-1.868394	0.344525
41	15	0	2.224159	0.439044	-0.480147
42	6	0	-2.043099	-3.747482	-0.357916
43	6	0	0.515703	-1.892402	2.085771
44	6	0	1.583571	-0.791520	3.958424
45	6	0	-1.690332	-2.690493	0.484198
46	6	0	1.507808	-1.964752	4.701518
47	6	0	0.400402	-3.055612	2.856558
48	6	0	1.078232	-0.754476	2.661185
49	6	0	0.901448	-3.093982	4.152670
50	6	0	-2.593417	-2.245457	1.454310
51	6	0	-3.825455	-2.874839	1.595282
52	6	0	3.433806	-0.925139	-0.473691
53	6	0	4.139834	-1.413563	-1.617310
54	6	0	2.631116	1.291930	-2.064464
55	6	0	2.406982	-4.854380	-0.985249
56	6	0	3.808326	-1.744635	0.642521
57	6	0	4.933625	-2.520783	-1.213525
58	6	0	-3.279873	-4.370286	-0.214440
59	6	0	4.735543	-2.719525	0.181516
60	6	0	3.598233	2.297249	-2.159712
61	6	0	0.964791	-3.122444	-0.479149
62	6	0	1.904745	0.936189	-3.208442
63	6	0	2.112328	-4.162326	-2.193846
64	6	0	1.697421	-4.223120	0.071206
65	6	0	1.220846	-3.101498	-1.889308
66	6	0	2.933056	1.598839	0.756356
67	6	0	4.220801	1.477566	1.288237
68	6	0	2.133662	1.581703	-4.421147
69	6	0	3.830622	2.935829	-3.373865
70	6	0	3.096842	2.583452	-4.505439
71	6	0	-4.169099	-3.940885	0.767591
72	6	0	2.647768	3.667066	1.978980
73	6	0	2.147601	2.697081	1.116071
74	6	0	3.925409	3.534884	2.516307
75	6	0	4.709155	2.436064	2.172383
76	1	0	0.824012	-2.363881	-2.573996
77	1	0	2.535367	-4.373957	-3.166321
78	1	0	3.099413	-5.678372	-0.876875
79	1	0	1.767148	-4.480387	1.118148
80	1	0	3.424411	-1.655429	1.649808
81	1	0	5.167974	-3.509934	0.779908
82	1	0	5.546976	-3.130445	-1.862760
83	1	0	4.045202	-1.025719	-2.622197
84	1	0	1.107826	0.167858	2.091953
85	1	0	2.029719	0.101702	4.386027
86	1	0	1.902196	-1.997195	5.712946
87	1	0	0.811031	-4.003914	4.738393
88	1	0	-0.098121	-3.929603	2.446816
89	1	0	-2.352140	-1.402124	2.094268
90	1	0	-4.525055	-2.511004	2.340970
91	1	0	-5.133964	-4.427548	0.879527
92	1	0	-3.546458	-5.192086	-0.872678
93	1	0	-1.356781	-4.086512	-1.127419
94	1	0	1.145802	0.157568	-3.146892
95	1	0	1.554121	1.302230	-5.295717
96	1	0	3.274965	3.089440	-5.449712
97	1	0	4.583964	3.715720	-3.434956
98	1	0	4.163744	2.593559	-1.281925
99	1	0	1.136031	2.786179	0.732200
100	1	0	2.028253	4.521310	2.234621
101	1	0	4.309753	4.285366	3.201055
102	1	0	5.706566	2.326022	2.587942
103	1	0	4.848489	0.637166	1.010090
104	45	0	0.022946	0.030670	-0.773758

Zero-point correction= 0.824086 (Hartree/Particle)
Thermal correction to Energy= 0.877459
Thermal correction to Enthalpy= 0.878403
Thermal correction to Gibbs Free Energy= 0.735239
Sum of electronic and zero-point Energies= -3985.170035
Sum of electronic and thermal Energies= -3985.116662
Sum of electronic and thermal Enthalpies= -3985.115717

Sum of electronic and thermal Free Energies= -3985.258882

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3589584

INT13c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-3.675501	-2.221263	-0.808661
2	15	0	-2.767215	0.550055	0.894184
3	15	0	-0.502328	-1.159900	-0.989754
4	6	0	-2.595702	3.283768	1.422803
5	6	0	-3.571709	0.331589	2.526435
6	6	0	-3.689781	-0.840159	4.636105
7	6	0	-3.072743	2.330312	0.512857
8	6	0	-4.876304	-0.179002	4.940861
9	6	0	-4.761044	0.996307	2.838997
10	6	0	-3.035012	-0.581453	3.434804
11	6	0	-5.409373	0.744275	4.043085
12	6	0	-3.702024	2.768041	-0.654883
13	6	0	-3.845611	4.130171	-0.914667
14	6	0	-1.691134	-2.533676	-0.942179
15	6	0	-2.363821	-3.224295	-2.001800
16	6	0	-0.753392	-0.375657	-2.630118
17	6	0	-5.692668	-1.797779	-0.735590
18	6	0	-2.190904	-3.064878	0.293446
19	6	0	-3.275032	-4.148264	-1.422205
20	6	0	-2.756940	4.641154	1.169215
21	6	0	-3.167089	-4.050749	-0.006095
22	6	0	-1.105969	0.974373	-2.670903
23	6	0	-4.000086	-0.328565	-0.142896
24	6	0	-0.588522	-1.072879	-3.833049
25	6	0	-5.120504	-1.286771	-1.932500
26	6	0	-5.013934	-1.207196	0.363039
27	6	0	-4.077769	-0.389801	-1.575052
28	6	0	1.087417	-2.050488	-1.250394
29	6	0	1.314514	-3.299029	-0.664891
30	6	0	-0.822765	-0.442092	-5.049637
31	6	0	-1.343422	1.606442	-3.889109
32	6	0	-1.212022	0.897336	-5.078394
33	6	0	-3.377877	5.070367	-0.003121
34	6	0	3.393175	-2.011371	-1.996969
35	6	0	2.135434	-1.421384	-1.928434
36	6	0	3.613877	-3.250781	-1.401012
37	6	0	2.568774	-3.897694	-0.746126
38	1	0	-3.422115	0.110752	-2.272442
39	1	0	-5.387016	-1.569443	-2.941876
40	1	0	-6.476633	-2.539658	-0.668889
41	1	0	-5.192861	-1.420058	1.407196
42	1	0	-1.909677	-2.704201	1.274409
43	1	0	-3.762541	-4.593042	0.715659
44	1	0	-3.968602	-4.775249	-1.966179
45	1	0	-2.258957	-3.022569	-3.058124
46	1	0	-2.086489	-1.059164	3.209250
47	1	0	-3.262431	-1.546655	5.341440
48	1	0	-5.381404	-0.374503	5.882493
49	1	0	-6.330851	1.267687	4.280887
50	1	0	-5.181692	1.710964	2.136792
51	1	0	-4.098117	2.054077	-1.367209
52	1	0	-4.337677	4.451787	-1.828209
53	1	0	-3.500211	6.131553	-0.200623
54	1	0	-2.389374	5.365766	1.889985
55	1	0	-2.082904	2.955609	2.322370
56	1	0	-0.253838	-2.106758	-3.817845
57	1	0	-0.694139	-0.990917	-5.978029
58	1	0	-1.393447	1.388493	-6.030076
59	1	0	-1.616298	2.657212	-3.899288
60	1	0	-1.183873	1.533037	-1.741926
61	1	0	1.970273	-0.457653	-2.400359
62	1	0	4.198297	-1.490438	-2.507651
63	1	0	4.595987	-3.712258	-1.447615
64	1	0	2.731578	-4.868059	-0.286385
65	1	0	0.510568	-3.803607	-0.136404
66	17	0	-0.255741	1.291334	2.985466
67	45	0	-0.518538	0.171894	0.829676
68	6	0	3.990107	-0.305324	1.131770
69	6	0	3.799606	0.717272	0.233070
70	16	0	2.470737	-0.838813	1.704858
71	6	0	4.935559	1.385285	-0.464601
72	8	0	5.125495	1.339240	-1.661350
73	8	0	5.735988	2.002895	0.403170
74	6	0	6.933820	2.598424	-0.127126
75	1	0	7.204271	3.353578	0.612490
76	1	0	6.697952	3.086516	-1.075575
77	6	0	2.412436	1.016801	0.066440
78	6	0	5.249505	-0.943705	1.547897
79	6	0	5.527290	-1.166257	2.900000
80	6	0	6.172892	-1.353104	0.579805
81	6	0	6.717019	-1.779973	3.277152
82	1	0	4.819314	-0.836774	3.655212
83	6	0	7.362844	-1.961716	0.961623
84	1	0	5.947702	-1.200457	-0.471482
85	6	0	7.637654	-2.176401	2.310366

86	1	0	6.926562	-1.942976	4.329761
87	1	0	8.075127	-2.273158	0.203585
88	1	0	8.566604	-2.653868	2.606978
89	6	0	8.031962	1.563452	-0.292351
90	1	0	8.959067	2.057061	-0.601745
91	1	0	8.210634	1.037884	0.650015
92	1	0	7.759390	0.831899	-1.057459
93	7	0	1.615749	0.244674	0.787624
94	6	0	1.821963	2.094602	-0.761554
95	6	0	0.833534	2.916117	-0.202707
96	6	0	2.209934	2.287005	-2.090903
97	6	0	0.231986	3.904484	-0.973961
98	1	0	0.540430	2.775257	0.833883
99	6	0	1.604339	3.279267	-2.855641
100	1	0	2.984880	1.664585	-2.524051
101	6	0	0.615467	4.086519	-2.300841
102	1	0	-0.544205	4.523543	-0.535053
103	1	0	1.901063	3.412548	-3.891503
104	1	0	0.142017	4.857930	-2.902062

Zero-point correction= 0.824718 (Hartree/Particle)
Thermal correction to Energy= 0.878713
Thermal correction to Enthalpy= 0.879658
Thermal correction to Gibbs Free Energy= 0.734577
Sum of electronic and zero-point Energies= -3985.189796
Sum of electronic and thermal Energies= -3985.135801
Sum of electronic and thermal Enthalpies= -3985.134857
Sum of electronic and thermal Free Energies= -3985.279937

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3768489

3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.460160	-0.826926	-0.077533
2	6	0	0.221936	-0.236841	-0.181501
3	16	0	1.220841	-2.525663	0.094008
4	6	0	-0.042837	1.227452	-0.237729
5	8	0	0.417387	2.001251	-1.047776
6	8	0	-0.907606	1.573127	0.719002
7	6	0	-1.474811	2.889211	0.635930
8	1	0	-1.711838	3.102809	-0.410515
9	1	0	-0.728055	3.616982	0.967929
10	6	0	-0.826259	-1.221107	-0.117060
11	6	0	2.814838	-0.247666	-0.046379
12	6	0	3.746622	-0.713605	0.890664
13	6	0	3.200571	0.739833	-0.960482
14	6	0	5.036469	-0.198042	0.917894
15	1	0	3.451059	-1.466733	1.615793
16	6	0	4.492162	1.253097	-0.926016
17	1	0	2.482373	1.104144	-1.685036
18	6	0	5.412274	0.787132	0.008943
19	1	0	5.746575	-0.562521	1.653777
20	1	0	4.780692	2.019174	-1.639042
21	1	0	6.419228	1.192985	0.031065
22	6	0	-2.712576	2.892257	1.507781
23	1	0	-3.189345	3.876727	1.471392
24	1	0	-3.426531	2.142553	1.153653
25	1	0	-2.458888	2.668288	2.547773
26	7	0	-0.433614	-2.467345	0.029683
27	6	0	-2.275338	-0.930873	-0.226012
28	6	0	-3.182841	-1.606781	0.591195
29	6	0	-2.751577	0.007051	-1.146785
30	6	0	-4.543346	-1.332534	0.504717
31	1	0	-2.810861	-2.341549	1.297848
32	6	0	-4.112128	0.278706	-1.233985
33	1	0	-2.057991	0.519143	-1.808922
34	6	0	-5.011328	-0.386533	-0.403609
35	1	0	-5.239934	-1.859058	1.150170
36	1	0	-4.470620	1.005587	-1.956676
37	1	0	-6.074220	-0.174505	-0.471124

Zero-point correction= 0.293562 (Hartree/Particle)
Thermal correction to Energy= 0.312189
Thermal correction to Enthalpy= 0.313133
Thermal correction to Gibbs Free Energy= 0.245198
Sum of electronic and zero-point Energies= -1297.742696
Sum of electronic and thermal Energies= -1297.724069
Sum of electronic and thermal Enthalpies= -1297.723125
Sum of electronic and thermal Free Energies= -1297.791060

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -1298.3324806

TS9c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.601041	-2.412901	-1.646272
2	15	0	-0.552240	-1.858226	-0.441177
3	15	0	2.174431	0.376195	0.470675
4	6	0	-3.260760	-2.491071	-0.158478

5	6	0	-0.298148	-2.960877	1.004353
6	6	0	0.815541	-3.420218	3.108266
7	6	0	-2.194694	-2.366441	-1.056928
8	6	0	0.271804	-4.701144	3.124918
9	6	0	-0.849044	-4.247591	1.034442
10	6	0	0.526079	-2.558873	2.055109
11	6	0	-0.562864	-5.111316	2.087332
12	6	0	-2.413050	-2.585964	-2.416294
13	6	0	-3.681573	-2.931473	-2.872792
14	6	0	3.177177	-0.926179	-0.341213
15	6	0	3.880791	-0.797640	-1.577299
16	6	0	3.073825	1.890108	-0.072103
17	6	0	1.998841	-4.090857	-2.687894
18	6	0	3.471516	-2.231013	0.180790
19	6	0	4.609781	-1.996263	-1.806518
20	6	0	-4.524008	-2.837977	-0.618081
21	6	0	4.365986	-2.877207	-0.716028
22	6	0	2.823423	2.391918	-1.354934
23	6	0	0.583128	-2.584624	-1.654572
24	6	0	4.003638	2.542955	0.742247
25	6	0	1.898777	-2.939263	-3.517252
26	6	0	1.185609	-3.883266	-1.544485
27	6	0	1.026760	-2.011771	-2.892665
28	6	0	2.743762	0.203745	2.217740
29	6	0	4.004952	-0.314104	2.544319
30	6	0	4.683313	3.664877	0.274304
31	6	0	3.510777	3.507047	-1.820180
32	6	0	4.444917	4.144991	-1.008982
33	6	0	-4.737107	-3.056603	-1.977680
34	6	0	2.317652	0.538652	4.582474
35	6	0	1.914974	0.646076	3.253131
36	6	0	3.559716	-0.002195	4.896043
37	6	0	4.406877	-0.419224	3.871288
38	1	0	0.775466	-1.021424	-3.240499
39	1	0	2.437770	-2.771212	-4.439718
40	1	0	2.629522	-4.951668	-2.864258
41	1	0	1.086803	-4.558743	-0.707206
42	1	0	3.075348	-2.652801	1.093898
43	1	0	4.741030	-3.886565	-0.614901
44	1	0	5.206246	-2.214418	-2.681771
45	1	0	3.844676	0.060339	-2.233555
46	1	0	0.940304	-1.559990	2.064407
47	1	0	1.456937	-3.077713	3.914923
48	1	0	0.489462	-5.376456	3.947104
49	1	0	-0.995971	-6.107009	2.096857
50	1	0	-1.499878	-4.578412	0.231007
51	1	0	-1.598621	-2.480373	-3.125007
52	1	0	-3.842730	-3.095347	-3.933850
53	1	0	-5.726794	-3.323372	-2.336722
54	1	0	-5.343783	-2.929397	0.088364
55	1	0	-3.105608	-2.318250	0.902291
56	1	0	4.204077	2.186065	1.746404
57	1	0	5.401987	4.162071	0.919456
58	1	0	4.974680	5.021512	-1.370846
59	1	0	3.294916	3.889366	-2.812959
60	1	0	2.066898	1.927290	-1.978906
61	1	0	0.953182	1.090811	3.029994
62	1	0	1.652522	0.881589	5.368979
63	1	0	3.872541	-0.090420	5.932337
64	1	0	5.386634	-0.826002	4.103841
65	1	0	4.682176	-0.632039	1.759115
66	45	0	-0.355242	0.441558	0.053013
67	17	0	-0.154275	0.999857	-2.301264
68	6	0	-2.793831	0.533521	1.221768
69	6	0	-2.339204	0.691216	-0.037052
70	16	0	-1.399524	0.175349	2.222705
71	6	0	-4.148262	0.712494	1.777703
72	6	0	-5.271832	0.315306	1.042183
73	6	0	-4.326576	1.272041	3.047359
74	6	0	-6.548386	0.486308	1.568251
75	1	0	-5.139882	-0.136642	0.064044
76	6	0	-5.604248	1.438925	3.568964
77	1	0	-3.456829	1.589043	3.616274
78	6	0	-6.719456	1.046632	2.831478
79	1	0	-7.412717	0.173848	0.989061
80	1	0	-5.730101	1.881405	4.552894
81	1	0	-7.717127	1.176600	3.240789
82	6	0	-3.146511	1.044788	-1.229825
83	8	0	-3.699632	0.257676	-1.964243
84	8	0	-3.214209	2.377678	-1.384778
85	6	0	-3.955982	2.850223	-2.519759
86	6	0	-3.128007	2.794421	-3.791793
87	1	0	-4.220575	3.876616	-2.257142
88	1	0	-4.868159	2.256176	-2.617900
89	1	0	-3.708601	3.203557	-4.626040
90	1	0	-2.208869	3.378817	-3.687430
91	1	0	-2.853001	1.763357	-4.023667
92	6	0	1.112071	4.552338	0.696324
93	6	0	1.542800	5.686155	0.021416
94	6	0	0.991192	6.014592	-1.215677
95	6	0	0.009060	5.203519	-1.776186
96	6	0	-0.417797	4.055484	-1.116206
97	6	0	0.135240	3.732713	0.120353

98	1	0	1.540949	4.283676	1.655779
99	1	0	2.314382	6.310726	0.460741
100	1	0	1.328944	6.903095	-1.741528
101	1	0	-0.425907	5.458358	-2.738278
102	1	0	-1.176509	3.411979	-1.540023
103	6	0	-0.319301	2.546435	0.873415
104	7	0	-0.581441	2.417971	2.046924

Zero-point correction= 0.820248 (Hartree/Particle)
Thermal correction to Energy= 0.874498
Thermal correction to Enthalpy= 0.875442
Thermal correction to Gibbs Free Energy= 0.731866
Sum of electronic and zero-point Energies= -3985.088620
Sum of electronic and thermal Energies= -3985.034370
Sum of electronic and thermal Enthalpies= -3985.033426
Sum of electronic and thermal Free Energies= -3985.177002

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.2687964

TS10c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.783928	0.356781	2.441592
2	6	0	3.716447	-2.119012	0.664176
3	6	0	4.799468	-1.388745	1.163435
4	6	0	3.949342	-3.351901	0.045129
5	6	0	6.095420	-1.875024	1.027286
6	1	0	4.616331	-0.432692	1.646329
7	6	0	5.245034	-3.838600	-0.083627
8	1	0	3.106346	-3.930635	-0.322590
9	6	0	6.321987	-3.099050	0.401939
10	1	0	6.930983	-1.296447	1.410341
11	1	0	5.414104	-4.800275	-0.559646
12	1	0	7.334141	-3.479443	0.299421
13	6	0	1.536608	-1.974867	-1.600503
14	8	0	0.759373	-2.626590	-2.265341
15	8	0	2.681061	-1.478943	-2.110312
16	6	0	2.973822	-1.803542	-3.474849
17	6	0	3.653495	-3.156792	-3.580263
18	1	0	3.632773	-0.997348	-3.806795
19	1	0	2.047888	-1.771831	-4.053785
20	1	0	3.941965	-3.349967	-4.619025
21	1	0	4.549761	-3.186825	-2.953641
22	1	0	2.971217	-3.948507	-3.258766
23	26	0	-2.421283	3.003122	-0.600815
24	15	0	-1.745582	-0.314046	-0.968049
25	15	0	0.711251	1.823559	0.651622
26	6	0	-4.154553	-1.736742	-0.599193
27	6	0	-1.041849	-0.153873	-2.655013
28	6	0	0.680442	0.783017	-4.080767
29	6	0	-2.845611	-1.778002	-1.086107
30	6	0	0.009077	0.317739	-5.207795
31	6	0	-1.711855	-0.616386	-3.791177
32	6	0	0.155282	0.541498	-2.816027
33	6	0	-1.185114	-0.384963	-5.058320
34	6	0	-2.359017	-2.964052	-1.651989
35	6	0	-3.190879	-4.074246	-1.761191
36	6	0	-0.499236	3.102937	0.146334
37	6	0	-1.404745	3.817918	0.989682
38	6	0	1.347595	2.442989	2.277005
39	6	0	-4.136241	2.883722	-1.742349
40	6	0	-0.590910	3.687003	-1.163567
41	6	0	-2.018602	4.843774	0.221263
42	6	0	-4.977122	-2.856066	-0.699414
43	6	0	-1.512533	4.767725	-1.106547
44	6	0	2.699491	2.775708	2.425811
45	6	0	-2.914056	1.074743	-0.987160
46	6	0	0.507710	2.544632	3.391117
47	6	0	-4.448927	2.683207	-0.368569
48	6	0	-3.201829	1.890420	-2.132386
49	6	0	-3.703184	1.572713	0.102651
50	6	0	2.131611	2.278717	-0.432935
51	6	0	2.413141	3.619916	-0.733979
52	6	0	1.001892	2.995485	4.610698
53	6	0	3.190535	3.219078	3.650049
54	6	0	2.343281	3.338323	4.746066
55	6	0	-4.501761	-4.022911	-1.289755
56	6	0	4.137314	1.627591	-1.629139
57	6	0	3.016947	1.295526	-0.869842
58	6	0	4.393534	2.955783	-1.946379
59	6	0	3.530573	3.952445	-1.489138
60	1	0	-3.663401	1.202799	1.116301
61	1	0	-4.503263	3.684639	-2.369773
62	1	0	-2.742955	1.799781	-3.106114
63	1	0	-0.051426	3.359545	-2.041128
64	1	0	-1.820322	5.379735	-1.943340
65	1	0	-2.780707	5.524474	0.575186
66	1	0	-1.615131	3.592567	2.023801
67	1	0	0.703552	0.877758	-1.946661
68	1	0	1.620599	1.319447	-4.173164
69	1	0	0.415082	0.495891	-6.199278
70	1	0	-1.711689	-0.754806	-5.933051

71	1	0	-2.647089	-1.157587	-3.689744
72	1	0	-1.331058	-3.017550	-1.998917
73	1	0	-2.806756	-4.985284	-2.210240
74	1	0	-5.146953	-4.892548	-1.375782
75	1	0	-5.992406	-2.809777	-0.317409
76	1	0	-4.542708	-0.831918	-0.145241
77	1	0	-0.523650	2.223374	3.322647
78	1	0	2.727553	3.685447	5.700728
79	1	0	4.243502	3.468719	3.741960
80	1	0	3.387492	2.684297	1.594148
81	1	0	2.836615	0.260318	-0.630098
82	1	0	4.804674	0.836015	-1.956272
83	1	0	5.265994	3.220795	-2.536651
84	1	0	3.732763	4.995052	-1.715859
85	1	0	1.765901	4.409294	-0.367156
86	45	0	-0.124726	-0.447222	0.782346
87	6	0	2.344676	-1.592891	0.776345
88	6	0	1.370229	-1.577007	-0.186070
89	16	0	1.719233	-0.894431	2.230032
90	6	0	-2.679696	-3.774541	1.901006
91	6	0	-3.597037	-4.225455	2.842403
92	6	0	-3.443709	-3.887401	4.184860
93	6	0	-2.375149	-3.089206	4.587795
94	6	0	-1.466859	-2.611180	3.651452
95	6	0	-1.618194	-2.964992	2.310655
96	1	0	-2.780053	-4.043232	0.856027
97	1	0	-4.428246	-4.847089	2.523544
98	1	0	-4.159608	-4.245128	4.919298
99	1	0	-2.257455	-2.821279	5.633006
100	1	0	-0.648613	-1.963004	3.942698
101	6	0	-0.641536	-2.521958	1.319074
102	7	0	0.025399	-2.968078	0.419451
103	1	0	0.330400	3.065121	5.461312
104	1	0	-5.095856	3.306421	0.233806

Zero-point correction= 0.819624 (Hartree/Particle)
Thermal correction to Energy= 0.874153
Thermal correction to Enthalpy= 0.875097
Thermal correction to Gibbs Free Energy= 0.730022
Sum of electronic and zero-point Energies= -3985.092977
Sum of electronic and thermal Energies= -3985.038449
Sum of electronic and thermal Enthalpies= -3985.037505
Sum of electronic and thermal Free Energies= -3985.182580

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.2729167

INT14c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.326056	-2.754078	-1.535140
2	15	0	-0.728125	-1.877994	-0.374213
3	15	0	2.182655	0.222816	0.408622
4	6	0	-3.469606	-2.231832	0.039439
5	6	0	-0.545232	-2.866948	1.165122
6	6	0	0.450057	-3.124738	3.364309
7	6	0	-2.429841	-2.304960	-0.893678
8	6	0	-0.118413	-4.388616	3.481500
9	6	0	-1.125899	-4.135046	1.300466
10	6	0	0.228143	-2.370608	2.214824
11	6	0	-0.911345	-4.889278	2.449110
12	6	0	-2.721486	-2.640320	-2.215928
13	6	0	-4.033573	-2.903049	-2.598338
14	6	0	3.015758	-1.247024	-0.299212
15	6	0	3.748536	-1.258226	-1.525215
16	6	0	3.281988	1.578405	-0.180596
17	6	0	1.627382	-4.426561	-2.508982
18	6	0	3.162826	-2.547534	0.293161
19	6	0	4.364102	-2.530274	-1.671128
20	6	0	-4.777696	-2.500057	-0.343835
21	6	0	4.014842	-3.322564	-0.542331
22	6	0	3.037503	2.165956	-1.426316
23	6	0	0.302382	-2.799910	-1.544754
24	6	0	4.360737	2.031228	0.585725
25	6	0	1.598577	-3.305726	-3.385535
26	6	0	0.823492	-4.123911	-1.378699
27	6	0	0.783817	-2.303311	-2.800927
28	6	0	2.666733	0.129428	2.191090
29	6	0	3.697388	-0.685486	2.675602
30	6	0	5.180079	3.051934	0.113434
31	6	0	3.863808	3.181446	-1.896148
32	6	0	4.935020	3.628441	-1.128809
33	6	0	-5.062510	-2.832879	-1.665933
34	6	0	2.325789	0.953948	4.451523
35	6	0	2.006882	0.968595	3.096856
36	6	0	3.321058	0.106245	4.926893
37	6	0	4.014854	-0.702270	4.031036
38	1	0	0.600216	-1.310346	-3.184160
39	1	0	2.147250	-3.208804	-4.312510
40	1	0	2.203893	-5.331140	-2.648486
41	1	0	0.684909	-4.754209	-0.511706
42	1	0	2.695886	-2.886265	1.207483
43	1	0	4.284192	-4.357377	-0.380096

44	1	0	4.953722	-2.852378	-2.518528
45	1	0	3.808590	-0.436159	-2.225042
46	1	0	0.664404	-1.382942	2.143963
47	1	0	1.062306	-2.713305	4.161460
48	1	0	0.044891	-4.979873	4.377703
49	1	0	-1.368202	-5.870184	2.541090
50	1	0	-1.752153	-4.529708	0.505540
51	1	0	-1.927544	-2.690753	-2.954065
52	1	0	-4.249422	-3.156510	-3.631828
53	1	0	-6.086062	-3.036018	-1.967001
54	1	0	-5.573918	-2.438997	0.392283
55	1	0	-3.261170	-1.971331	1.073365
56	1	0	4.566209	1.597376	1.558029
57	1	0	6.010875	3.396427	0.722489
58	1	0	5.572034	4.429232	-1.493303
59	1	0	3.649547	3.639209	-2.856689
60	1	0	2.184047	1.848809	-2.016079
61	1	0	1.249363	1.660064	2.749686
62	1	0	1.790261	1.609904	5.130917
63	1	0	3.565355	0.086670	5.984877
64	1	0	4.813862	-1.347957	4.383487
65	1	0	4.271787	-1.303571	1.996638
66	45	0	-0.287111	0.550723	-0.041134
67	17	0	0.008600	0.911481	-2.417033
68	6	0	-2.735916	0.973926	1.077677
69	6	0	-2.274220	0.936322	-0.174469
70	16	0	-1.250485	0.862737	2.100401
71	6	0	-4.066687	1.179803	1.664818
72	6	0	-5.208695	0.755638	0.971701
73	6	0	-4.215961	1.792384	2.913582
74	6	0	-6.471260	0.951199	1.520414
75	1	0	-5.099415	0.264304	0.010089
76	6	0	-5.480527	1.979526	3.459853
77	1	0	-3.337909	2.139206	3.452199
78	6	0	-6.612680	1.559055	2.765687
79	1	0	-7.349070	0.618460	0.973871
80	1	0	-5.582336	2.460808	4.427992
81	1	0	-7.599780	1.704112	3.194643
82	6	0	-3.040017	1.219995	-1.412187
83	8	0	-3.674908	0.416762	-2.056107
84	8	0	-2.943426	2.522750	-1.712117
85	6	0	-3.599136	2.955776	-2.914358
86	6	0	-2.745359	2.685556	-4.140105
87	1	0	-3.756044	4.025315	-2.761052
88	1	0	-4.568168	2.455733	-2.989115
89	1	0	-3.242360	3.088553	-5.029493
90	1	0	-1.763901	3.158107	-4.041072
91	1	0	-2.595360	1.612233	-4.274065
92	6	0	1.483312	4.334624	0.721365
93	6	0	2.102353	5.433152	0.137975
94	6	0	1.709665	5.863700	-1.127494
95	6	0	0.702231	5.187441	-1.811783
96	6	0	0.096910	4.071560	-1.244513
97	6	0	0.482824	3.645696	0.028267
98	1	0	1.788970	3.988893	1.704068
99	1	0	2.895790	5.950104	0.669258
100	1	0	2.192086	6.724773	-1.581486
101	1	0	0.392453	5.523664	-2.797227
102	1	0	-0.676374	3.523247	-1.769525
103	6	0	-0.153094	2.462605	0.635476
104	7	0	-0.630041	2.547711	1.826434

Zero-point correction= 0.821682 (Hartree/Particle)
Thermal correction to Energy= 0.876097
Thermal correction to Enthalpy= 0.877042
Thermal correction to Gibbs Free Energy= 0.731748
Sum of electronic and zero-point Energies= -3985.104860
Sum of electronic and thermal Energies= -3985.050445
Sum of electronic and thermal Enthalpies= -3985.049501
Sum of electronic and thermal Free Energies= -3985.194794

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.2918955

INT15c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.272798	1.182742	-2.532531
2	6	0	-1.059286	-2.482051	-1.101781
3	6	0	0.064151	-2.545904	-0.216687
4	6	0	-2.400242	-3.022695	-0.789837
5	6	0	-3.558560	-2.354713	-1.198071
6	6	0	-2.517584	-4.261550	-0.148315
7	6	0	-4.811280	-2.891252	-0.927556
8	1	0	-3.469566	-1.406391	-1.717531
9	6	0	-3.769950	-4.807896	0.101140
10	1	0	-1.622785	-4.807664	0.136739
11	6	0	-4.920604	-4.116926	-0.275902
12	1	0	-5.702670	-2.350638	-1.230682
13	1	0	-3.848463	-5.775936	0.586864
14	1	0	-5.899451	-4.541996	-0.074246
15	6	0	-0.010560	-2.895579	1.236665
16	8	0	0.908340	-3.392345	1.850566

17	8	0	-1.171097	-2.552463	1.806498
18	6	0	-1.323615	-2.843143	3.202951
19	6	0	-1.838786	-4.255335	3.407968
20	1	0	-2.035991	-2.095645	3.556236
21	1	0	-0.366100	-2.684194	3.701267
22	1	0	-2.002403	-4.437919	4.475194
23	1	0	-2.784918	-4.403635	2.878727
24	1	0	-1.109607	-4.984792	3.043663
25	26	0	0.580460	3.716469	0.531519
26	15	0	1.673179	0.412385	0.932553
27	15	0	-1.660161	1.232135	-0.600498
28	6	0	4.492735	0.656080	1.012802
29	6	0	0.949336	0.105684	2.594095
30	6	0	-0.929507	0.477064	4.084434
31	6	0	3.393236	-0.203363	1.091330
32	6	0	-0.211823	-0.084669	5.138274
33	6	0	1.659059	-0.465097	3.653041
34	6	0	-0.349268	0.564135	2.825496
35	6	0	1.077519	-0.560195	4.916486
36	6	0	3.611905	-1.580033	1.231631
37	6	0	4.907000	-2.083562	1.261499
38	6	0	-1.191865	2.968865	-0.242427
39	6	0	-0.574698	3.873966	-1.158086
40	6	0	-2.653618	1.371138	-2.158273
41	6	0	2.071565	4.371132	1.791858
42	6	0	-1.410722	3.688131	0.980178
43	6	0	-0.447889	5.138851	-0.522378
44	6	0	5.787071	0.144566	1.036449
45	6	0	-0.964181	5.025858	0.798206
46	6	0	-4.031239	1.122971	-2.192560
47	6	0	1.882081	2.213425	0.992429
48	6	0	-1.997401	1.652040	-3.362792
49	6	0	2.529238	4.359554	0.443483
50	6	0	1.684553	3.051400	2.138399
51	6	0	2.411581	3.036881	-0.055618
52	6	0	-3.011804	0.987257	0.628814
53	6	0	-3.976062	1.972291	0.891034
54	6	0	-2.704221	1.713379	-4.558600
55	6	0	-4.734109	1.174064	-3.394072
56	6	0	-4.075613	1.476274	-4.580426
57	6	0	5.997401	-1.225462	1.150691
58	6	0	-4.189073	-0.511476	2.126612
59	6	0	-3.132843	-0.251499	1.254618
60	6	0	-5.131378	0.475048	2.391170
61	6	0	-5.021070	1.720810	1.771685
62	1	0	2.618290	2.706430	-1.062196
63	1	0	2.847537	5.221208	-0.127466
64	1	0	1.986652	5.241306	2.428588
65	1	0	1.275188	2.737094	3.087583
66	1	0	-1.838544	3.285095	1.887052
67	1	0	-0.967991	5.801343	1.551928
68	1	0	0.015731	6.016069	-0.952548
69	1	0	-0.218509	3.621322	-2.145905
70	1	0	-0.907929	1.013986	2.017527
71	1	0	-1.943199	0.839075	4.231158
72	1	0	-0.658101	-0.158177	6.125697
73	1	0	1.641495	-1.005070	5.730758
74	1	0	2.668665	-0.829683	3.501955
75	1	0	2.778226	-2.270989	1.307527
76	1	0	5.058052	-3.154097	1.356478
77	1	0	7.007473	-1.624349	1.155344
78	1	0	6.631111	0.823863	0.961704
79	1	0	4.347639	1.726097	0.917652
80	1	0	-0.921518	1.785691	-3.374267
81	1	0	-2.172416	1.931744	-5.479807
82	1	0	-4.623907	1.516385	-5.517052
83	1	0	-5.802361	0.976742	-3.395964
84	1	0	-4.570651	0.879191	-1.284356
85	1	0	-2.392768	-1.020165	1.077437
86	1	0	-4.272428	-1.491930	2.586662
87	1	0	-5.953728	0.277895	3.072958
88	1	0	-5.758914	2.493528	1.966461
89	1	0	-3.915872	2.934649	0.392274
90	45	0	0.433120	-0.419693	-0.927298
91	16	0	-0.778249	-1.684597	-2.581981
92	6	0	3.553744	-3.052121	-2.566179
93	6	0	4.798963	-3.139985	-3.174681
94	6	0	5.620171	-2.016302	-3.248752
95	6	0	5.182871	-0.804099	-2.723458
96	6	0	3.929200	-0.708848	-2.130610
97	6	0	3.109725	-1.833955	-2.034538
98	1	0	2.910574	-3.922363	-2.490574
99	1	0	5.131142	-4.086965	-3.590183
100	1	0	6.596499	-2.086335	-3.720102
101	1	0	5.817110	0.075730	-2.777099
102	1	0	3.586067	0.237029	-1.735091
103	6	0	1.818802	-1.821658	-1.319570
104	7	0	1.354834	-2.876560	-0.779669

Zero-point correction= 0.824489 (Hartree/Particle)
Thermal correction to Energy= 0.878159
Thermal correction to Enthalpy= 0.879104
Thermal correction to Gibbs Free Energy= 0.737751

Sum of electronic and zero-point Energies= -3985.136099
Sum of electronic and thermal Energies= -3985.082428
Sum of electronic and thermal Enthalpies= -3985.081484
Sum of electronic and thermal Free Energies= -3985.222837

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3199267

INT16c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.480339	1.708655	2.758211
2	15	0	-1.415846	1.486140	-0.489944
3	15	0	1.915341	0.437506	0.625260
4	6	0	-3.058434	1.403028	-2.714178
5	6	0	-1.036940	3.255364	-0.782446
6	6	0	0.582353	4.998598	-1.228026
7	6	0	-3.034853	1.311682	-1.317687
8	6	0	-0.420043	5.960126	-1.143543
9	6	0	-2.044161	4.225902	-0.726254
10	6	0	0.275062	3.651335	-1.053010
11	6	0	-1.736170	5.571341	-0.898172
12	6	0	-4.219907	1.062070	-0.624869
13	6	0	-5.418073	0.913899	-1.318435
14	6	0	1.425984	1.447538	2.074134
15	6	0	1.318986	0.978884	3.422878
16	6	0	2.797925	-0.935686	1.467184
17	6	0	-2.407685	1.919580	3.458627
18	6	0	1.066341	2.838031	2.086914
19	6	0	0.898924	2.058241	4.244782
20	6	0	-4.257120	1.261576	-3.402348
21	6	0	0.752726	3.208034	3.421602
22	6	0	2.024921	-1.963210	2.010220
23	6	0	-1.834725	1.423947	1.273756
24	6	0	4.188862	-0.998961	1.576982
25	6	0	-2.042834	0.544178	3.404516
26	6	0	-2.283882	2.462221	2.150944
27	6	0	-1.688299	0.238016	2.064633
28	6	0	3.306234	1.387270	-0.101095
29	6	0	3.841565	2.542882	0.475765
30	6	0	4.790902	-2.082856	2.210969
31	6	0	2.625486	-3.043028	2.647366
32	6	0	4.013731	-3.108317	2.743176
33	6	0	-5.438343	1.015074	-2.705509
34	6	0	5.020960	1.477396	-1.809339
35	6	0	3.910988	0.859408	-1.247741
36	6	0	5.535875	2.640074	-1.242412
37	6	0	4.944957	3.169765	-0.099316
38	1	0	-1.294454	-0.705461	1.717860
39	1	0	-1.982609	-0.132801	4.246168
40	1	0	-2.672908	2.472508	4.349719
41	1	0	-2.434420	3.496952	1.876097
42	1	0	1.011779	3.490742	1.228731
43	1	0	0.406637	4.182411	3.738638
44	1	0	0.688047	1.998644	5.303804
45	1	0	1.495664	-0.035598	3.750904
46	1	0	1.056280	2.905222	-1.151348
47	1	0	1.607455	5.287585	-1.439758
48	1	0	-0.182314	7.010383	-1.285541
49	1	0	-2.524813	6.316426	-0.850611
50	1	0	-3.075498	3.925642	-0.560416
51	1	0	-4.211249	0.970872	0.456713
52	1	0	-6.333004	0.707215	-0.772005
53	1	0	-6.373667	0.895225	-3.244667
54	1	0	-4.266936	1.334787	-4.485709
55	1	0	-2.134687	1.579550	-3.259089
56	1	0	4.808049	-0.214156	1.156323
57	1	0	5.873512	-2.127416	2.283043
58	1	0	4.488091	-3.957448	3.226216
59	1	0	2.008244	-3.841772	3.048442
60	1	0	0.945501	-1.926783	1.927685
61	1	0	3.521620	-0.040512	-1.705176
62	1	0	5.473422	1.046054	-2.696743
63	1	0	6.398604	3.128529	-1.686105
64	1	0	5.347666	4.068909	0.357750
65	1	0	3.414332	2.953631	1.383164
66	45	0	0.238798	-0.335835	-1.033135
67	17	0	1.120894	0.921162	-2.837383
68	6	0	-1.661138	-2.165226	-1.152488
69	6	0	-0.695211	-2.711256	-0.309077
70	16	0	-1.124416	-1.409508	-2.621237
71	6	0	-3.120195	-2.235145	-0.869213
72	6	0	-3.653413	-2.094096	0.415983
73	6	0	-4.005111	-2.462229	-1.930717
74	6	0	-5.021477	-2.203577	0.639893
75	1	0	-3.005206	-1.869589	1.251971
76	6	0	-5.370388	-2.576272	-1.707271
77	1	0	-3.615338	-2.555219	-2.939223
78	6	0	-5.886791	-2.451750	-0.419610
79	1	0	-5.407956	-2.083739	1.648241
80	1	0	-6.035419	-2.761101	-2.545437
81	1	0	-6.955251	-2.541093	-0.247087
82	6	0	-1.108357	-3.559363	0.873135

83	8	0	-1.484067	-4.696878	0.769552
84	8	0	-0.959908	-2.919900	2.048964
85	6	0	-1.291372	-3.656279	3.239421
86	6	0	-2.771988	-3.546741	3.554484
87	1	0	-0.677354	-3.197938	4.018135
88	1	0	-0.990664	-4.697153	3.101971
89	1	0	-2.989363	-4.068770	4.491892
90	1	0	-3.068588	-2.498473	3.666456
91	1	0	-3.367902	-3.999801	2.757752
92	6	0	1.233990	-2.076760	-1.328938
93	6	0	2.553161	-2.323161	-1.940232
94	6	0	3.553005	-2.942829	-1.182017
95	6	0	2.830236	-1.914481	-3.248291
96	6	0	4.826761	-3.110603	-1.713528
97	1	0	3.329229	-3.272529	-0.172803
98	6	0	4.100037	-2.107195	-3.782230
99	1	0	2.052202	-1.434462	-3.829719
100	6	0	5.104646	-2.690690	-3.012232
101	1	0	5.602339	-3.572988	-1.109850
102	1	0	4.305840	-1.793179	-4.801217
103	1	0	6.099606	-2.824543	-3.427320
104	7	0	0.613854	-3.021970	-0.726531

Zero-point correction= 0.823505 (Hartree/Particle)
Thermal correction to Energy= 0.877691
Thermal correction to Enthalpy= 0.878635
Thermal correction to Gibbs Free Energy= 0.735231
Sum of electronic and zero-point Energies= -3985.122724
Sum of electronic and thermal Energies= -3985.068538
Sum of electronic and thermal Enthalpies= -3985.067594
Sum of electronic and thermal Free Energies= -3985.210998

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3107102

TS11c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.046023	-3.637404	-0.818816
2	15	0	1.306023	-1.567017	0.624678
3	15	0	-2.240394	-0.504827	-0.316348
4	6	0	2.623808	-0.583014	2.856973
5	6	0	2.711774	-1.702285	-0.554670
6	6	0	3.472139	-1.914123	-2.852016
7	6	0	2.132308	-1.740861	2.246553
8	6	0	4.792143	-1.751625	-2.439067
9	6	0	4.040053	-1.553472	-0.151566
10	6	0	2.443661	-1.883526	-1.918070
11	6	0	5.070125	-1.576719	-1.088691
12	6	0	2.333610	-2.981685	2.859299
13	6	0	3.013890	-3.061551	4.070397
14	6	0	-2.190197	-2.026126	-1.313742
15	6	0	-3.003728	-3.200036	-1.208183
16	6	0	-3.416736	-0.991005	1.006806
17	6	0	-0.066592	-5.340108	-0.199639
18	6	0	-1.226160	-2.276973	-2.340889
19	6	0	-2.531941	-4.156532	-2.146881
20	6	0	3.316270	-0.669894	4.061306
21	6	0	-1.433990	-3.585573	-2.848801
22	6	0	-2.975500	-1.215292	2.311798
23	6	0	0.510083	-3.192730	0.433001
24	6	0	-4.768712	-1.198853	0.700291
25	6	0	-0.994749	-4.911510	0.790219
26	6	0	0.866394	-4.290538	-0.413047
27	6	0	-0.643946	-3.592678	1.179785
28	6	0	-3.274058	0.612872	-1.336917
29	6	0	-3.354473	0.492126	-2.724727
30	6	0	-5.653432	-1.644210	1.675465
31	6	0	-3.864296	-1.661097	3.288488
32	6	0	-5.200654	-1.880781	2.972728
33	6	0	3.507353	-1.906096	4.672043
34	6	0	-4.610766	2.627730	-1.452341
35	6	0	-3.913863	1.685344	-0.707032
36	6	0	-4.682353	2.504396	-2.837823
37	6	0	-4.059596	1.433076	-3.470290
38	1	0	-1.178387	-2.981742	1.892267
39	1	0	-1.854298	-5.465213	1.142525
40	1	0	-0.092629	-6.281175	-0.732225
41	1	0	1.681008	-4.299464	-1.123190
42	1	0	-0.466679	-1.579458	-2.660754
43	1	0	-0.833563	-4.076307	-3.602768
44	1	0	-2.909709	-5.162934	-2.266771
45	1	0	-3.794050	-3.354046	-0.487081
46	1	0	1.421749	-2.028905	-2.247649
47	1	0	3.241219	-2.056720	-3.903726
48	1	0	5.596998	-1.753931	-3.167435
49	1	0	6.095333	-1.442996	-0.757662
50	1	0	4.276608	-1.407292	0.897012
51	1	0	1.961162	-3.888266	2.392046
52	1	0	3.161364	-4.028680	4.542331
53	1	0	4.037387	-1.971124	5.618120
54	1	0	3.693813	0.236808	4.524092
55	1	0	2.470129	0.388282	2.397772

56	1	0	-5.130209	-1.010216	-0.306523
57	1	0	-6.698163	-1.802607	1.424616
58	1	0	-5.893117	-2.224689	3.735618
59	1	0	-3.506429	-1.823643	4.300741
60	1	0	-1.944414	-1.005005	2.572797
61	1	0	-3.856960	1.794081	0.371671
62	1	0	-5.078628	3.468184	-0.949013
63	1	0	-5.222544	3.242801	-3.423146
64	1	0	-4.117853	1.327987	-4.549691
65	1	0	-2.870079	-0.337208	-3.231051
66	45	0	-0.058656	0.523653	0.123918
67	17	0	-0.379771	0.896270	2.468038
68	6	0	1.985140	1.665424	-1.114311
69	6	0	1.317214	2.142009	-0.044022
70	16	0	0.676659	0.928188	-2.159852
71	6	0	3.383747	1.659228	-1.548799
72	6	0	4.422618	1.755217	-0.610646
73	6	0	3.706013	1.605079	-2.912152
74	6	0	5.743354	1.830078	-1.033829
75	1	0	4.184456	1.763414	0.446719
76	6	0	5.029994	1.667562	-3.328671
77	1	0	2.915072	1.530075	-3.652098
78	6	0	6.052163	1.787567	-2.391090
79	1	0	6.535806	1.910451	-0.295753
80	1	0	5.261374	1.630356	-4.388945
81	1	0	7.086553	1.844516	-2.717706
82	6	0	1.856043	2.915920	1.101599
83	8	0	2.701840	2.517583	1.878265
84	8	0	1.285639	4.114945	1.179624
85	6	0	1.611969	4.915536	2.328974
86	6	0	0.757554	4.517124	3.518613
87	1	0	1.407027	5.938512	2.008941
88	1	0	2.677439	4.806187	2.544624
89	1	0	1.011919	5.142523	4.381291
90	1	0	-0.302674	4.649997	3.287025
91	1	0	0.927712	3.469356	3.778864
92	6	0	-0.476720	2.385902	-0.677975
93	6	0	-1.306705	3.523756	-0.209084
94	6	0	-1.873044	3.574808	1.065358
95	6	0	-1.571959	4.559234	-1.113305
96	6	0	-2.708194	4.629841	1.420418
97	1	0	-1.665171	2.778086	1.769926
98	6	0	-2.405726	5.611468	-0.757473
99	1	0	-1.126227	4.517954	-2.101009
100	6	0	-2.980745	5.649007	0.511323
101	1	0	-3.150609	4.650547	2.412554
102	1	0	-2.607960	6.403803	-1.472526
103	1	0	-3.633254	6.471384	0.791806
104	7	0	-0.456086	2.197973	-1.989278

Zero-point correction= 0.820827 (Hartree/Particle)
Thermal correction to Energy= 0.874767
Thermal correction to Enthalpy= 0.875711
Thermal correction to Gibbs Free Energy= 0.728892
Sum of electronic and zero-point Energies= -3985.071073
Sum of electronic and thermal Energies= -3985.017134
Sum of electronic and thermal Enthalpies= -3985.016190
Sum of electronic and thermal Free Energies= -3985.163009

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.2524147

TS12c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.410120	1.764262	2.769000
2	15	0	-1.246718	1.641511	-0.511952
3	15	0	1.936373	0.330157	0.718035
4	6	0	-2.751277	1.391494	-2.812440
5	6	0	-0.815953	3.394746	-0.800362
6	6	0	0.863215	5.093797	-1.180368
7	6	0	-2.819889	1.446380	-1.415043
8	6	0	-0.120699	6.078107	-1.155691
9	6	0	-1.803028	4.386409	-0.801268
10	6	0	0.517596	3.755683	-1.008823
11	6	0	-1.455813	5.722848	-0.971178
12	6	0	-4.054572	1.308544	-0.778623
13	6	0	-5.212460	1.135063	-1.532062
14	6	0	1.510552	1.365724	2.167388
15	6	0	1.309852	0.911938	3.508638
16	6	0	2.695631	-1.127796	1.532094
17	6	0	-2.339587	2.110837	3.402062
18	6	0	1.246690	2.775799	2.159793
19	6	0	0.929468	2.022365	4.309819
20	6	0	-3.910847	1.222954	-3.560037
21	6	0	0.900142	3.175299	3.478532
22	6	0	1.831985	-2.060791	2.109709
23	6	0	-1.733075	1.591303	1.233000
24	6	0	4.071295	-1.369197	1.555207
25	6	0	-2.081335	0.711571	3.344582
26	6	0	-2.130254	2.654368	2.105831
27	6	0	-1.704782	0.390177	2.014447
28	6	0	3.397706	1.170494	0.000080

29	6	0	4.056317	2.237870	0.617472
30	6	0	4.567619	-2.530286	2.142475
31	6	0	2.327379	-3.216634	2.701373
32	6	0	3.699101	-3.457462	2.712704
33	6	0	-5.142211	1.095438	-2.920959
34	6	0	5.063951	1.190266	-1.756714
35	6	0	3.914277	0.650039	-1.192863
36	6	0	5.703266	2.266778	-1.147228
37	6	0	5.197676	2.788855	0.039904
38	1	0	-1.383086	-0.581454	1.667610
39	1	0	-2.103936	0.024218	4.179538
40	1	0	-2.593270	2.674263	4.289906
41	1	0	-2.194064	3.699529	1.836284
42	1	0	1.274809	3.423899	1.296318
43	1	0	0.611452	4.173802	3.777540
44	1	0	0.670556	1.984082	5.359162
45	1	0	1.403265	-0.110296	3.846964
46	1	0	1.283088	2.988386	-1.063754
47	1	0	1.902931	5.359101	-1.346464
48	1	0	0.148000	7.121042	-1.296284
49	1	0	-2.228201	6.486108	-0.969016
50	1	0	-2.847428	4.111266	-0.678259
51	1	0	-4.114373	1.328116	0.305369
52	1	0	-6.167319	1.014766	-1.030064
53	1	0	-6.046770	0.953179	-3.505230
54	1	0	-3.849864	1.180417	-4.643420
55	1	0	-1.786540	1.472741	-3.307579
56	1	0	4.759175	-0.661603	1.104976
57	1	0	5.638479	-2.711158	2.149099
58	1	0	4.090245	-4.366568	3.159873
59	1	0	1.638795	-3.939459	3.129689
60	1	0	0.761811	-1.890965	2.085275
61	1	0	3.422081	-0.180664	-1.684137
62	1	0	5.449639	0.767605	-2.679196
63	1	0	6.595555	2.695813	-1.593983
64	1	0	5.695790	3.622369	0.526648
65	1	0	3.690762	2.638073	1.556763
66	45	0	0.219000	-0.224121	-0.965401
67	17	0	1.109678	0.976119	-2.808073
68	6	0	-1.665096	-2.156589	-1.022571
69	6	0	-0.770001	-2.830173	-0.157485
70	16	0	-0.925354	-1.571770	-2.471023
71	6	0	-3.136521	-2.132044	-0.867979
72	6	0	-3.746013	-1.949384	0.379060
73	6	0	-3.963697	-2.309921	-1.985739
74	6	0	-5.130173	-1.974852	0.511190
75	1	0	-3.139856	-1.765195	1.255910
76	6	0	-5.345216	-2.330774	-1.853913
77	1	0	-3.517002	-2.439319	-2.966720
78	6	0	-5.937978	-2.169902	-0.603522
79	1	0	-5.574415	-1.831204	1.492275
80	1	0	-5.962320	-2.475027	-2.735664
81	1	0	-7.019018	-2.190025	-0.501860
82	6	0	-1.253516	-3.625226	1.029864
83	8	0	-1.605550	-4.773328	0.972228
84	8	0	-1.209061	-2.899941	2.164366
85	6	0	-1.630695	-3.552406	3.375132
86	6	0	-3.126131	-3.397305	3.582347
87	1	0	-1.059532	-3.056099	4.163100
88	1	0	-1.343614	-4.604798	3.323887
89	1	0	-3.419781	-3.871168	4.524485
90	1	0	-3.405000	-2.339156	3.626066
91	1	0	-3.676941	-3.874256	2.767015
92	6	0	0.944377	-2.134945	-1.392519
93	6	0	2.198782	-2.419764	-2.117918
94	6	0	3.222236	-3.062188	-1.406704
95	6	0	2.441250	-1.990800	-3.425545
96	6	0	4.475755	-3.230635	-1.982887
97	1	0	3.027923	-3.404910	-0.396000
98	6	0	3.692692	-2.177845	-4.002376
99	1	0	1.655423	-1.495136	-3.983068
100	6	0	4.717824	-2.785411	-3.280347
101	1	0	5.265086	-3.712807	-1.413391
102	1	0	3.867111	-1.840351	-5.019708
103	1	0	5.697253	-2.918923	-3.730692
104	7	0	0.501365	-3.027864	-0.516828

Zero-point correction= 0.821261 (Hartree/Particle)
Thermal correction to Energy= 0.875198
Thermal correction to Enthalpy= 0.876142
Thermal correction to Gibbs Free Energy= 0.732360
Sum of electronic and zero-point Energies= -3985.116973
Sum of electronic and thermal Energies= -3985.063036
Sum of electronic and thermal Enthalpies= -3985.062092
Sum of electronic and thermal Free Energies= -3985.205873

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.302862

INT17c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.519429	-3.382355	-0.704474

2	15	0	2.418025	-0.152222	0.145183
3	15	0	-1.376898	-1.833272	0.152280
4	6	0	3.474870	1.316755	2.348212
5	6	0	3.160037	0.422296	-1.432521
6	6	0	3.504859	0.232393	-3.824539
7	6	0	3.710817	0.387740	1.337727
8	6	0	4.213418	1.431663	-3.826530
9	6	0	3.865785	1.629692	-1.446484
10	6	0	2.978892	-0.266671	-2.637860
11	6	0	4.389031	2.127672	-2.635558
12	6	0	5.002416	-0.132058	1.175248
13	6	0	6.036891	0.277130	2.006044
14	6	0	-0.463264	-2.971187	-0.944156
15	6	0	-0.258527	-4.383446	-0.823827
16	6	0	-1.809214	-2.982741	1.525723
17	6	0	3.358846	-4.123932	-0.155530
18	6	0	0.274110	-2.541446	-2.091781
19	6	0	0.602295	-4.803918	-1.873458
20	6	0	4.515568	1.729333	3.178715
21	6	0	0.930488	-3.665029	-2.660328
22	6	0	-1.258552	-2.797951	2.794733
23	6	0	2.663647	-1.946895	0.171798
24	6	0	-2.660213	-4.076357	1.306554
25	6	0	2.481247	-4.105497	0.965343
26	6	0	3.482136	-2.795170	-0.643700
27	6	0	2.057184	-2.769433	1.173516
28	6	0	-3.001219	-1.723536	-0.710104
29	6	0	-3.107836	-1.807821	-2.099800
30	6	0	-2.931387	-4.976989	2.328889
31	6	0	-1.532139	-3.703781	3.820117
32	6	0	-2.361845	-4.794645	3.589354
33	6	0	5.794989	1.213780	3.010080
34	6	0	-5.401090	-1.416537	-0.576914
35	6	0	-4.160717	-1.509766	0.042847
36	6	0	-5.498559	-1.513684	-1.961505
37	6	0	-4.348557	-1.703477	-2.720772
38	1	0	1.366601	-2.418642	1.928019
39	1	0	2.148567	-4.966224	1.529065
40	1	0	3.813544	-5.001906	-0.594095
41	1	0	4.063780	-2.485796	-1.500796
42	1	0	0.337862	-1.519396	-2.436346
43	1	0	1.597264	-3.649518	-3.512252
44	1	0	0.985055	-5.805630	-2.014664
45	1	0	-0.637066	-5.010760	-0.029777
46	1	0	2.435672	-1.203778	-2.649247
47	1	0	3.359815	-0.317251	-4.749927
48	1	0	4.623610	1.822028	-4.753192
49	1	0	4.926669	3.070600	-2.623850
50	1	0	4.006397	2.192252	-0.528558
51	1	0	5.203551	-0.858339	0.393132
52	1	0	7.031720	-0.136713	1.870768
53	1	0	6.602797	1.533954	3.661819
54	1	0	4.314875	2.450615	3.965215
55	1	0	2.474499	1.691968	2.507108
56	1	0	-3.114652	-4.218992	0.330191
57	1	0	-3.591277	-5.819836	2.144109
58	1	0	-2.575206	-5.498771	4.388600
59	1	0	-1.096627	-3.544961	4.802187
60	1	0	-0.632066	-1.933012	2.988063
61	1	0	-4.097806	-1.429882	1.124750
62	1	0	-6.290163	-1.248613	0.022357
63	1	0	-6.466567	-1.429257	-2.446421
64	1	0	-4.414037	-1.773140	-3.802646
65	1	0	-2.222210	-1.959570	-2.707197
66	45	0	0.206516	0.346888	0.339130
67	17	0	0.399236	0.236441	2.711808
68	6	0	0.020817	2.284002	-0.513732
69	6	0	-1.326707	2.440508	-0.074216
70	16	0	-0.127600	1.179317	-1.915203
71	6	0	1.101396	3.302193	-0.425868
72	6	0	1.648676	3.658216	0.810148
73	6	0	1.569158	3.930405	-1.583316
74	6	0	2.665684	4.602115	0.880587
75	1	0	1.251313	3.194933	1.704718
76	6	0	2.581161	4.882777	-1.509244
77	1	0	1.146586	3.667671	-2.548392
78	6	0	3.140527	5.213283	-0.279006
79	1	0	3.091521	4.856974	1.846286
80	1	0	2.937638	5.357786	-2.418513
81	1	0	3.936169	5.950312	-0.221213
82	6	0	-1.660545	3.478335	0.932037
83	8	0	-1.070796	3.646835	1.976552
84	8	0	-2.670504	4.263753	0.519242
85	6	0	-3.100727	5.283419	1.432054
86	6	0	-4.052712	4.729954	2.477720
87	1	0	-3.595005	6.020408	0.796011
88	1	0	-2.221899	5.736000	1.897539
89	1	0	-4.401048	5.540314	3.126940
90	1	0	-4.919894	4.265092	2.000438
91	1	0	-3.545612	3.986836	3.099310
92	6	0	-2.273196	1.803094	-0.954240
93	6	0	-3.738659	1.820501	-0.747994
94	6	0	-4.281471	1.745240	0.537647

95	6	0	-4.592790	1.895039	-1.848598
96	6	0	-5.658070	1.775510	0.720403
97	1	0	-3.622168	1.647612	1.396019
98	6	0	-5.970401	1.932369	-1.663773
99	1	0	-4.164367	1.930193	-2.844638
100	6	0	-6.506527	1.879697	-0.380100
101	1	0	-6.069256	1.712506	1.723859
102	1	0	-6.627470	2.001237	-2.525814
103	1	0	-7.582861	1.912085	-0.236653
104	7	0	-1.802663	1.164309	-2.007558

Zero-point correction= 0.823644 (Hartree/Particle)
Thermal correction to Energy= 0.876907
Thermal correction to Enthalpy= 0.877851
Thermal correction to Gibbs Free Energy= 0.735389
Sum of electronic and zero-point Energies= -3985.131468
Sum of electronic and thermal Energies= -3985.078205
Sum of electronic and thermal Enthalpies= -3985.077261
Sum of electronic and thermal Free Energies= -3985.219723

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.3180901

INT18c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.409451	0.086826	2.835327
2	15	0	0.303730	2.033033	0.066351
3	15	0	2.182090	-0.863240	0.153849
4	6	0	-0.836225	4.169648	-1.375865
5	6	0	1.411657	3.322024	0.751102
6	6	0	3.661609	4.158570	1.062157
7	6	0	-1.088118	3.026079	-0.610032
8	6	0	3.167275	5.217860	1.817620
9	6	0	0.919138	4.407542	1.484073
10	6	0	2.785945	3.218290	0.525130
11	6	0	1.794174	5.346192	2.020881
12	6	0	-2.411277	2.652512	-0.362825
13	6	0	-3.468642	3.396911	-0.878891
14	6	0	2.050623	-0.700353	1.969489
15	6	0	1.509085	-1.636228	2.910109
16	6	0	1.930175	-2.677245	-0.005653
17	6	0	-1.348797	0.828126	3.619119
18	6	0	2.400684	0.479648	2.703345
19	6	0	1.496806	-1.024086	4.192131
20	6	0	-1.892564	4.915556	-1.885765
21	6	0	2.050997	0.279570	4.064538
22	6	0	0.655144	-3.189661	0.250554
23	6	0	-0.505301	1.298324	1.518978
24	6	0	2.949527	-3.560040	-0.368665
25	6	0	-1.623553	-0.287907	2.778443
26	6	0	-0.673187	1.811124	2.845840
27	6	0	-1.113975	0.003288	1.485354
28	6	0	4.001044	-0.673516	-0.064900
29	6	0	4.901633	-1.124260	0.906985
30	6	0	2.698326	-4.927525	-0.456097
31	6	0	0.404188	-4.554207	0.170892
32	6	0	1.428453	-5.428992	-0.182475
33	6	0	-3.209409	4.529955	-1.643045
34	6	0	5.871324	0.085410	-1.405604
35	6	0	4.499145	-0.067515	-1.222873
36	6	0	6.758802	-0.368359	-0.434285
37	6	0	6.271917	-0.973534	0.722908
38	1	0	-1.129857	-0.644689	0.619142
39	1	0	-2.090103	-1.215640	3.079056
40	1	0	-1.565260	0.897424	4.676589
41	1	0	-0.278128	2.745600	3.217849
42	1	0	2.812214	1.386452	2.283295
43	1	0	2.145828	1.013949	4.852807
44	1	0	1.097311	-1.462236	5.096628
45	1	0	1.127720	-2.619315	2.675918
46	1	0	3.160543	2.398184	-0.082318
47	1	0	4.728008	4.064568	0.881044
48	1	0	3.848987	5.954023	2.233652
49	1	0	1.403546	6.185243	2.589072
50	1	0	-0.152095	4.530658	1.618203
51	1	0	-2.633082	1.779957	0.241281
52	1	0	-4.489574	3.088313	-0.674330
53	1	0	-4.031264	5.114506	-2.046703
54	1	0	-1.683275	5.800136	-2.479851
55	1	0	0.185022	4.468046	-1.583597
56	1	0	3.943745	-3.185271	-0.588518
57	1	0	3.500399	-5.602386	-0.741335
58	1	0	1.236892	-6.495718	-0.255786
59	1	0	-0.604909	-4.911256	0.350762
60	1	0	-0.163955	-2.527127	0.501883
61	1	0	3.812022	0.308566	-1.978197
62	1	0	6.243269	0.565792	-2.305521
63	1	0	7.828637	-0.245445	-0.575139
64	1	0	6.961074	-1.325459	1.484922
65	1	0	4.526442	-1.594254	1.811848
66	45	0	1.268483	0.599173	-1.354186
67	17	0	1.302744	2.330069	-3.036865

68	6	0	-3.685376	-0.828725	-1.080718
69	6	0	-3.205137	-2.028517	-0.604893
70	16	0	-2.637890	-0.278342	-2.342136
71	6	0	-4.820756	0.011364	-0.655011
72	6	0	-4.963454	0.381087	0.686861
73	6	0	-5.727736	0.502447	-1.598437
74	6	0	-5.999796	1.220096	1.074908
75	1	0	-4.252345	0.016468	1.420827
76	6	0	-6.769068	1.337974	-1.205922
77	1	0	-5.621087	0.222044	-2.642434
78	6	0	-6.907427	1.698932	0.131146
79	1	0	-6.098208	1.502912	2.118388
80	1	0	-7.471131	1.706669	-1.947417
81	1	0	-7.716810	2.354485	0.438085
82	6	0	-3.800079	-2.801432	0.515846
83	8	0	-4.898474	-2.610548	0.987279
84	8	0	-2.949826	-3.742420	0.961357
85	6	0	-3.413667	-4.552219	2.049618
86	6	0	-3.159156	-3.875218	3.384692
87	1	0	-2.845551	-5.480626	1.960666
88	1	0	-4.476706	-4.762684	1.911993
89	1	0	-3.455864	-4.539046	4.203233
90	1	0	-2.096023	-3.639107	3.500130
91	1	0	-3.745112	-2.954804	3.461002
92	6	0	-1.643001	-1.695268	-2.134009
93	6	0	-0.367558	-1.891099	-2.837182
94	6	0	0.219256	-3.153456	-2.868434
95	6	0	0.327249	-0.791911	-3.370050
96	6	0	1.511842	-3.313184	-3.365656
97	1	0	-0.325991	-4.000806	-2.470144
98	6	0	1.635648	-0.949195	-3.832468
99	1	0	-0.154571	0.175423	-3.476132
100	6	0	2.233251	-2.214109	-3.813278
101	1	0	1.962458	-4.300171	-3.367370
102	1	0	2.151152	-0.086785	-4.243071
103	1	0	3.250768	-2.337333	-4.172025
104	7	0	-2.069119	-2.502141	-1.206831

Zero-point correction=	0.824351 (Hartree/Particle)
Thermal correction to Energy=	0.878595
Thermal correction to Enthalpy=	0.879539
Thermal correction to Gibbs Free Energy=	0.733771
Sum of electronic and zero-point Energies=	-3985.173824
Sum of electronic and thermal Energies=	-3985.119580
Sum of electronic and thermal Enthalpies=	-3985.118636
Sum of electronic and thermal Free Energies=	-3985.264404

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3988.358178

INT9a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.034113	1.746289	-2.313186
2	6	0	2.443448	-0.751324	1.214848
3	6	0	1.208961	-0.332396	1.507709
4	16	0	2.810685	-0.137876	-0.444093
5	6	0	3.431894	-1.496921	2.006451
6	6	0	4.805703	-1.373311	1.774647
7	6	0	2.995369	-2.361689	3.018989
8	6	0	5.721074	-2.081290	2.547503
9	1	0	5.161033	-0.717879	0.983168
10	6	0	3.910455	-3.064076	3.792424
11	1	0	1.929258	-2.504368	3.170348
12	6	0	5.278269	-2.926310	3.561295
13	1	0	6.784491	-1.969950	2.356473
14	1	0	3.554506	-3.735627	4.568686
15	1	0	5.992539	-3.482199	4.161446
16	26	0	-3.832885	-0.263251	-0.903670
17	15	0	-1.427329	1.470655	0.821104
18	15	0	-0.620412	-1.591318	-0.905391
19	6	0	-1.537740	4.191853	0.171412
20	6	0	-1.958913	0.771310	2.434746
21	6	0	-2.242039	-1.180148	3.848759
22	6	0	-1.194242	3.253254	1.147181
23	6	0	-2.932013	-0.413897	4.783651
24	6	0	-2.658021	1.531533	3.379440
25	6	0	-1.761348	-0.588675	2.684702
26	6	0	-3.138838	0.942827	4.545497
27	6	0	-0.546432	3.682848	2.310770
28	6	0	-0.276389	5.032360	2.509382
29	6	0	-2.440447	-1.780402	-0.999800
30	6	0	-3.160267	-1.677345	-2.232218
31	6	0	-0.128659	-2.164621	-2.582217
32	6	0	-5.255641	1.181933	-0.539456
33	6	0	-3.414926	-2.012676	0.031022
34	6	0	-4.542622	-1.869804	-1.970730
35	6	0	-1.260583	5.541135	0.370623
36	6	0	-4.699973	-2.085492	-0.574887
37	6	0	-0.548969	-3.425258	-3.031068
38	6	0	-2.998479	1.400883	-0.092802
39	6	0	0.709991	-1.395417	-3.386974
40	6	0	-4.586749	1.449077	-1.766276

41	6	0	-4.285502	1.157094	0.495065
42	6	0	-3.200503	1.585335	-1.501217
43	6	0	-0.022120	-3.040936	0.067464
44	6	0	-0.739816	-3.699807	1.066984
45	6	0	1.121303	-1.879857	-4.629593
46	6	0	-0.141487	-3.901773	-4.268918
47	6	0	0.697915	-3.126991	-5.071319
48	6	0	-0.635488	5.964937	1.539672
49	6	0	1.903512	-4.422554	0.600664
50	6	0	1.307769	-3.425014	-0.158260
51	6	0	1.179785	-5.066947	1.601739
52	6	0	-0.143227	-4.707043	1.826774
53	1	0	-2.410385	1.738231	-2.223062
54	1	0	-5.044934	1.483197	-2.745363
55	1	0	-6.310560	0.976144	-0.417812
56	1	0	-4.477231	0.936084	1.535160
57	1	0	-3.239184	-2.066934	1.094534
58	1	0	-5.636502	-2.219346	-0.050821
59	1	0	-5.337214	-1.809292	-2.701627
60	1	0	-2.716275	-1.459403	-3.193371
61	1	0	-1.220642	-1.195703	1.967808
62	1	0	-2.068017	-2.238264	4.022447
63	1	0	-3.306669	-0.870164	5.695013
64	1	0	-3.679938	1.546948	5.267523
65	1	0	-2.837465	2.586932	3.200084
66	1	0	-0.250182	2.961252	3.067228
67	1	0	0.221420	5.353422	3.419424
68	1	0	-0.422542	7.018708	1.692616
69	1	0	-1.532459	6.261615	-0.394549
70	1	0	-2.007762	3.870740	-0.751747
71	1	0	1.019754	-0.409906	-3.058272
72	1	0	1.770919	-1.270018	-5.249964
73	1	0	1.020097	-3.501742	-6.038766
74	1	0	-0.473596	-4.878532	-4.608534
75	1	0	-1.193399	-4.034900	-2.403278
76	1	0	1.882765	-2.944290	-0.944790
77	1	0	2.940379	-4.686675	0.418715
78	1	0	1.646967	-5.843671	2.199534
79	1	0	-0.725291	-5.214805	2.590856
80	1	0	-1.779622	-3.460541	1.250425
81	45	0	0.454352	0.534841	-0.127436
82	6	0	1.677258	2.173478	0.372079
83	6	0	3.082634	1.674488	0.079183
84	1	0	1.362698	2.984082	-0.285477
85	1	0	1.577558	2.472720	1.414948
86	1	0	3.674017	1.574482	0.992962
87	6	0	3.907275	2.381012	-0.963348
88	6	0	3.360002	2.809807	-2.176120
89	6	0	5.268840	2.586983	-0.723998
90	6	0	4.165016	3.436241	-3.122415
91	1	0	2.304797	2.645565	-2.379601
92	6	0	6.071869	3.217522	-1.669390
93	1	0	5.704489	2.253900	0.215859
94	6	0	5.519691	3.644604	-2.873776
95	1	0	3.726418	3.765155	-4.060102
96	1	0	7.126725	3.376361	-1.464530
97	1	0	6.142245	4.137999	-3.614764
98	1	0	0.761428	-0.474843	2.489783

Zero-point correction=	0.785417 (Hartree/Particle)
Thermal correction to Energy=	0.833596
Thermal correction to Enthalpy=	0.834540
Thermal correction to Gibbs Free Energy=	0.703901
Sum of electronic and zero-point Energies=	-3703.223983
Sum of electronic and thermal Energies=	-3703.175804
Sum of electronic and thermal Enthalpies=	-3703.174860
Sum of electronic and thermal Free Energies=	-3703.305500

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3706.2886311

TS7a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.004322	-2.318770	-1.981402
2	16	0	-2.841373	0.491423	-0.510242
3	26	0	3.711497	-0.589629	-1.146497
4	15	0	1.256766	-1.302112	1.116827
5	15	0	0.718089	1.264218	-1.213835
6	6	0	0.672292	-4.043962	1.123385
7	6	0	1.804838	-0.304309	2.553401
8	6	0	1.950353	1.841965	3.668257
9	6	0	0.685634	-2.867068	1.878759
10	6	0	2.719760	1.272676	4.676907
11	6	0	2.583255	-0.870288	3.572711
12	6	0	1.494018	1.052438	2.615489
13	6	0	3.033930	-0.086153	4.628006
14	6	0	0.105992	-2.867384	3.152726
15	6	0	-0.456326	-4.030240	3.670845
16	6	0	2.433654	0.918612	-1.737043
17	6	0	2.801445	0.102549	-2.849862
18	6	0	-0.139437	1.679755	-2.794839
19	6	0	5.105110	-1.713929	-0.131846

20	6	0	3.643333	1.441157	-1.169101
21	6	0	4.215562	0.149906	-2.987037
22	6	0	0.110540	-5.204271	1.645900
23	6	0	4.736380	0.979284	-1.953774
24	6	0	-0.476558	2.993325	-3.138332
25	6	0	2.839705	-1.689549	0.322135
26	6	0	-0.506688	0.637595	-3.655434
27	6	0	4.449359	-2.511938	-1.110368
28	6	0	4.121637	-1.206904	0.756158
29	6	0	3.057201	-2.497926	-0.841995
30	6	0	0.877026	2.930752	-0.446306
31	6	0	1.797558	3.887763	-0.894218
32	6	0	-1.168498	0.912130	-4.847150
33	6	0	-1.147296	3.260466	-4.329274
34	6	0	-1.489765	2.223105	-5.189596
35	6	0	-0.452772	-5.201726	2.919212
36	6	0	-0.018914	4.569880	1.105234
37	6	0	-0.039474	3.296963	0.540723
38	6	0	0.921306	5.501103	0.676474
39	6	0	1.823684	5.158671	-0.329495
40	1	0	2.276791	-2.927380	-1.453823
41	1	0	4.919473	-2.993570	-1.956870
42	1	0	6.161951	-1.486511	-0.096826
43	1	0	4.303045	-0.537932	1.584520
44	1	0	3.711102	2.065625	-0.289453
45	1	0	5.782152	1.175066	-1.759702
46	1	0	4.796546	-0.397775	-3.716426
47	1	0	2.119427	-0.486668	-3.446875
48	1	0	0.888257	1.495374	1.837049
49	1	0	1.700074	2.898600	3.688855
50	1	0	3.075517	1.882067	5.502459
51	1	0	3.633708	-0.534999	5.414061
52	1	0	2.836483	-1.926165	3.538123
53	1	0	0.093988	-1.959254	3.747985
54	1	0	-0.900499	-4.017179	4.661689
55	1	0	-0.894286	-6.108250	3.322182
56	1	0	0.105184	-6.110709	1.048518
57	1	0	1.067578	-4.049054	0.114358
58	1	0	-0.301410	-0.393224	-3.379138
59	1	0	-1.445643	0.091607	-5.502288
60	1	0	-2.012895	2.433306	-6.118037
61	1	0	-1.402390	4.286389	-4.578514
62	1	0	-0.226727	3.818809	-2.482002
63	1	0	-0.782643	2.580692	0.867869
64	1	0	-0.749382	4.822503	1.868448
65	1	0	0.945490	6.495192	1.113335
66	1	0	2.546945	5.887433	-0.683558
67	1	0	2.486812	3.647475	-1.696819
68	45	0	-0.504183	-0.455154	-0.072493
69	6	0	-2.446939	1.038573	1.153952
70	6	0	-1.531048	0.103461	1.565124
71	6	0	-3.074892	2.159775	1.830982
72	6	0	-2.567238	2.624411	3.060307
73	6	0	-4.157140	2.853251	1.265493
74	6	0	-3.134809	3.719451	3.699093
75	1	0	-1.706733	2.131102	3.505672
76	6	0	-4.716951	3.951423	1.906722
77	1	0	-4.558840	2.526120	0.310562
78	6	0	-4.213409	4.393640	3.127511
79	1	0	-2.724217	4.055238	4.647651
80	1	0	-5.555000	4.466568	1.445605
81	1	0	-4.650737	5.254086	3.624479
82	6	0	-2.183037	-1.554053	1.020629
83	6	0	-3.444638	-1.119988	0.276205
84	1	0	-1.679444	-2.382789	0.499926
85	1	0	-2.353849	-1.907130	2.039957
86	1	0	-4.192252	-0.770614	0.993683
87	6	0	-4.112058	-2.076290	-0.672394
88	6	0	-3.440464	-2.685250	-1.735831
89	6	0	-5.471520	-2.346481	-0.487270
90	6	0	-4.120081	-3.551060	-2.586433
91	1	0	-2.383026	-2.494370	-1.899036
92	6	0	-6.149160	-3.215488	-1.336649
93	1	0	-6.005959	-1.872701	0.333212
94	6	0	-5.472922	-3.820768	-2.391663
95	1	0	-3.582172	-4.017481	-3.406595
96	1	0	-7.204413	-3.415439	-1.174481
97	1	0	-5.998118	-4.498175	-3.058983
98	1	0	-1.147188	0.076790	2.584563

Zero-point correction= 0.784381 (Hartree/Particle)
Thermal correction to Energy= 0.833117
Thermal correction to Enthalpy= 0.834061
Thermal correction to Gibbs Free Energy= 0.700064
Sum of electronic and zero-point Energies= -3703.177138
Sum of electronic and thermal Energies= -3703.128402
Sum of electronic and thermal Enthalpies= -3703.127458
Sum of electronic and thermal Free Energies= -3703.261454

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3706.2387

INT12a'

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	17	0	1.219417	-1.883976	-2.519414
2	16	0	-1.400992	-2.460799	-1.041942
3	26	0	0.900352	3.595144	0.121868
4	15	0	2.157636	0.475973	-0.332567
5	15	0	-1.172368	0.870452	0.306557
6	6	0	4.471267	0.784761	-1.956030
7	6	0	2.715446	0.327697	1.421080
8	6	0	2.205276	-0.170932	3.740249
9	6	0	3.671277	-0.079467	-1.208228
10	6	0	3.533016	0.061209	4.090486
11	6	0	4.049265	0.547630	1.781855
12	6	0	1.805133	-0.042659	2.413080
13	6	0	4.453544	0.419422	3.107837
14	6	0	4.046598	-1.419693	-1.080309
15	6	0	5.213195	-1.883390	-1.670444
16	6	0	-0.714941	2.576540	0.790931
17	6	0	-1.132092	3.788960	0.150783
18	6	0	-2.449947	1.288201	-0.957668
19	6	0	2.623649	4.532359	-0.509980
20	6	0	0.126350	2.946822	1.890426
21	6	0	-0.536846	4.882948	0.835151
22	6	0	5.637881	0.314188	-2.558786
23	6	0	0.235774	4.363078	1.910565
24	6	0	-3.704379	1.820596	-0.650778
25	6	0	2.212911	2.262781	-0.629375
26	6	0	-2.062498	1.198050	-2.299808
27	6	0	1.755380	4.300973	-1.614877
28	6	0	2.915569	3.279288	0.093402
29	6	0	1.505367	2.905301	-1.695472
30	6	0	-2.072454	0.394810	1.843473
31	6	0	-2.857597	1.292304	2.579139
32	6	0	-2.900011	1.661259	-3.311001
33	6	0	-4.536799	2.288486	-1.661193
34	6	0	-4.133082	2.220976	-2.992507
35	6	0	6.012966	-1.016790	-2.413826
36	6	0	-2.537622	-1.314861	3.501309
37	6	0	-1.905416	-0.900306	2.332147
38	6	0	-3.348026	-0.427333	4.201466
39	6	0	-3.501645	0.880059	3.740154
40	1	0	0.851858	2.403800	-2.396698
41	1	0	1.318433	5.059971	-2.249436
42	1	0	2.958879	5.497889	-0.155500
43	1	0	3.504899	3.123021	0.986330
44	1	0	0.631672	2.264716	2.559722
45	1	0	0.846994	4.939196	2.591952
46	1	0	-0.622640	5.924614	0.557154
47	1	0	-1.749312	3.851639	-0.734262
48	1	0	0.776863	-0.246704	2.133839
49	1	0	1.479302	-0.461402	4.494168
50	1	0	3.852171	-0.045469	5.123223
51	1	0	5.493148	0.590906	3.371226
52	1	0	4.779838	0.803703	1.019874
53	1	0	3.413757	-2.104092	-0.528775
54	1	0	5.485815	-2.929223	-1.562284
55	1	0	6.922027	-1.380970	-2.884080
56	1	0	6.251498	0.993577	-3.143402
57	1	0	4.193839	1.827367	-2.075200
58	1	0	-1.098773	0.755292	-2.546300
59	1	0	-2.583265	1.582983	-4.346823
60	1	0	-4.786400	2.589325	-3.778374
61	1	0	-5.510587	2.696496	-1.407385
62	1	0	-4.044609	1.868184	0.377456
63	1	0	-1.271745	-1.583062	1.777220
64	1	0	-2.394702	-2.329822	3.861854
65	1	0	-3.845431	-0.744300	5.113461
66	1	0	-4.113233	1.583867	4.296931
67	1	0	-2.948167	2.325513	2.256121
68	45	0	0.213156	-0.622462	-0.719242
69	6	0	-2.956039	-2.616374	-0.171112
70	6	0	-2.967939	-3.589100	0.744364
71	6	0	-4.115785	-1.782861	-0.535443
72	6	0	-4.985704	-1.331463	0.464034
73	6	0	-4.409658	-1.497112	-1.873371
74	6	0	-6.153814	-0.655901	0.127572
75	1	0	-4.736316	-1.504903	1.506958
76	6	0	-5.578317	-0.823300	-2.205241
77	1	0	-3.728927	-1.822970	-2.654245
78	6	0	-6.459919	-0.412655	-1.208189
79	1	0	-6.823968	-0.316529	0.912145
80	1	0	-5.797339	-0.613907	-3.247581
81	1	0	-7.373693	0.112276	-1.471576
82	6	0	-1.668507	-4.287164	0.992234
83	6	0	-0.738136	-4.009740	-0.206874
84	1	0	-1.219807	-3.927923	1.929453
85	1	0	-1.790386	-5.369527	1.110187
86	1	0	-0.913226	-4.775282	-0.967097
87	6	0	0.728066	-4.022605	0.150669
88	6	0	1.235262	-3.303488	1.237302
89	6	0	1.599920	-4.834605	-0.573140
90	6	0	2.569457	-3.417077	1.610057
91	1	0	0.589972	-2.638481	1.801347

92	6	0	2.937123	-4.955141	-0.204350
93	1	0	1.231238	-5.372114	-1.442037
94	6	0	3.422974	-4.256311	0.896019
95	1	0	2.943263	-2.836235	2.448343
96	1	0	3.597702	-5.593708	-0.783070
97	1	0	4.466338	-4.346131	1.184123
98	1	0	-3.864370	-3.840796	1.302956

Zero-point correction= 0.787443 (Hartree/Particle)
Thermal correction to Energy= 0.835251
Thermal correction to Enthalpy= 0.836196
Thermal correction to Gibbs Free Energy= 0.707916
Sum of electronic and zero-point Energies= -3703.267895
Sum of electronic and thermal Energies= -3703.220087
Sum of electronic and thermal Enthalpies= -3703.219143
Sum of electronic and thermal Free Energies= -3703.347422

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3706.3316757

INT11a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.613598	-0.736795	2.138108
2	15	0	2.480370	0.703614	-0.827211
3	15	0	-0.442632	-1.556002	0.632432
4	6	0	2.107908	2.651084	-2.753224
5	6	0	4.003164	0.017177	-1.592545
6	6	0	5.202778	-1.804648	-2.635297
7	6	0	2.516880	2.432220	-1.433069
8	6	0	6.368348	-1.046723	-2.638534
9	6	0	5.177208	0.782865	-1.615459
10	6	0	4.021438	-1.276633	-2.115326
11	6	0	6.353285	0.252356	-2.130866
12	6	0	2.901233	3.518216	-0.646352
13	6	0	2.883047	4.807028	-1.176056
14	6	0	1.057051	-1.924448	1.576186
15	6	0	1.230859	-1.972119	3.001018
16	6	0	-1.620563	-0.990504	1.917272
17	6	0	4.075502	0.484492	2.921275
18	6	0	2.267261	-2.398260	0.979264
19	6	0	2.538873	-2.458351	3.264609
20	6	0	2.098340	3.935435	-3.281916
21	6	0	3.176818	-2.717402	2.018177
22	6	0	-1.288744	0.089287	2.740427
23	6	0	2.999452	0.829083	0.907111
24	6	0	-2.863595	-1.607754	2.080247
25	6	0	2.790208	1.030870	3.199195
26	6	0	4.213241	0.370597	1.511211
27	6	0	2.129413	1.248060	1.963343
28	6	0	-1.066605	-3.244187	0.267977
29	6	0	-0.895669	-4.237313	1.240583
30	6	0	-3.765110	-1.135225	3.030206
31	6	0	-2.182084	0.549583	3.698602
32	6	0	-3.428508	-0.055074	3.838360
33	6	0	2.484461	5.017145	-2.491839
34	6	0	-2.337977	-4.810333	-1.065643
35	6	0	-1.785767	-3.544671	-0.888631
36	6	0	-2.169768	-5.790638	-0.093399
37	6	0	-1.443182	-5.502144	1.059118
38	1	0	1.137564	1.648650	1.805313
39	1	0	2.370903	1.205499	4.180909
40	1	0	4.802249	0.162613	3.654700
41	1	0	5.055087	-0.058917	0.986539
42	1	0	2.446017	-2.473469	-0.084346
43	1	0	4.196959	-3.048839	1.881148
44	1	0	2.988578	-2.561444	4.242772
45	1	0	0.502115	-1.664049	3.737176
46	1	0	3.103874	-1.854657	-2.151280
47	1	0	5.202297	-2.808777	-3.048692
48	1	0	7.286225	-1.460061	-3.046665
49	1	0	7.257770	0.853625	-2.142150
50	1	0	5.168853	1.797953	-1.227574
51	1	0	3.210170	3.361953	0.383069
52	1	0	3.178906	5.647557	-0.555097
53	1	0	2.468187	6.022371	-2.902409
54	1	0	1.781015	4.094745	-4.307975
55	1	0	1.793439	1.811218	-3.369955
56	1	0	-3.138683	-2.458038	1.465152
57	1	0	-4.732380	-1.616776	3.135349
58	1	0	-4.135071	0.317540	4.573634
59	1	0	-1.915753	1.400825	4.316777
60	1	0	-0.330047	0.577193	2.622510
61	1	0	-1.895087	-2.803944	-1.666682
62	1	0	-2.886976	-5.028617	-1.976513
63	1	0	-2.598303	-6.778408	-0.234831
64	1	0	-1.300745	-6.262751	1.820822
65	1	0	-0.339977	-4.024945	2.148429
66	17	0	0.689893	-2.021124	-2.506681
67	45	0	0.010804	-0.183920	-1.080803
68	6	0	-2.331451	1.888090	0.241494
69	6	0	-3.259265	0.981651	-0.110710
70	16	0	-0.616021	1.865805	-0.197895

71	6	0	-2.725164	3.031178	1.118144
72	6	0	-1.880961	3.521314	2.122088
73	6	0	-3.973791	3.643893	0.952027
74	6	0	-2.285581	4.558101	2.955740
75	1	0	-0.898168	3.080065	2.250028
76	6	0	-4.381262	4.679922	1.786025
77	1	0	-4.624901	3.312414	0.148414
78	6	0	-3.540619	5.139572	2.795920
79	1	0	-1.613679	4.915948	3.731129
80	1	0	-5.354098	5.139280	1.635581
81	1	0	-3.855219	5.952201	3.444291
82	6	0	-1.883646	-0.257978	-1.882058
83	6	0	-3.150328	-0.195314	-1.040575
84	1	0	-1.812904	0.635033	-2.520930
85	1	0	-1.901835	-1.126897	-2.543165
86	1	0	-3.215529	-1.109567	-0.433841
87	6	0	-4.346377	-0.237156	-1.984090
88	6	0	-4.775256	0.913989	-2.649777
89	6	0	-5.001877	-1.443127	-2.237851
90	6	0	-5.837704	0.860149	-3.546461
91	1	0	-4.269581	1.857243	-2.456782
92	6	0	-6.064907	-1.501044	-3.134983
93	1	0	-4.673400	-2.345861	-1.725923
94	6	0	-6.486554	-0.348154	-3.791829
95	1	0	-6.160611	1.764137	-4.055123
96	1	0	-6.565606	-2.447463	-3.318949
97	1	0	-7.315484	-0.390174	-4.492343
98	1	0	-4.240515	1.085795	0.349640

Zero-point correction=	0.786144 (Hartree/Particle)
Thermal correction to Energy=	0.835333
Thermal correction to Enthalpy=	0.836277
Thermal correction to Gibbs Free Energy=	0.700701
Sum of electronic and zero-point Energies=	-3703.240197
Sum of electronic and thermal Energies=	-3703.191008
Sum of electronic and thermal Enthalpies=	-3703.190064
Sum of electronic and thermal Free Energies=	-3703.325639

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3706.309377

TS8a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.539604	-1.163328	-2.293787
2	15	0	2.449298	-0.268505	0.965279
3	15	0	-0.149435	0.620410	-1.232223
4	6	0	3.712406	-0.247743	3.473914
5	6	0	3.508127	1.200778	0.680334
6	6	0	3.660270	3.570589	0.192299
7	6	0	3.263975	-1.042489	2.414797
8	6	0	5.048348	3.479952	0.163635
9	6	0	4.906212	1.128352	0.689526
10	6	0	2.897198	2.435694	0.457108
11	6	0	5.670398	2.258952	0.422715
12	6	0	3.422807	-2.427363	2.485302
13	6	0	4.031008	-3.008766	3.594721
14	6	0	1.103382	0.233283	-2.511407
15	6	0	1.005280	-0.725080	-3.573411
16	6	0	-1.630239	-0.078211	-2.068209
17	6	0	3.937040	-2.655139	-2.017005
18	6	0	2.398208	0.841663	-2.612434
19	6	0	2.231767	-0.726276	-4.288766
20	6	0	4.325496	-0.829661	4.576344
21	6	0	3.089333	0.241989	-3.697322
22	6	0	-1.752190	-1.469869	-2.124770
23	6	0	2.903669	-1.446894	-0.339365
24	6	0	-2.625598	0.710924	-2.646465
25	6	0	2.624201	-3.178016	-1.847495
26	6	0	4.117279	-1.597379	-1.085604
27	6	0	1.989241	-2.445422	-0.810365
28	6	0	-0.306912	2.435212	-1.530624
29	6	0	-0.191804	2.952809	-2.828002
30	6	0	-3.725408	0.117995	-3.261228
31	6	0	-2.834711	-2.061958	-2.764137
32	6	0	-3.829959	-1.267441	-3.326442
33	6	0	4.486152	-2.211789	4.639887
34	6	0	-0.661391	4.690386	-0.707177
35	6	0	-0.539711	3.321467	-0.477104
36	6	0	-0.549956	5.191036	-1.999802
37	6	0	-0.314655	4.317684	-3.060470
38	1	0	0.976859	-2.567699	-0.445252
39	1	0	2.171817	-3.963340	-2.437616
40	1	0	4.654335	-2.967608	-2.763734
41	1	0	4.990525	-0.965327	-1.015343
42	1	0	2.796533	1.595906	-1.949250
43	1	0	4.109339	0.454482	-3.987153
44	1	0	2.480988	-1.381992	-5.111855
45	1	0	0.159885	-1.367517	-3.770354
46	1	0	1.814394	2.507634	0.486776
47	1	0	3.165508	4.520296	0.012814
48	1	0	5.647544	4.361701	-0.043603
49	1	0	6.754216	2.190016	0.427190

50	1	0	5.397718	0.190155	0.930059
51	1	0	3.074705	-3.061428	1.675779
52	1	0	4.149353	-4.087372	3.638950
53	1	0	4.960502	-2.665916	5.504937
54	1	0	4.667676	-0.201570	5.393296
55	1	0	3.573271	0.827991	3.441727
56	1	0	-2.559065	1.793295	-2.606095
57	1	0	-4.500789	0.745527	-3.690560
58	1	0	-4.689141	-1.728825	-3.803609
59	1	0	-2.922558	-3.143353	-2.785076
60	1	0	-1.003447	-2.094259	-1.646617
61	1	0	-0.615104	2.947171	0.537796
62	1	0	-0.842557	5.359746	0.128433
63	1	0	-0.644058	6.257362	-2.182081
64	1	0	-0.222745	4.701637	-4.072042
65	1	0	-0.007292	2.281472	-3.661545
66	17	0	0.428178	0.059348	3.434489
67	45	0	0.125887	0.133479	1.056644
68	6	0	-3.183299	-1.435977	0.677684
69	6	0	-3.791166	-0.271321	0.423733
70	16	0	-1.570397	-1.493735	1.407355
71	6	0	-3.803150	-2.754877	0.394596
72	6	0	-3.037267	-3.872880	0.041552
73	6	0	-5.193517	-2.904403	0.473977
74	6	0	-3.643195	-5.089856	-0.252885
75	1	0	-1.956630	-3.783214	-0.012404
76	6	0	-5.800190	-4.118163	0.172902
77	1	0	-5.800804	-2.062691	0.792950
78	6	0	-5.028147	-5.217381	-0.195380
79	1	0	-3.028089	-5.942593	-0.526417
80	1	0	-6.880208	-4.210463	0.242913
81	1	0	-5.501477	-6.168440	-0.420728
82	6	0	-1.953095	0.757151	1.718845
83	6	0	-3.112929	1.017516	0.774547
84	1	0	-2.254213	0.502750	2.732011
85	1	0	-1.287176	1.632875	1.806881
86	1	0	-2.731794	1.482337	-0.143301
87	6	0	-4.054570	2.025996	1.415216
88	6	0	-4.914010	1.642212	2.448014
89	6	0	-4.054918	3.357589	0.997831
90	6	0	-5.757529	2.570886	3.047940
91	1	0	-4.919806	0.605455	2.776165
92	6	0	-4.898950	4.289730	1.596612
93	1	0	-3.389323	3.665352	0.193965
94	6	0	-5.752994	3.898449	2.623648
95	1	0	-6.422274	2.257945	3.847982
96	1	0	-4.890608	5.322004	1.257729
97	1	0	-6.413660	4.622913	3.090833
98	1	0	-4.749616	-0.233770	-0.085782

Zero-point correction= 0.784364 (Hartree/Particle)
Thermal correction to Energy= 0.832242
Thermal correction to Enthalpy= 0.833187
Thermal correction to Gibbs Free Energy= 0.701164
Sum of electronic and zero-point Energies= -3703.206409
Sum of electronic and thermal Energies= -3703.158531
Sum of electronic and thermal Enthalpies= -3703.157587
Sum of electronic and thermal Free Energies= -3703.289610

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3706.275102

TS8a''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	4.028413	-0.099099	-1.539234
2	15	0	1.268521	-1.749972	-0.751547
3	15	0	1.869071	1.276305	0.801724
4	6	0	-0.694321	-3.685817	-0.609118
5	6	0	2.112369	-2.612309	0.635218
6	6	0	2.667584	-2.745058	2.990999
7	6	0	0.303266	-3.144346	-1.425983
8	6	0	3.411785	-3.896364	2.757949
9	6	0	2.818166	-3.802682	0.420259
10	6	0	2.013745	-2.114804	1.934290
11	6	0	3.474152	-4.432549	1.471505
12	6	0	0.539401	-3.690449	-2.685652
13	6	0	-0.213618	-4.779326	-3.123148
14	6	0	3.539716	0.989752	0.116331
15	6	0	4.229083	1.817412	-0.828398
16	6	0	1.611993	3.043023	0.353175
17	6	0	4.538864	-1.263643	-3.160754
18	6	0	4.425566	-0.083300	0.463845
19	6	0	5.509184	1.251779	-1.066789
20	6	0	-1.437723	-4.773278	-1.046099
21	6	0	5.633355	0.085052	-0.262892
22	6	0	1.319597	3.351266	-0.983237
23	6	0	2.563561	-1.426772	-1.974284
24	6	0	1.590812	4.062689	1.304156
25	6	0	3.688818	-0.200795	-3.578173
26	6	0	3.849168	-2.023836	-2.178358
27	6	0	2.471369	-0.302156	-2.858334

28	6	0	2.222625	1.346163	2.600151
29	6	0	3.492733	1.676555	3.087417
30	6	0	1.272990	5.367418	0.927426
31	6	0	1.004525	4.651046	-1.356821
32	6	0	0.975225	5.662476	-0.397901
33	6	0	-1.197886	-5.323185	-2.304873
34	6	0	1.418406	1.184230	4.878179
35	6	0	1.185741	1.108706	3.507361
36	6	0	2.686734	1.501220	5.355315
37	6	0	3.722039	1.751238	4.457087
38	1	0	1.616540	0.358850	-2.924415
39	1	0	3.943701	0.574738	-4.287309
40	1	0	5.556210	-1.430624	-3.488080
41	1	0	4.260929	-2.856494	-1.627316
42	1	0	4.203147	-0.890550	1.146961
43	1	0	6.474692	-0.594456	-0.249175
44	1	0	6.242252	1.623849	-1.769401
45	1	0	3.831375	2.703576	-1.300967
46	1	0	1.415490	-1.232773	2.125435
47	1	0	2.585270	-2.330650	3.991314
48	1	0	3.923783	-4.390784	3.578273
49	1	0	4.022155	-5.352638	1.291166
50	1	0	2.831582	-4.254048	-0.567842
51	1	0	1.302342	-3.265595	-3.331625
52	1	0	-0.029722	-5.199789	-4.107479
53	1	0	-1.781613	-6.172409	-2.648232
54	1	0	-2.210838	-5.183334	-0.403341
55	1	0	-0.901558	-3.242487	0.361844
56	1	0	1.803554	3.845305	2.345830
57	1	0	1.249350	6.150144	1.679568
58	1	0	0.713035	6.676308	-0.684937
59	1	0	0.754743	4.867945	-2.390360
60	1	0	1.304181	2.561996	-1.730871
61	1	0	0.192172	0.856264	3.148420
62	1	0	0.605029	0.990756	5.570799
63	1	0	2.868842	1.556849	6.424492
64	1	0	4.712568	2.003956	4.823425
65	1	0	4.304575	1.877023	2.395528
66	17	0	-1.464405	-0.472116	-1.910088
67	45	0	0.044880	0.144055	-0.147427
68	6	0	-3.118012	-0.231028	1.069414
69	6	0	-3.624679	0.877173	0.517698
70	16	0	-1.437953	-0.285604	1.615213
71	6	0	-3.867912	-1.490660	1.324619
72	6	0	-3.882704	-2.493555	0.350153
73	6	0	-4.553032	-1.681146	2.524306
74	6	0	-4.591166	-3.667450	0.576285
75	1	0	-3.352581	-2.326810	-0.583203
76	6	0	-5.254278	-2.864167	2.750945
77	1	0	-4.542646	-0.897040	3.276137
78	6	0	-5.275742	-3.857937	1.777551
79	1	0	-4.616983	-4.434395	-0.192888
80	1	0	-5.786242	-3.005073	3.687327
81	1	0	-5.824663	-4.779161	1.951179
82	6	0	-5.072618	1.020961	0.218246
83	8	0	-5.736246	1.964297	0.590612
84	8	0	-5.547316	-0.000297	-0.507814
85	6	0	-6.966861	-0.072686	-0.680484
86	6	0	-7.600494	-0.810838	0.485595
87	1	0	-7.102612	-0.615507	-1.618148
88	1	0	-7.369859	0.937504	-0.784852
89	1	0	-8.675242	-0.934523	0.314217
90	1	0	-7.144358	-1.798417	0.605594
91	1	0	-7.460232	-0.248916	1.413547
92	6	0	-1.268490	1.839467	0.537901
93	6	0	-2.770733	2.117503	0.421499
94	1	0	-0.817863	2.353252	1.383645
95	1	0	-0.776480	2.168053	-0.394746
96	6	0	-3.010299	2.978970	-0.808835
97	6	0	-3.380539	2.436235	-2.039557
98	6	0	-2.755329	4.350315	-0.725318
99	6	0	-3.499915	3.253459	-3.160892
100	1	0	-3.550541	1.367992	-2.126448
101	6	0	-2.867639	5.166902	-1.845644
102	1	0	-2.457687	4.780565	0.228455
103	6	0	-3.243183	4.618779	-3.070028
104	1	0	-3.788048	2.815051	-4.112000
105	1	0	-2.669591	6.231918	-1.759581
106	1	0	-3.336105	5.252561	-3.947595
107	1	0	-3.046022	2.726826	1.295138

Zero-point correction= 0.856608 (Hartree/Particle)
Thermal correction to Energy= 0.910681
Thermal correction to Enthalpy= 0.911625
Thermal correction to Gibbs Free Energy= 0.764774
Sum of electronic and zero-point Energies= -3970.239825
Sum of electronic and thermal Energies= -3970.185753
Sum of electronic and thermal Enthalpies= -3970.184808
Sum of electronic and thermal Free Energies= -3970.331659

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.4645329

INT13a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.313110	-1.801408	2.241059
2	15	0	2.584154	0.182053	-0.506490
3	15	0	-0.499146	-1.089977	0.454776
4	6	0	4.173031	2.118242	-1.839098
5	6	0	3.540518	-0.988064	-1.539559
6	6	0	3.518182	-2.845023	-3.091597
7	6	0	3.462429	1.791711	-0.680760
8	6	0	4.909223	-2.884044	-3.072640
9	6	0	4.939682	-1.021797	-1.540072
10	6	0	2.836989	-1.896216	-2.333481
11	6	0	5.620273	-1.966531	-2.300969
12	6	0	3.360450	2.742522	0.338584
13	6	0	3.975281	3.984883	0.213876
14	6	0	0.501974	-2.227580	1.468575
15	6	0	0.470743	-2.404816	2.888912
16	6	0	-1.552159	-0.340935	1.772557
17	6	0	4.162094	-1.276036	2.989175
18	6	0	1.482389	-3.130611	0.945113
19	6	0	1.442774	-3.383810	3.233993
20	6	0	4.789799	3.359190	-1.961040
21	6	0	2.062471	-3.834576	2.034266
22	6	0	-1.101613	0.880508	2.280969
23	6	0	3.110267	-0.282911	1.179971
24	6	0	-2.728136	-0.887689	2.294452
25	6	0	3.159462	-0.404138	3.494303
26	6	0	4.140569	-1.199579	1.570383
27	6	0	2.513566	0.208127	2.387292
28	6	0	-1.529152	-2.374875	-0.386066
29	6	0	-2.110173	-3.445015	0.307263
30	6	0	-3.424786	-0.232224	3.306241
31	6	0	-1.780789	1.526407	3.308483
32	6	0	-2.946766	0.969293	3.824925
33	6	0	4.695001	4.295895	-0.936119
34	6	0	-2.407201	-3.292544	-2.454207
35	6	0	-1.656773	-2.333705	-1.777283
36	6	0	-3.031513	-4.315209	-1.747073
37	6	0	-2.868909	-4.397987	-0.364850
38	1	0	1.670456	0.880069	2.445846
39	1	0	2.894407	-0.270032	4.534154
40	1	0	4.794261	-1.927439	3.577125
41	1	0	4.746232	-1.791423	0.899801
42	1	0	1.770848	-3.216372	-0.094368
43	1	0	2.870525	-4.550051	1.965409
44	1	0	1.695667	-3.696496	4.238020
45	1	0	-0.141840	-1.838676	3.577059
46	1	0	1.752087	-1.834979	-2.364850
47	1	0	2.959844	-3.543444	-3.707650
48	1	0	5.441853	-3.619618	-3.668435
49	1	0	6.706223	-1.983302	-2.296192
50	1	0	5.498799	-0.300243	-0.950424
51	1	0	2.796600	2.524911	1.239444
52	1	0	3.891811	4.709020	1.019710
53	1	0	5.174859	5.265109	-1.035610
54	1	0	5.334853	3.597183	-2.869525
55	1	0	4.226944	1.410587	-2.658367
56	1	0	-3.132684	-1.811035	1.895122
57	1	0	-4.345429	-0.663358	3.688325
58	1	0	-3.490244	1.475116	4.617748
59	1	0	-1.416414	2.481809	3.673003
60	1	0	-0.242184	1.358275	1.820291
61	1	0	-1.144433	-1.549538	-2.330538
62	1	0	-2.498811	-3.239143	-3.535029
63	1	0	-3.622058	-5.060188	-2.272052
64	1	0	-3.320377	-5.216108	0.188544
65	1	0	-1.946847	-3.552270	1.375800
66	17	0	1.211135	1.408194	-3.076701
67	45	0	0.383065	0.348176	-1.065738
68	6	0	-2.434760	2.231909	-0.365594
69	6	0	-3.535855	1.592749	0.047125
70	16	0	-1.712194	1.475840	-1.827758
71	6	0	-1.752011	3.373216	0.268675
72	6	0	-0.424653	3.693855	-0.044634
73	6	0	-2.415750	4.139882	1.236404
74	6	0	0.227559	4.730072	0.618015
75	1	0	0.120325	3.129028	-0.797563
76	6	0	-1.763774	5.175083	1.893529
77	1	0	-3.453418	3.927088	1.474314
78	6	0	-0.434681	5.469762	1.592522
79	1	0	1.258956	4.951253	0.360897
80	1	0	-2.297473	5.758371	2.638512
81	1	0	0.074174	6.280873	2.105328
82	6	0	-3.268396	0.558540	-2.109367
83	6	0	-3.904692	0.357284	-0.730345
84	1	0	-3.902195	1.192231	-2.737842
85	1	0	-3.071571	-0.378245	-2.629944
86	1	0	-3.402630	-0.492765	-0.248472
87	6	0	-5.372363	0.016324	-0.824385
88	6	0	-6.345479	1.008867	-0.954787
89	6	0	-5.766778	-1.323650	-0.827996

90	6	0	-7.689295	0.669636	-1.082063
91	1	0	-6.045383	2.054336	-0.955288
92	6	0	-7.109514	-1.665130	-0.958816
93	1	0	-5.011860	-2.102268	-0.731720
94	6	0	-8.074626	-0.668965	-1.084759
95	1	0	-8.437151	1.451339	-1.179125
96	1	0	-7.402544	-2.711171	-0.960423
97	1	0	-9.123126	-0.933504	-1.185231
98	1	0	-4.063947	1.848119	0.960419

Zero-point correction= 0.787031 (Hartree/Particle)
Thermal correction to Energy= 0.836106
Thermal correction to Enthalpy= 0.837050
Thermal correction to Gibbs Free Energy= 0.702120
Sum of electronic and zero-point Energies= -3703.266665
Sum of electronic and thermal Energies= -3703.217590
Sum of electronic and thermal Enthalpies= -3703.216645
Sum of electronic and thermal Free Energies= -3703.351576

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3706.3317946

INT13a''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-3.917880	-0.817490	-1.503877
2	15	0	-1.783451	1.597571	-0.693371
3	15	0	-1.500813	-1.369029	0.886219
4	6	0	-0.495166	4.055270	-0.631219
5	6	0	-2.903332	2.246068	0.613866
6	6	0	-3.599366	2.290145	2.935562
7	6	0	-1.238049	3.181227	-1.431810
8	6	0	-4.619799	3.180992	2.620431
9	6	0	-3.898804	3.185258	0.316529
10	6	0	-2.741347	1.835538	1.936408
11	6	0	-4.758596	3.639414	1.310114
12	6	0	-1.538364	3.537539	-2.744248
13	6	0	-1.099409	4.758612	-3.254233
14	6	0	-3.166872	-1.665865	0.192836
15	6	0	-3.520270	-2.683265	-0.749667
16	6	0	-0.681589	-2.963082	0.465257
17	6	0	-4.701664	0.125109	-3.158440
18	6	0	-4.358666	-0.925903	0.487618
19	6	0	-4.906044	-2.561891	-1.039242
20	6	0	-0.064441	5.273161	-1.139669
21	6	0	-5.423415	-1.481358	-0.271391
22	6	0	-0.097816	-3.071836	-0.804938
23	6	0	-2.893712	0.872816	-1.929445
24	6	0	-0.568520	-4.030917	1.358112
25	6	0	-3.566654	-0.648627	-3.533639
26	6	0	-4.291840	1.066773	-2.177057
27	6	0	-2.452779	-0.188044	-2.786914
28	6	0	-1.848723	-1.522644	2.686109
29	6	0	-2.896325	-2.309148	3.179046
30	6	0	0.121549	-5.184404	0.988927
31	6	0	0.584623	-4.225914	-1.173786
32	6	0	0.699014	-5.283417	-0.273605
33	6	0	-0.364145	5.626440	-2.455200
34	6	0	-1.256898	-0.933772	4.960658
35	6	0	-1.033279	-0.835361	3.589669
36	6	0	-2.299336	-1.720708	5.441758
37	6	0	-3.118379	-2.408808	4.548881
38	1	0	-1.443036	-0.575642	-2.811214
39	1	0	-3.564174	-1.475052	-4.231099
40	1	0	-5.713451	-0.015975	-3.514281
41	1	0	-4.944135	1.747934	-1.650372
42	1	0	-4.425618	-0.073850	1.149807
43	1	0	-6.437834	-1.107117	-0.300631
44	1	0	-5.458237	-3.159896	-1.751312
45	1	0	-2.835561	-3.393327	-1.191830
46	1	0	-1.933976	1.156899	2.182730
47	1	0	-3.461923	1.943814	3.955733
48	1	0	-5.294866	3.535441	3.393882
49	1	0	-5.531486	4.361907	1.065069
50	1	0	-3.987457	3.581293	-0.691481
51	1	0	-2.104913	2.860603	-3.376587
52	1	0	-1.329350	5.025275	-4.281609
53	1	0	-0.020446	6.575808	-2.855433
54	1	0	0.508076	5.949406	-0.511107
55	1	0	-0.243568	3.774678	0.389038
56	1	0	-1.002447	-3.961395	2.350324
57	1	0	0.214653	-6.002088	1.697784
58	1	0	1.252573	-6.174725	-0.553485
59	1	0	1.063559	-4.279392	-2.145974
60	1	0	-0.136190	-2.227086	-1.488684
61	1	0	-0.226003	-0.211618	3.215585
62	1	0	-0.617560	-0.390195	5.649754
63	1	0	-2.476286	-1.797160	6.510588
64	1	0	-3.934313	-3.022444	4.919206
65	1	0	-3.541279	-2.845651	2.489084
66	17	0	1.202798	1.110253	-1.838451
67	45	0	-0.135098	0.201898	-0.039290
68	6	0	3.331110	0.309703	0.883801

69	6	0	4.258325	-0.540516	0.418158
70	16	0	1.805840	-0.511433	1.329615
71	6	0	3.502056	1.729784	1.278213
72	6	0	2.810916	2.780044	0.670220
73	6	0	4.379525	2.004533	2.333522
74	6	0	3.014432	4.085756	1.107300
75	1	0	2.145346	2.572717	-0.160705
76	6	0	4.576071	3.310879	2.767379
77	1	0	4.911414	1.185543	2.810242
78	6	0	3.893171	4.357570	2.152145
79	1	0	2.486666	4.895995	0.612342
80	1	0	5.264318	3.509864	3.583833
81	1	0	4.046908	5.379624	2.486507
82	6	0	5.643173	-0.166139	0.032803
83	8	0	6.582387	-0.926407	0.142078
84	8	0	5.724906	1.075392	-0.451928
85	6	0	7.038064	1.585217	-0.717439
86	6	0	7.642715	2.174386	0.544885
87	1	0	6.883298	2.349704	-1.480883
88	1	0	7.659046	0.783541	-1.123898
89	1	0	8.609456	2.636300	0.318569
90	1	0	6.977338	2.934147	0.965652
91	1	0	7.802005	1.391445	1.292339
92	6	0	2.605845	-2.160783	1.209789
93	6	0	3.891328	-2.006877	0.366535
94	1	0	2.841563	-2.461436	2.233596
95	1	0	1.909279	-2.877015	0.780504
96	6	0	3.737510	-2.563602	-1.038855
97	6	0	3.115430	-1.824449	-2.044728
98	6	0	4.171356	-3.860637	-1.318822
99	6	0	2.928752	-2.377439	-3.309255
100	1	0	2.762418	-0.815361	-1.848479
101	6	0	3.988161	-4.414382	-2.582691
102	1	0	4.664035	-4.440737	-0.541749
103	6	0	3.364747	-3.671868	-3.584220
104	1	0	2.442469	-1.783931	-4.078302
105	1	0	4.340848	-5.421361	-2.787780
106	1	0	3.226596	-4.099009	-4.573652
107	1	0	4.695491	-2.566022	0.857045

Zero-point correction= 0.858677 (Hartree/Particle)
Thermal correction to Energy= 0.913069
Thermal correction to Enthalpy= 0.914013
Thermal correction to Gibbs Free Energy= 0.767282
Sum of electronic and zero-point Energies= -3970.306081
Sum of electronic and thermal Energies= -3970.251689
Sum of electronic and thermal Enthalpies= -3970.250745
Sum of electronic and thermal Free Energies= -3970.397476

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3973.52622