Electronic Supporting Information (SI-2)

Triggering the approach of an Arene or Heteroarene towards an aldehyde *via* Lewis acid-aldehyde communication

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ESI

The Cartesian coordinates of the optimized geometries, Frequency data, and NImag Obtained at the B3LYP/LANL2DZ/6-31G* Level of Theory

Optimized Geometry:

Benzaldehyde

Cartesian Coordinates (Angstroms):

1	6	0	1.630463	-1.216505	0.000000
2	6	0	1.333296	0.145726	0.000000
3	6	0	0.000000	0.575158	0.000000
4	6	0	-1.039163	-0.368134	0.000000
5	6	0	-0.741952	-1.726711	0.000000
6	6	0	0.592410	-2.150981	0.000000
7	6	0	-0.306260	2.023585	0.000000
8	8	0	-1.426688	2.496533	0.000000
9	1	0	2.664468	-1.549839	0.000000
10	1	0	2.133761	0.882881	0.000000
11	1	0	-2.064300	-0.010306	0.000000
12	1	0	-1.544001	-2.459708	0.000000
13	1	0	0.821614	-3.213387	0.000000
14	1	0	0.589205	2.685269	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.110226 (Hartree/Particle)
Thermal correction to Energy= 0.116512
Thermal correction to Enthalpy= 0.117456
Thermal correction to Gibbs Free Energy= 0.079711
Sum of electronic and zero-point Energies= -345.463229
Sum of electronic and thermal Energies= -345.456944
Sum of electronic and thermal Enthalpies= -345.455999
Sum of electronic and thermal Free Energies= -345.493744

C-1

Cartesian Coordinates (Angstroms):

1	6	0	3.964674	-1.278538	-0.011807
2	6	0	5.331487	-1.018117	-0.006424
3	6	0	5.782392	0.305463	0.005271
4	6	0	4.874106	1.373297	0.011531
5	6	0	3.508914	1.121525	0.006106
6	6	0	3.048434	-0.210524	-0.005517
7	1	0	3.598928	-2.302294	-0.020935
8	1	0	6.043412	-1.837555	-0.011274
9	1	0	5.238652	2.395899	0.020588
10	1	0	2.784884	1.929775	0.010611
11	6	0	1.630243	-0.507059	-0.011389
12	8	0	0.753801	0.373744	-0.007221
13	1	0	1.337408	-1.566711	-0.021129
14	50	0	-1.508400	0.038606	0.000382
15	17	0	-1.030205	-1.049514	2.029911
16	17	0	-3.848466	-0.263189	0.012586

17	17	0	-1.460462	2.369998	-0.104963
18	17	0	-1.031742	-1.219916	-1.930202
19	1	0	6.849674	0.508874	0.009532

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.116875 (Hartree/Particle)
Thermal correction to Energy= 0.132553
Thermal correction to Enthalpy= 0.133497
Thermal correction to Gibbs Free Energy= 0.068890
Sum of electronic and zero-point Energies= -2189.776131
Sum of electronic and thermal Energies= -2189.760453
Sum of electronic and thermal Enthalpies= -2189.759509
Sum of electronic and thermal Free Energies= -2189.824116

C-2

Cartesian Coordinates (Angstroms):

1	6	0	-4.895057	1.163797	-0.005182
2	6	0	-6.259800	1.418050	-0.004509
3	6	0	-7.170129	0.351957	-0.003199
4	6	0	-6.722242	-0.972665	-0.002226
5	6	0	-5.356070	-1.236031	-0.002201
6	6	0	-4.437828	-0.169480	-0.003882
7	1	0	-4.169248	1.970388	-0.006145
8	1	0	-6.622375	2.441415	-0.004958
9	1	0	-7.435898	-1.790672	-0.001351
10	1	0	-4.990911	-2.259852	-0.001297
11	6	0	-3.023378	-0.473875	-0.004005
12	1	0	-8.237077	0.557662	-0.002838
13	50	0	-0.000002	0.000090	0.001327
14	8	0	2.146239	-0.413138	0.011936
15	6	0	3.023390	0.473787	0.002982
16	6	0	4.437826	0.169310	0.001552
17	6	0	4.894999	-1.163987	0.003940
18	6	0	5.356123	1.235811	-0.002480
19	6	0	6.259726	-1.418307	0.001998
20	1	0	4.169151	-1.970540	0.006670
21	6	0	6.722279	0.972382	-0.003664
22	1	0	4.991010	2.259648	-0.004239
23	6	0	7.170105	-0.352261	-0.001611
24	1	0	6.622254	-2.441688	0.003231
25	1	0	7.435972	1.790352	-0.006334
26	1	0	8.237041	-0.558020	-0.002947
27	1	0	2.723050	1.529162	-0.002542
28	17	0	-0.310045	-1.606185	1.775261
29	17	0	-0.314640	-1.756171	-1.625696
30	17	0	0.316116	1.756230	1.627971
31	17	0	0.308609	1.606490	-1.772951
32	8	0	-2.146271	0.413109	-0.010292

33	1	0	-2.722932	-1.529227	0.000236

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.229342 (Hartree/Particle)
Thermal correction to Energy= 0.252866
Thermal correction to Enthalpy= 0.253810
Thermal correction to Gibbs Free Energy= 0.170082
Sum of electronic and zero-point Energies= -2535.247731
Sum of electronic and thermal Energies= -2535.224207
Sum of electronic and thermal Enthalpies= -2535.223263
Sum of electronic and thermal Free Energies= -2535.306991

C-3

Cartesian Coordinates (Angstroms):

1	6	0	5.000700	-1.810398	-0.000294
2	6	0	6.391900	-1.824998	-0.000594
3	6	0	4.313500	-0.582098	-0.000294
4	1	0	4.438400	-2.740598	-0.000094
5	6	0	7.095100	-0.616398	-0.000794
6	1	0	6.928000	-2.768898	-0.000594
7	6	0	6.415800	0.609902	-0.000794
8	1	0	8.181700	-0.627598	-0.000994
9	6	0	5.027800	0.633102	-0.000494
10	1	0	6.975300	1.540302	-0.000994
11	1	0	4.477800	1.568502	-0.000494
12	6	0	2.866900	-0.599198	0.000006
13	8	0	2.183900	0.444502	-0.000094
14	1	0	2.361800	-1.572898	0.000606
15	50	0	0.000000	0.485202	0.000306
16	17	0	0.000200	2.125202	1.729506
17	17	0	-0.000200	2.125302	-1.728794
18	17	0	0.000100	-1.298498	1.682006
19	17	0	-0.000100	-1.298398	-1.681394
20	8	0	-2.183900	0.444502	0.000306
21	6	0	-2.866900	-0.599198	0.000506
22	6	0	-4.313500	-0.582098	0.000006
23	1	0	-2.361800	-1.572898	0.000806
24	6	0	-5.027800	0.633102	-0.000994
25	6	0	-5.000700	-1.810398	0.000506
26	6	0	-6.415800	0.609902	-0.001494
27	1	0	-4.477800	1.568502	-0.001394
28	6	0	-6.391900	-1.824998	0.000006
29	1	0	-4.438400	-2.740598	0.001206
30	6	0	-7.095100	-0.616398	-0.000994
31	1	0	-6.975300	1.540302	-0.002194
32	1	0	-6.928000	-2.768898	0.000406
33	1	0	-8.181700	-0.627598	-0.001394

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.229482 (Hartree/Particle)
Thermal correction to Energy= 0.252934
Thermal correction to Enthalpy= 0.253878
Thermal correction to Gibbs Free Energy= 0.170918
Sum of electronic and zero-point Energies= -2535.248609
Sum of electronic and thermal Energies= -2535.225158
Sum of electronic and thermal Enthalpies= -2535.224213
Sum of electronic and thermal Free Energies= -2535.307173

C-4

Cartesian Coordinates (Angstroms):

1	6	0	2.516889	0.307769	0.287194
2	8	0	1.375582	0.262442	-0.204204
3	50	0	0.000054	-1.490986	-0.000067
4	8	0	-1.376036	0.262037	0.205908
5	6	0	-2.517418	0.307082	-0.285438
6	6	0	-3.425991	1.416083	-0.061713
7	6	0	-4.685951	1.390963	-0.686105
8	6	0	-3.066425	2.495740	0.768440
9	6	0	-5.579502	2.439384	-0.486842
10	1	0	-4.954226	0.550756	-1.321438
11	6	0	-3.963664	3.537156	0.964734
12	1	0	-2.092704	2.489606	1.247255
13	6	0	-5.216899	3.508694	0.337352
14	1	0	-6.553161	2.425228	-0.966745
15	1	0	-3.697076	4.371829	1.606072
16	1	0	-5.915270	4.325913	0.495831
17	1	0	-2.869564	-0.520088	-0.915147
18	17	0	-1.859244	-2.972978	0.201146
19	17	0	0.276231	-1.089987	2.357653
20	17	0	1.859862	-2.972095	-0.203134
21	17	0	-0.276053	-1.087453	-2.357372
22	6	0	3.425622	1.416475	0.062702
23	6	0	3.066239	2.495502	-0.768351
24	6	0	4.685535	1.391672	0.687181
25	6	0	3.963633	3.536630	-0.965454
26	1	0	2.092545	2.489089	-1.247217
27	6	0	5.579246	2.439803	0.487094
28	1	0	4.953662	0.551945	1.323209
29	6	0	5.216837	3.508489	-0.337993
30	1	0	3.697203	4.370817	-1.607488
31	1	0	6.552882	2.425897	0.967050
32	1	0	5.915346	4.325463	-0.497121
33	1	0	2.868856	-0.518925	0.917669

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.229463 (Hartree/Particle)
Thermal correction to Energy= 0.252864
Thermal correction to Enthalpy= 0.253808
Thermal correction to Gibbs Free Energy= 0.171165

Sum of electronic and zero-point Energies= -2535.251994
Sum of electronic and thermal Energies= -2535.228592
Sum of electronic and thermal Enthalpies= -2535.227648
Sum of electronic and thermal Free Energies= -2535.310291

$SnCl_4$

Cartesian Coordinates (Angstroms):

1	50	0	0.000000	0.000000	0.000000
2	17	0	0.000000	2.366193	0.000000
3	17	0	2.366193	0.000000	0.000000
4	17	0	-2.366193	0.000000	0.000000
5	17	0	0.000000	-2.366193	0.000000

Frequency Data:
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.004374 (Hartree/Particle)
Thermal correction to Energy= 0.011316
Thermal correction to Enthalpy= 0.012260
Thermal correction to Gibbs Free Energy= -0.027764
Sum of electronic and zero-point Energies= -1844.237862
Sum of electronic and thermal Energies= -1844.230920
Sum of electronic and thermal Enthalpies= -1844.229976
Sum of electronic and thermal Free Energies= -1844.270001

4-Methoxy Benzaldehyde

Cartesian Coordinates (Angstroms):

1	6	0	-0.537989	1.286012	0.000006
2	6	0	0.834755	1.043985	0.000004
3	6	0	1.295246	-0.280705	0.000002
4	6	0	0.375571	-1.348336	0.000002
5	6	0	-0.982303	-1.091570	0.000004
6	6	0	-1.458882	0.233522	0.000005
7	1	0	-0.899204	2.312628	0.000007
8	1	0	1.528233	1.876682	0.000002
9	1	0	0.764391	-2.361749	0.000001
10	1	0	-1.705173	-1.901710	0.000004
11	6	0	-2.905027	0.511796	0.000005
12	8	0	-3.779781	-0.335987	-0.000046
13	1	0	-3.166395	1.594622	-0.000044
14	8	0	2.604210	-0.640699	-0.000001
15	6	0	3.593529	0.380245	0.000023
16	1	0	4.554010	-0.137307	0.000039
17	1	0	3.519673	1.010323	-0.895384
18	1	0	3.519639	1.010314	0.895434

Frequency Data:
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.143085 (Hartree/Particle)
Thermal correction to Energy= 0.151908

Thermal correction to Enthalpy= 0.152852
Thermal correction to Gibbs Free Energy= 0.109118
Sum of electronic and zero-point Energies= -459.955596
Sum of electronic and thermal Energies= -459.946773
Sum of electronic and thermal Enthalpies= -459.945828
Sum of electronic and thermal Free Energies= -459.989563

4-Methyl Benzaldehyde

Cartesian Coordinates (Angstroms):

1	6	0	-0.915133	-1.200550	-0.000005
2	6	0	-1.754575	-0.074922	-0.000009
3	6	0	-1.165753	1.199354	-0.000006
4	6	0	0.217710	1.343391	0.000006
5	6	0	1.047289	0.213507	0.000013
6	6	0	0.468265	-1.063269	0.000007
7	6	0	-3.257217	-0.223008	0.000007
8	6	0	2.516471	0.372559	0.000026
9	8	0	3.316094	-0.544814	-0.000031
10	1	0	-1.358194	-2.193516	-0.000012
11	1	0	-1.801116	2.082117	-0.000015
12	1	0	0.663378	2.336239	0.000007
13	1	0	1.121917	-1.930373	0.000009
14	1	0	-3.557414	-1.275091	-0.000277
15	1	0	-3.703227	0.253378	0.881804
16	1	0	-3.703305	0.253891	-0.881470
17	1	0	2.866868	1.429492	-0.000032

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.137673 (Hartree/Particle)
Thermal correction to Energy= 0.144964
Thermal correction to Enthalpy= 0.145908
Thermal correction to Gibbs Free Energy= 0.105753
Sum of electronic and zero-point Energies= -384.754577
Sum of electronic and thermal Energies= -384.747285
Sum of electronic and thermal Enthalpies= -384.746341
Sum of electronic and thermal Free Energies= -384.786496

4-Chloro Benzaldehyde

Cartesian Coordinates (Angstroms):

1	6	0	-0.545855	-1.171681	-0.000011
2	6	0	-1.326669	-0.010723	-0.000005
3	6	0	-0.748685	1.259650	0.000007
4	6	0	0.640247	1.363292	0.000013
5	6	0	1.441275	0.214794	0.000007
6	6	0	0.838195	-1.052111	-0.000004
7	17	0	-3.074477	-0.155939	-0.000012
8	6	0	2.916227	0.339269	0.000014

9	8	0	3.687978	-0.600333	0.000007
10	1	0	-1.023856	-2.145424	-0.000020
11	1	0	-1.377205	2.143499	0.000011
12	1	0	1.106965	2.345942	0.000022
13	1	0	1.474784	-1.931588	-0.000009
14	1	0	3.293183	1.386246	0.000021

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.100530 (Hartree/Particle)
Thermal correction to Energy= 0.108005
Thermal correction to Enthalpy= 0.108949
Thermal correction to Gibbs Free Energy= 0.067787
Sum of electronic and zero-point Energies= -805.068330
Sum of electronic and thermal Energies= -805.060855
Sum of electronic and thermal Enthalpies= -805.059911
Sum of electronic and thermal Free Energies= -805.101073

4-(trifluromethyl) Benzaldehyde

Cartesian Coordinates (Angstroms):

1	6	0	-0.070811	1.152608	-0.000036
2	6	0	0.712260	-0.006293	-0.000042
3	6	0	0.113042	-1.270680	-0.000032
4	6	0	-1.274198	-1.371880	-0.000011
5	6	0	-2.065600	-0.215430	-0.000005
6	6	0	-1.457616	1.046991	-0.000020
7	6	0	2.217721	0.075611	0.000003
8	6	0	-3.545113	-0.331124	0.000012
9	8	0	-4.307852	0.614460	0.000026
10	1	0	0.407539	2.125504	-0.000052
11	1	0	0.730858	-2.163394	-0.000051
12	1	0	-1.749560	-2.350079	-0.000005
13	1	0	-2.089476	1.929558	-0.000021
14	1	0	-3.929791	-1.374743	0.000037
15	9	0	2.741400	-0.538136	1.085312
16	9	0	2.663214	1.348073	-0.000461
17	9	0	2.741512	-0.538976	-1.084775

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.114836 (Hartree/Particle)
Thermal correction to Energy= 0.123844
Thermal correction to Enthalpy= 0.124788
Thermal correction to Gibbs Free Energy= 0.079952
Sum of electronic and zero-point Energies= -682.493934
Sum of electronic and thermal Energies= -682.484926
Sum of electronic and thermal Enthalpies= -682.483982
Sum of electronic and thermal Free Energies= -682.528818

4-cyano Benzaldehyde

Cartesian Coordinates (Angstroms):

1	6	0	-0.864162	1.256927	0.000001
2	6	0	0.522728	1.361968	-0.000004
3	6	0	1.319944	0.210559	-0.000010
4	6	0	0.720749	-1.058254	-0.000011
5	6	0	-0.661690	-1.175708	-0.000006
6	6	0	-1.460201	-0.015433	0.000000
7	6	0	2.799605	0.334438	-0.000018
8	8	0	3.564490	-0.608985	0.000023
9	6	0	-2.889890	-0.132854	0.000005
10	7	0	-4.049138	-0.228090	0.000009
11	1	0	-1.489747	2.143331	0.000005
12	1	0	0.992461	2.342751	-0.000003
13	1	0	1.359939	-1.935461	-0.000015
14	1	0	-1.136579	-2.151353	-0.000007
15	1	0	3.179477	1.379377	0.000032

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.108639 (Hartree/Particle)
Thermal correction to Energy= 0.116743
Thermal correction to Enthalpy= 0.117687
Thermal correction to Gibbs Free Energy= 0.075347
Sum of electronic and zero-point Energies= -437.705317
Sum of electronic and thermal Energies= -437.697214
Sum of electronic and thermal Enthalpies= -437.696270
Sum of electronic and thermal Free Energies= -437.738610

(4-Methoxy Benzaldehyde)$_2$SnCl$_4$ Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	2.459611	-0.274999	0.342665
2	8	0	1.328422	-0.335487	-0.182115
3	50	0	-0.044042	-2.060177	0.042171
4	8	0	-1.424419	-0.332252	0.112229
5	6	0	-2.533850	-0.301665	-0.460380
6	6	0	-3.460378	0.790498	-0.310450
7	6	0	-4.681907	0.764911	-1.018573
8	6	0	-3.178284	1.879604	0.537106
9	6	0	-5.589893	1.797377	-0.888162
10	1	0	-4.906001	-0.075498	-1.670407
11	6	0	-4.083734	2.918760	0.677843
12	1	0	-2.241473	1.886645	1.084939
13	6	0	-5.298240	2.882927	-0.037619
14	1	0	-6.533817	1.798880	-1.422491
15	1	0	-3.852898	3.745948	1.338332
16	1	0	-2.829457	-1.136792	-1.107573
17	17	0	-1.901310	-3.553089	0.235970

18	17	0	0.141564	-1.576471	2.399031
19	17	0	1.817884	-3.562021	-0.017299
20	17	0	-0.220545	-1.793692	-2.350148
21	6	0	3.369866	0.817496	0.115895
22	6	0	3.043079	1.889436	-0.747404
23	6	0	4.618029	0.811333	0.763050
24	6	0	3.939923	2.916596	-0.946645
25	1	0	2.081990	1.882783	-1.250984
26	6	0	5.528770	1.841781	0.569891
27	1	0	4.873427	-0.013100	1.423934
28	6	0	5.191044	2.902462	-0.289477
29	1	0	3.716975	3.748700	-1.606210
30	1	0	6.485041	1.817512	1.077928
31	1	0	2.790238	-1.084390	1.005523
32	8	0	-6.246048	3.839113	0.026723
33	8	0	5.991834	3.953449	-0.554844
34	6	0	-6.041342	4.968086	0.873808
35	6	0	7.280094	4.018288	0.053941
36	1	0	7.732394	4.939765	-0.313878
37	1	0	7.200474	4.059822	1.146691
38	1	0	7.900123	3.163041	-0.239337
39	1	0	-5.939208	4.663750	1.922007
40	1	0	-6.932421	5.585969	0.758849
41	1	0	-5.157424	5.539528	0.566812

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.295433 (Hartree/Particle)
Thermal correction to Energy= 0.323939
Thermal correction to Enthalpy= 0.324883
Thermal correction to Gibbs Free Energy= 0.230503
Sum of electronic and zero-point Energies= -2764.239131
Sum of electronic and thermal Energies= -2764.210625
Sum of electronic and thermal Enthalpies= -2764.209681
Sum of electronic and thermal Free Energies= -2764.304061

(4-Methyl Benzaldehyde)$_2$SnCl$_4$ Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	-2.507607	-0.007818	-0.356931
2	8	0	-1.378146	-0.051843	0.165662
3	50	0	0.000023	-1.795192	-0.000046
4	8	0	1.377975	-0.051667	-0.165439
5	6	0	2.507350	-0.007570	0.357343
6	6	0	3.421396	1.096336	0.157822
7	6	0	4.666109	1.074240	0.809842
8	6	0	3.091976	2.181356	-0.680168
9	6	0	5.564969	2.120282	0.631075
10	1	0	4.921789	0.236274	1.453427
11	6	0	3.996321	3.215846	-0.851975
12	1	0	2.131436	2.183441	-1.185126

13	6	0	5.246572	3.203857	-0.200689
14	1	0	6.525755	2.099212	1.137718
15	1	0	3.743541	4.050405	-1.501134
16	1	0	2.840077	-0.835040	0.996913
17	17	0	1.861661	-3.283992	-0.151322
18	17	0	-0.211240	-1.403248	-2.368122
19	17	0	-1.861454	-3.284238	0.151018
20	17	0	0.211202	-1.403665	2.368123
21	6	0	-3.421556	1.096195	-0.157549
22	6	0	-3.091946	2.181403	0.680124
23	6	0	-4.666357	1.074025	-0.809396
24	6	0	-3.996197	3.215998	0.851797
25	1	0	-2.131338	2.183547	1.184952
26	6	0	-5.565112	2.120182	-0.630784
27	1	0	-4.922186	0.235908	-1.452725
28	6	0	-5.246525	3.203948	0.200661
29	1	0	-3.743276	4.050688	1.500732
30	1	0	-6.525969	2.099055	-1.137289
31	1	0	-2.840503	-0.835449	-0.996207
32	6	0	-6.218698	4.337866	0.407229
33	6	0	6.218875	4.337621	-0.407491
34	1	0	-7.126007	4.205964	-0.188816
35	1	0	-5.766991	5.298758	0.132301
36	1	0	-6.513898	4.412940	1.461205
37	1	0	5.767195	5.298659	-0.133037
38	1	0	6.514268	4.412270	-1.461448
39	1	0	7.126066	4.205859	0.188760

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284495 (Hartree/Particle)
Thermal correction to Energy= 0.311644
Thermal correction to Enthalpy= 0.312588
Thermal correction to Gibbs Free Energy= 0.220378
Sum of electronic and zero-point Energies= -2613.835638
Sum of electronic and thermal Energies= -2613.808489
Sum of electronic and thermal Enthalpies= -2613.807545
Sum of electronic and thermal Free Energies= -2613.899754

(4-chloro Benzaldehyde)$_2$SnCl$_4$ Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	2.512155	-0.290117	0.387460
2	8	0	1.387791	-0.324963	-0.141945
3	50	0	0.000002	-2.081974	0.000035
4	8	0	-1.387829	-0.325002	0.142008
5	6	0	-2.512189	-0.290165	-0.387406
6	6	0	-3.430310	0.817100	-0.202663
7	6	0	-4.669320	0.790672	-0.866888
8	6	0	-3.103092	1.903852	0.631516
9	6	0	-5.573082	1.835049	-0.710409

10	1	0	-4.921213	-0.051128	-1.506455
11	6	0	-3.999691	2.948704	0.795467
12	1	0	-2.147495	1.905747	1.145467
13	6	0	-5.227865	2.905251	0.120513
14	1	0	-6.531101	1.827101	-1.217787
15	1	0	-3.765393	3.791010	1.436870
16	1	0	-2.840706	-1.124044	-1.020925
17	17	0	-1.867020	-3.560982	0.119519
18	17	0	0.170575	-1.669410	2.364199
19	17	0	1.867079	-3.560913	-0.119432
20	17	0	-0.170592	-1.669422	-2.364126
21	6	0	3.430288	0.817129	0.202660
22	6	0	3.103076	1.903845	-0.631567
23	6	0	4.669303	0.790717	0.866876
24	6	0	3.999685	2.948680	-0.795574
25	1	0	2.147477	1.905726	-1.145514
26	6	0	5.573075	1.835078	0.710344
27	1	0	4.921191	-0.051057	1.506479
28	6	0	5.227864	2.905245	-0.120625
29	1	0	3.765393	3.790957	-1.437015
30	1	0	6.531097	1.827143	1.217715
31	1	0	2.840670	-1.123975	1.021008
32	17	0	6.355153	4.220783	-0.326179
33	17	0	-6.355142	4.220810	0.325998

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.209941 (Hartree/Particle)
Thermal correction to Energy= 0.235796
Thermal correction to Enthalpy= 0.236740
Thermal correction to Gibbs Free Energy= 0.147193
Sum of electronic and zero-point Energies= -3454.453351
Sum of electronic and thermal Energies= -3454.427496
Sum of electronic and thermal Enthalpies= -3454.426552
Sum of electronic and thermal Free Energies= -3454.516100

(4-trifluromethyl Benzaldehyde)$_2$SnCl$_4$ Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	2.516610	-0.794165	0.420048
2	8	0	1.394371	-0.820943	-0.108373
3	50	0	0.000000	-2.592178	-0.000010
4	8	0	-1.394440	-0.821012	0.108494
5	6	0	-2.516630	-0.794207	-0.420029
6	6	0	-3.430229	0.328381	-0.263856
7	6	0	-4.666114	0.289815	-0.929150
8	6	0	-3.091407	1.434010	0.538965
9	6	0	-5.560089	1.348934	-0.799083
10	1	0	-4.921219	-0.567053	-1.546801
11	6	0	-3.984053	2.487449	0.668307

12	1	0	-2.134405	1.443035	1.049736
13	6	0	-5.216178	2.442769	-0.001172
14	1	0	-6.513843	1.331485	-1.313773
15	1	0	-3.733791	3.347860	1.279860
16	1	0	-2.852576	-1.643041	-1.029810
17	17	0	-1.871053	-4.064841	0.077734
18	17	0	0.116664	-2.163568	2.360983
19	17	0	1.871219	-4.064633	-0.077812
20	17	0	-0.116747	-2.163424	-2.360956
21	6	0	3.430169	0.328458	0.263901
22	6	0	3.091102	1.434323	-0.538483
23	6	0	4.666286	0.289675	0.928764
24	6	0	3.983727	2.487788	-0.667829
25	1	0	2.133925	1.443522	-1.048921
26	6	0	5.560250	1.348789	0.798661
27	1	0	4.921571	-0.567365	1.546100
28	6	0	5.216089	2.442872	0.001184
29	1	0	3.733259	3.348391	-1.279022
30	1	0	6.514189	1.331165	1.313007
31	1	0	2.852645	-1.643066	1.029683
32	6	0	6.192679	3.579923	-0.192539
33	6	0	-6.192668	3.579911	0.192505
34	9	0	-7.125826	3.613123	-0.778588
35	9	0	-6.836962	3.464235	1.372374
36	9	0	-5.559255	4.771113	0.198414
37	9	0	5.559303	4.771129	-0.199555
38	9	0	7.125202	3.613668	0.779159
39	9	0	6.837778	3.463532	-1.371899

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.238626 (Hartree/Particle)
Thermal correction to Energy= 0.269389
Thermal correction to Enthalpy= 0.270333
Thermal correction to Gibbs Free Energy= 0.167907
Sum of electronic and zero-point Energies= -3209.302662
Sum of electronic and thermal Energies= -3209.271898
Sum of electronic and thermal Enthalpies= -3209.270954
Sum of electronic and thermal Free Energies= -3209.373381

(4-Cyano Benzaldehyde)$_2$SnCl$_4$ Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	2.525775	-0.186728	0.379661
2	8	0	1.398530	-0.213223	-0.136628
3	50	0	0.000004	-1.988809	0.000003
4	8	0	-1.398538	-0.213238	0.136665
5	6	0	-2.525748	-0.186712	-0.379698
6	6	0	-3.446252	0.926911	-0.192445
7	6	0	-4.689077	0.893823	-0.847346
8	6	0	-3.106893	2.014857	0.633676

9	6	0	-5.589082	1.940409	-0.687909
10	1	0	-4.944774	0.047901	-1.479513
11	6	0	-4.001551	3.060478	0.799007
12	1	0	-2.146531	2.015711	1.138169
13	6	0	-5.245379	3.026243	0.136274
14	1	0	-6.550729	1.927671	-1.189021
15	1	0	-3.757266	3.904694	1.434711
16	1	0	-2.862119	-1.026449	-1.001694
17	17	0	-1.871160	-3.455996	0.110279
18	17	0	0.158355	-1.549659	2.355397
19	17	0	1.871181	-3.455977	-0.110295
20	17	0	-0.158350	-1.549623	-2.355383
21	6	0	3.446262	0.926911	0.192423
22	6	0	3.106843	2.014914	-0.633600
23	6	0	4.689131	0.893782	0.847239
24	6	0	4.001486	3.060549	-0.798918
25	1	0	2.146448	2.015799	-1.138029
26	6	0	5.589120	1.940383	0.687815
27	1	0	4.944873	0.047817	1.479329
28	6	0	5.245358	3.026273	-0.136270
29	1	0	3.757156	3.904809	-1.434547
30	1	0	6.550801	1.927615	1.188862
31	1	0	2.862191	-1.026508	1.001575
32	6	0	-6.169213	4.110250	0.306024
33	7	0	-6.916344	4.990584	0.443470
34	6	0	6.169176	4.110296	-0.306006
35	7	0	6.916295	4.990642	-0.443441

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.225978 (Hartree/Particle)
Thermal correction to Energy= 0.253131
Thermal correction to Enthalpy= 0.254075
Thermal correction to Gibbs Free Energy= 0.161997
Sum of electronic and zero-point Energies= -2719.723566
Sum of electronic and thermal Energies= -2719.696413
Sum of electronic and thermal Enthalpies= -2719.695469
Sum of electronic and thermal Free Energies= -2719.787548

(Benzaldehyde)$SnCl_4$ Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	3.964480	-1.278502	-0.009972
2	6	0	5.331323	-1.018213	-0.005372
3	6	0	5.782365	0.305333	0.004525
4	6	0	4.874191	1.373269	0.009772
5	6	0	3.508972	1.121632	0.005133
6	6	0	3.048355	-0.210387	-0.004700
7	1	0	3.598627	-2.302231	-0.017693
8	1	0	6.043163	-1.837731	-0.009436
9	1	0	5.238847	2.395843	0.017434
10	1	0	2.785022	1.929956	0.008907
11	6	0	1.630128	-0.506774	-0.009710
12	8	0	0.753774	0.374117	-0.006257
13	1	0	1.337199	-1.566416	-0.017922
14	50	0	-1.508391	0.038623	0.000324
15	17	0	-1.029896	-1.063626	2.022279
16	17	0	-3.848415	-0.263535	0.010813
17	17	0	-1.460798	2.370724	-0.088087
18	17	0	-1.031601	-1.206521	-1.938749
19	1	0	6.849669	0.508642	0.008170

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.116875 (Hartree/Particle)
Thermal correction to Energy= 0.132553
Thermal correction to Enthalpy= 0.133497
Thermal correction to Gibbs Free Energy= 0.068886
Sum of electronic and zero-point Energies= -2189.776132
Sum of electronic and thermal Energies= -2189.760453
Sum of electronic and thermal Enthalpies= -2189.759509
Sum of electronic and thermal Free Energies= -2189.824120

Anisole

Cartesian Coordinates (Angstroms):

1	6	0	-0.212750	-1.212867	-0.165036
2	6	0	-1.586170	-1.207825	0.083962
3	6	0	-2.274642	0.000771	0.211120
4	6	0	-1.585002	1.208644	0.083264
5	6	0	-0.211604	1.212229	-0.165787
6	6	0	0.470841	-0.000693	-0.290130
7	1	0	0.336693	-2.142693	-0.279678
8	1	0	-2.119623	-2.150529	0.174647
9	1	0	-3.344035	0.001349	0.402861
10	1	0	-2.117570	2.151903	0.173393
11	1	0	0.338687	2.141479	-0.281057
12	8	0	1.821083	-0.001547	-0.582492
13	6	0	2.670002	0.000841	0.562343

14	1	0	2.507840	-0.890828	1.184313
15	1	0	3.696424	-0.000643	0.187123
16	1	0	2.508859	0.895749	1.179919

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.132879 (Hartree/Particle)
Thermal correction to Energy= 0.139162
Thermal correction to Enthalpy= 0.140106
Thermal correction to Gibbs Free Energy= 0.102434
Sum of electronic and zero-point Energies= -346.633628
Sum of electronic and thermal Energies= -346.627346
Sum of electronic and thermal Enthalpies= -346.626402
Sum of electronic and thermal Free Energies= -346.664073

(Benzaldehyde)$SnCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	1.240733	3.343274	-1.153109
2	6	0	1.394866	4.707720	-0.913633
3	6	0	1.021301	5.248001	0.320149
4	6	0	0.490273	4.417828	1.308484
5	6	0	0.338071	3.049660	1.071846
6	6	0	0.715406	2.504239	-0.160885
7	1	0	1.517016	2.929038	-2.120347
8	1	0	1.794034	5.350973	-1.692947
9	1	0	0.184216	4.834742	2.263991
10	1	0	-0.095827	2.403613	1.827733
11	6	0	0.591449	1.026163	-0.433295
12	8	0	-0.321202	0.362776	0.490219
13	1	0	0.290362	0.860986	-1.471022
14	6	0	1.847203	0.164908	-0.088115
15	6	0	2.088780	-1.039833	-0.841026
16	6	0	2.940535	0.668524	0.706436
17	6	0	3.251034	-1.764244	-0.695028
18	1	0	1.294852	-1.422092	-1.478610
19	6	0	4.095569	-0.053502	0.857920
20	1	0	2.816853	1.617428	1.218548
21	6	0	4.265845	-1.277720	0.160879
22	1	0	3.375367	-2.694895	-1.234856
23	1	0	4.907056	0.290997	1.490080
24	1	0	0.989439	-0.287892	0.734970
25	8	0	5.423923	-1.898413	0.379516
26	6	0	5.702955	-3.147900	-0.269028
27	1	0	4.965456	-3.905047	0.015767
28	1	0	6.690405	-3.441198	0.085666
29	1	0	5.720421	-3.025817	-1.356832
30	50	0	-1.979136	-0.713767	0.037097
31	17	0	-1.303539	-1.946245	2.007388
32	17	0	-2.367756	0.832069	-1.793681

33	17	0	-1.402194	-2.489522	-1.445676
34	17	0	-4.182536	-0.451179	0.830267
35	1	0	1.133713	6.312820	0.504504

Frequency Data:
NImag: 1 (-1082.3)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.248306 (Hartree/Particle)
Thermal correction to Energy= 0.271324
Thermal correction to Enthalpy= 0.272268
Thermal correction to Gibbs Free Energy= 0.190475
Sum of electronic and zero-point Energies= -2536.337399
Sum of electronic and thermal Energies= -2536.314382
Sum of electronic and thermal Enthalpies= -2536.313438
Sum of electronic and thermal Free Energies= -2536.395231

(Benzaldehyde)$SnCl_4$(anisole) Intermediate 2

Cartesian Coordinates (Angstroms):

1	6	0	-0.907846	4.118392	1.205453
2	6	0	-1.413321	4.925891	0.186353
3	6	0	-1.721714	4.361497	-1.054058
4	6	0	-1.526918	2.998139	-1.268897
5	6	0	-1.024348	2.181591	-0.247112
6	6	0	-0.713576	2.751649	0.991246
7	6	0	-0.879798	0.697590	-0.523020
8	6	0	-2.155516	-0.107400	-0.394367
9	6	0	-2.350307	-1.242736	-1.203020
10	6	0	-3.489132	-2.022701	-1.074996
11	6	0	-4.469255	-1.689660	-0.124293
12	6	0	-4.288836	-0.563472	0.690295
13	6	0	-3.140272	0.216521	0.546293
14	8	0	0.132626	0.104012	0.393948
15	1	0	-0.654232	4.550924	2.169366
16	1	0	-1.558692	5.989551	0.353279
17	1	0	-2.106961	4.983855	-1.857021
18	1	0	-1.767732	2.563658	-2.236578
19	1	0	-0.295436	2.133952	1.778909
20	1	0	-0.460451	0.548617	-1.520786
21	1	0	-1.596211	-1.514223	-1.936661
22	1	0	-3.648211	-2.895877	-1.699413
23	1	0	-5.033254	-0.280993	1.425513
24	1	0	-3.022504	1.100395	1.166201
25	1	0	-0.314522	-0.508435	1.006827
26	50	0	2.294352	-0.578311	0.057647
27	17	0	1.462573	-1.574188	-1.899394
28	17	0	4.509054	-1.375716	-0.071159
29	17	0	1.747982	-1.598153	2.116934
30	17	0	2.726590	1.707848	-0.079920
31	8	0	-5.547502	-2.513672	-0.078398

32	6	0	-6.578758	-2.234401	0.858939
33	1	0	-7.036698	-1.254708	0.671682
34	1	0	-6.204405	-2.269811	1.890026
35	1	0	-7.327096	-3.015941	0.719159

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253732 (Hartree/Particle)
Thermal correction to Energy= 0.277266
Thermal correction to Enthalpy= 0.278211
Thermal correction to Gibbs Free Energy= 0.194624
Sum of electronic and zero-point Energies= -2536.404359
Sum of electronic and thermal Energies= -2536.380825
Sum of electronic and thermal Enthalpies= -2536.379881
Sum of electronic and thermal Free Energies= -2536.463467

$SnCl_4$(4-methoxy Benzaldehyde) Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	3.363225	1.335943	-0.000040
2	6	0	4.720201	1.045836	-0.000037
3	6	0	5.133579	-0.299617	0.000018
4	6	0	4.175992	-1.340147	0.000059
5	6	0	2.831532	-1.041717	0.000042
6	6	0	2.402163	0.307630	0.000004
7	1	0	3.037519	2.373283	-0.000086
8	1	0	5.443867	1.851743	-0.000076
9	1	0	4.532455	-2.364743	0.000098
10	1	0	2.086637	-1.830550	0.000064
11	6	0	1.007846	0.654837	-0.000007
12	8	0	0.094540	-0.196912	-0.000081
13	1	0	0.744378	1.720620	-0.000115
14	8	0	6.417320	-0.700712	0.000029
15	6	0	7.456806	0.277815	-0.000024
16	1	0	8.389558	-0.286505	0.000004
17	1	0	7.407687	0.905960	-0.896963
18	1	0	7.407691	0.906054	0.896849
19	50	0	-2.141313	-0.033787	-0.000008
20	17	0	-1.821224	2.306394	-0.001411
21	17	0	-4.506176	0.018808	0.000091
22	17	0	-1.854824	-1.165270	-2.031490
23	17	0	-1.854663	-1.162814	2.032866

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.149998 (Hartree/Particle)
Thermal correction to Energy= 0.168161
Thermal correction to Enthalpy= 0.169105
Thermal correction to Gibbs Free Energy= 0.098939
Sum of electronic and zero-point Energies= -2304.270569

Sum of electronic and thermal Energies= -2304.252406
Sum of electronic and thermal Enthalpies= -2304.251462
Sum of electronic and thermal Free Energies= -2304.321628

$SnCl_4$(4-Methyl Benzaldehyde) Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	3.597310	-1.388637	-0.002566
2	6	0	4.968006	-1.158166	-0.000602
3	6	0	5.474821	0.150527	0.002389
4	6	0	4.568500	1.230837	0.004643
5	6	0	3.201278	1.015062	0.002588
6	6	0	2.701410	-0.304525	-0.001072
7	1	0	3.213720	-2.405961	-0.004591
8	1	0	5.656942	-1.998020	-0.001140
9	1	0	4.953226	2.247336	0.008390
10	1	0	2.500966	1.844058	0.004473
11	6	0	1.281304	-0.566331	-0.002649
12	8	0	0.424163	0.336793	-0.001704
13	1	0	0.962160	-1.618128	-0.005271
14	50	0	-1.828720	0.054390	0.000002
15	17	0	-1.388551	-1.112167	1.996667
16	17	0	-4.177307	-0.194455	0.002792
17	17	0	-1.738917	2.388146	-0.027072
18	17	0	-1.389482	-1.156071	-1.971022
19	6	0	6.959690	0.408826	-0.001942
20	1	0	7.532411	-0.520423	0.062225
21	1	0	7.249745	1.048501	0.840159
22	1	0	7.261973	0.930509	-0.918671

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.144367 (Hartree/Particle)
Thermal correction to Energy= 0.161945
Thermal correction to Enthalpy= 0.162889
Thermal correction to Gibbs Free Energy= 0.092936
Sum of electronic and zero-point Energies= -2229.068338
Sum of electronic and thermal Energies= -2229.050760
Sum of electronic and thermal Enthalpies= -2229.049816
Sum of electronic and thermal Free Energies= -2229.119769

$SnCl_4$(4-chloro Benzaldehyde) Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	-3.354774	1.507740	0.000066
2	6	0	-4.720581	1.252158	0.000350
3	6	0	-5.157633	-0.076552	0.000053
4	6	0	-4.254753	-1.149502	-0.000490
5	6	0	-2.893751	-0.885825	-0.000765
6	6	0	-2.432415	0.445607	-0.000502
7	1	0	-2.997652	2.534399	0.000280

8	1	0	-5.441674	2.061631	0.000804
9	1	0	-4.626052	-2.168181	-0.000683
10	1	0	-2.171793	-1.695757	-0.001164
11	6	0	-1.014431	0.746250	-0.000770
12	8	0	-0.140035	-0.135326	-0.001227
13	1	0	-0.714727	1.803206	-0.000481
14	50	0	2.150376	-0.057881	-0.000054
15	17	0	1.885827	2.283744	-0.002324
16	17	0	4.507749	-0.101459	0.002215
17	17	0	1.780937	-1.167786	2.025317
18	17	0	1.783971	-1.170953	-2.024094
19	17	0	-6.868873	-0.408127	0.000421

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.107198 (Hartree/Particle)
Thermal correction to Energy= 0.124060
Thermal correction to Enthalpy= 0.125004
Thermal correction to Gibbs Free Energy= 0.057145
Sum of electronic and zero-point Energies= -2649.376737
Sum of electronic and thermal Energies= -2649.359876
Sum of electronic and thermal Enthalpies= -2649.358931
Sum of electronic and thermal Free Energies= -2649.426791

$SnCl_4$(4-trifluromethyl Benzaldehyde) Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	2.721033	-1.531975	-0.017977
2	6	0	4.098132	-1.336111	0.002440
3	6	0	4.606556	-0.034198	0.036273
4	6	0	3.748197	1.074404	0.052643
5	6	0	2.374439	0.881922	0.032224
6	6	0	1.854766	-0.425892	-0.004291
7	1	0	2.313911	-2.539329	-0.042268
8	1	0	4.775373	-2.182737	-0.000973
9	1	0	4.162093	2.076130	0.088766
10	1	0	1.689838	1.723447	0.046099
11	6	0	0.417815	-0.654940	-0.025355
12	8	0	-0.408668	0.267370	-0.014066
13	1	0	0.074054	-1.699121	-0.055915
14	50	0	-2.722822	0.069855	-0.000418
15	17	0	-2.285001	-0.872317	2.104972
16	17	0	-5.071786	-0.091716	0.025420
17	17	0	-2.512026	2.373179	-0.294615
18	17	0	-2.304124	-1.353054	-1.825076
19	6	0	6.101725	0.188086	-0.000273
20	9	0	6.451257	1.301114	0.674408
21	9	0	6.531917	0.334472	-1.270835
22	9	0	6.772285	-0.850190	0.536617

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.
Zero-point correction= 0.121436 (Hartree/Particle)
Thermal correction to Energy= 0.139880
Thermal correction to Enthalpy= 0.140825
Thermal correction to Gibbs Free Energy= 0.069789
Sum of electronic and zero-point Energies= -2526.800893
Sum of electronic and thermal Energies= -2526.782449
Sum of electronic and thermal Enthalpies= -2526.781505
Sum of electronic and thermal Free Energies= -2526.852540

$SnCl_4$(4-cyano Benzaldehyde) Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	3.437175	-1.450140	-0.021204
2	6	0	4.809866	-1.236373	-0.014182
3	6	0	5.303375	0.080251	0.001658
4	6	0	4.420462	1.179204	0.010277
5	6	0	3.051945	0.959852	0.002993
6	6	0	2.553949	-0.357001	-0.012616
7	1	0	3.045438	-2.463710	-0.033496
8	1	0	5.502444	-2.070841	-0.020765
9	1	0	4.820200	2.187399	0.022467
10	1	0	2.353009	1.789606	0.009149
11	6	0	1.118774	-0.607571	-0.020440
12	8	0	0.280949	0.302936	-0.015369
13	1	0	0.790675	-1.657267	-0.033467
14	50	0	-2.043831	0.062217	0.001245
15	17	0	-1.573274	-0.970452	2.056173
16	17	0	-4.387388	-0.141966	0.025249
17	17	0	-1.865698	2.378765	-0.181645
18	17	0	-1.593155	-1.267039	-1.883306
19	6	0	6.719553	0.307234	0.008968
20	7	0	7.867624	0.491360	0.014871

Frequency Data:
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.115075 (Hartree/Particle)
Thermal correction to Energy= 0.132669
Thermal correction to Enthalpy= 0.133613
Thermal correction to Gibbs Free Energy= 0.063292
Sum of electronic and zero-point Energies= -2282.011155
Sum of electronic and thermal Energies= -2281.993562
Sum of electronic and thermal Enthalpies= -2281.992618
Sum of electronic and thermal Free Energies= -2282.062938

(4-metoxy benzaldehyde)$SnCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	3.029574	-0.059442	1.461009
2	6	0	4.347218	-0.473017	1.339329

3	6	0	4.788383	-1.081195	0.151252
4	6	0	3.888225	-1.266537	-0.904988
5	6	0	2.563908	-0.839853	-0.770466
6	6	0	2.118343	-0.232107	0.405330
7	1	0	2.698745	0.393816	2.392899
8	1	0	5.054614	-0.352651	2.153565
9	1	0	4.198038	-1.747668	-1.825475
10	1	0	1.862453	-1.005447	-1.581481
11	6	0	0.704285	0.258724	0.554778
12	8	0	-0.198643	-0.334887	-0.428422
13	1	0	0.347403	0.079665	1.572575
14	6	0	0.449759	1.747742	0.146892
15	6	0	-0.617841	2.469922	0.789750
16	6	0	1.416754	2.527793	-0.584106
17	6	0	-0.799115	3.821488	0.594290
18	1	0	-1.341004	1.913451	1.381698
19	6	0	1.234752	3.871396	-0.786697
20	1	0	2.278874	2.021209	-1.006100
21	6	0	0.125597	4.534900	-0.201775
22	1	0	-1.644904	4.321270	1.050053
23	1	0	1.930717	4.461166	-1.373787
24	1	0	-0.232971	1.113080	-0.721032
25	8	0	0.043010	5.839734	-0.460765
26	6	0	-1.041724	6.610051	0.076340
27	1	0	-2.002850	6.230974	-0.285672
28	1	0	-0.882734	7.623994	-0.289248
29	1	0	-1.019707	6.602782	1.170920
30	50	0	-1.891721	-1.386049	-0.065416
31	17	0	-2.623114	-0.267753	-2.085571
32	17	0	-0.762280	-2.360204	1.849112
33	17	0	-3.373254	-0.132885	1.320471
34	17	0	-2.490150	-3.507764	-0.898417
35	8	0	6.096597	-1.454376	0.131707
36	6	0	6.594136	-2.112716	-1.024404
37	1	0	6.526633	-1.471646	-1.913205
38	1	0	7.642837	-2.330404	-0.815528
39	1	0	6.058205	-3.051495	-1.213871

Frequency Data:

NImag: 1 (-1103.9)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.280986 (Hartree/Particle)

Thermal correction to Energy= 0.306628

Thermal correction to Enthalpy= 0.307573

Thermal correction to Gibbs Free Energy= 0.219551

Sum of electronic and zero-point Energies= -2650.826831

Sum of electronic and thermal Energies= -2650.801189

Sum of electronic and thermal Enthalpies= -2650.800244

Sum of electronic and thermal Free Energies= -2650.888266

(4-methyl benzaldehyde)$SnCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	-1.918129	2.680187	1.260096
2	6	0	-2.410357	3.966291	1.055071
3	6	0	-2.221629	4.627216	-0.168130
4	6	0	-1.528409	3.951256	-1.179944
5	6	0	-1.035037	2.660647	-0.983578
6	6	0	-1.227136	2.011479	0.240969
7	1	0	-2.063831	2.196158	2.223515
8	1	0	-2.938488	4.471437	1.860492
9	1	0	-1.362218	4.444362	-2.134857
10	1	0	-0.478815	2.161435	-1.770240
11	6	0	-0.734667	0.606890	0.473015
12	8	0	0.308548	0.218683	-0.469875
13	6	0	-2.717976	6.039401	-0.371329
14	1	0	-1.987533	6.770481	-0.000215
15	1	0	-3.655698	6.217807	0.166206
16	1	0	-2.886178	6.257012	-1.431148
17	1	0	-0.394414	0.494401	1.505870
18	6	0	-1.735080	-0.535691	0.104653
19	6	0	-1.646045	-1.786880	0.813869
20	6	0	-2.936911	-0.301461	-0.656950
21	6	0	-2.590351	-2.777367	0.657177
22	1	0	-0.766339	-1.975822	1.425191
23	6	0	-3.874250	-1.288075	-0.820535
24	1	0	-3.070038	0.664785	-1.133087
25	6	0	-3.714238	-2.536803	-0.166091
26	1	0	-2.462527	-3.726387	1.163202
27	1	0	-4.760371	-1.140490	-1.428683
28	1	0	-0.801968	-0.726689	-0.737947
29	8	0	-4.683195	-3.423264	-0.390440
30	6	0	-4.625223	-4.720268	0.220720
31	1	0	-3.728890	-5.260351	-0.100643
32	1	0	-5.516040	-5.241866	-0.127614
33	1	0	-4.646940	-4.636874	1.312075
34	50	0	2.191425	-0.398176	-0.047895
35	17	0	1.820836	-1.769790	-2.008451
36	17	0	2.198097	1.199171	1.779279
37	17	0	2.120556	-2.260660	1.439751
38	17	0	4.239266	0.419229	-0.880517

Frequency Data:

NImag: 1 (-1093.4)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.275677 (Hartree/Particle)

Thermal correction to Energy= 0.300647

Thermal correction to Enthalpy= 0.301591

Thermal correction to Gibbs Free Energy= 0.214462

Sum of electronic and zero-point Energies= -2575.627816

Sum of electronic and thermal Energies= -2575.602846
Sum of electronic and thermal Enthalpies= -2575.601902
Sum of electronic and thermal Free Energies= -2575.689031

(4-chloro benzaldehyde)$SnCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	3.039083	-0.382820	1.308491
2	6	0	4.311419	-0.921992	1.133993
3	6	0	4.627506	-1.536080	-0.079450
4	6	0	3.689730	-1.622460	-1.107332
5	6	0	2.419657	-1.074817	-0.920200
6	6	0	2.084626	-0.447361	0.284736
7	1	0	2.786450	0.081854	2.258728
8	1	0	5.046812	-0.878382	1.930020
9	1	0	3.945894	-2.117834	-2.037655
10	1	0	1.674065	-1.155275	-1.703845
11	6	0	0.727404	0.176997	0.491128
12	8	0	-0.256814	-0.303701	-0.469151
13	1	0	0.391573	0.009093	1.518171
14	6	0	0.610706	1.688832	0.121066
15	6	0	-0.351572	2.499387	0.823652
16	6	0	1.616756	2.384569	-0.643497
17	6	0	-0.409653	3.864749	0.653468
18	1	0	-1.097627	2.002753	1.440010
19	6	0	1.557859	3.742555	-0.818248
20	1	0	2.404332	1.806932	-1.116710
21	6	0	0.545284	4.499810	-0.173761
22	1	0	-1.182560	4.435946	1.152765
23	1	0	2.280227	4.272503	-1.429879
24	1	0	-0.170833	1.153700	-0.729958
25	8	0	0.579524	5.809315	-0.411376
26	6	0	-0.398012	6.675118	0.184972
27	1	0	-1.406825	6.402909	-0.141335
28	1	0	-0.151104	7.674551	-0.171352
29	1	0	-0.330517	6.643110	1.277114
30	50	0	-2.021122	-1.222212	-0.054036
31	17	0	-2.744653	0.056145	-1.977761
32	17	0	-0.850235	-2.395638	1.717099
33	17	0	-3.266772	0.103897	1.484343
34	17	0	-2.904867	-3.226803	-0.918222
35	17	0	6.228867	-2.216724	-0.308647

Frequency Data:
NImag: 1 (-1080.2)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.238609 (Hartree/Particle)
Thermal correction to Energy= 0.262854
Thermal correction to Enthalpy= 0.263799
Thermal correction to Gibbs Free Energy= 0.178803

Sum of electronic and zero-point Energies= -2995.938894
Sum of electronic and thermal Energies= -2995.914649
Sum of electronic and thermal Enthalpies= -2995.913705
Sum of electronic and thermal Free Energies= -2995.998700

(4-trifluromethyl benzaldehyde)$SnCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	-2.598472	0.499612	-1.338525
2	6	0	-3.964601	0.294011	-1.174162
3	6	0	-4.445857	-0.268828	0.012900
4	6	0	-3.555768	-0.628310	1.026140
5	6	0	-2.186559	-0.417702	0.859687
6	6	0	-1.698912	0.150042	-0.321871
7	1	0	-2.228785	0.926565	-2.267745
8	1	0	-4.657198	0.567503	-1.963372
9	1	0	-3.929982	-1.070483	1.943267
10	1	0	-1.488506	-0.710765	1.635951
11	6	0	-0.224198	0.412884	-0.510983
12	8	0	0.596564	-0.302625	0.453365
13	6	0	-5.920257	-0.536050	0.165130
14	1	0	0.067114	0.170164	-1.536556
15	6	0	0.262140	1.844645	-0.129838
16	6	0	1.401231	2.393521	-0.821727
17	6	0	-0.544760	2.764887	0.634266
18	6	0	1.795584	3.700636	-0.642276
19	1	0	2.005183	1.728688	-1.435292
20	6	0	-0.151079	4.064375	0.818273
21	1	0	-1.453827	2.398726	1.100617
22	6	0	1.022536	4.549185	0.184055
23	1	0	2.689862	4.064379	-1.133252
24	1	0	-0.722528	4.754059	1.430269
25	1	0	0.879627	1.128881	0.722459
26	8	0	1.313882	5.823980	0.431462
27	6	0	2.481154	6.423019	-0.151564
28	1	0	3.386799	5.900643	0.172515
29	1	0	2.492324	7.447663	0.218193
30	1	0	2.412619	6.423067	-1.244076
31	50	0	2.061250	-1.658124	0.055378
32	17	0	3.050068	-0.643373	2.015478
33	17	0	0.644135	-2.472600	-1.736918
34	17	0	3.622221	-0.670359	-1.447757
35	17	0	2.402494	-3.836661	0.883919
36	9	0	-6.662079	0.418918	-0.441248
37	9	0	-6.273497	-1.716731	-0.387948
38	9	0	-6.292584	-0.577562	1.462773

Frequency Data:
NImag: 1 (-1079.6)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.

Zero-point correction= 0.253017 (Hartree/Particle)
Thermal correction to Energy= 0.279725
Thermal correction to Enthalpy= 0.280669
Thermal correction to Gibbs Free Energy= 0.188546
Sum of electronic and zero-point Energies= -2873.365915
Sum of electronic and thermal Energies= -2873.339207
Sum of electronic and thermal Enthalpies= -2873.338263
Sum of electronic and thermal Free Energies= -2873.430385

(4-cyano benzaldehyde)$SnCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	3.024140	-0.906180	1.277392
2	6	0	4.185652	-1.649398	1.104725
3	6	0	4.389659	-2.357005	-0.093317
4	6	0	3.414457	-2.315286	-1.102449
5	6	0	2.254956	-1.564845	-0.920007
6	6	0	2.053460	-0.851480	0.266988
7	1	0	2.865693	-0.372165	2.211094
8	1	0	4.933007	-1.695192	1.889987
9	1	0	3.567191	-2.873915	-2.020060
10	1	0	1.489966	-1.544640	-1.688126
11	6	0	0.819606	-0.005409	0.471487
12	8	0	-0.228998	-0.302475	-0.491639
13	1	0	0.460062	-0.122696	1.497790
14	6	0	0.969381	1.504291	0.113071
15	6	0	0.170071	2.466623	0.828639
16	6	0	2.074425	2.017345	-0.660077
17	6	0	0.346960	3.821656	0.659352
18	1	0	-0.643658	2.104408	1.452918
19	6	0	2.249858	3.365370	-0.832079
20	1	0	2.744941	1.314718	-1.144528
21	6	0	1.388396	4.284703	-0.177915
22	1	0	-0.310494	4.516582	1.167080
23	1	0	3.046741	3.763917	-1.450835
24	1	0	0.098400	1.121457	-0.737423
25	8	0	1.643173	5.568400	-0.417646
26	6	0	0.829802	6.588837	0.181945
27	1	0	-0.214224	6.483105	-0.129349
28	1	0	1.233226	7.530718	-0.187861
29	1	0	0.906772	6.554590	1.273344
30	50	0	-2.126118	-0.898600	-0.053164
31	17	0	-2.645740	0.586732	-1.892440
32	17	0	-1.131569	-2.356150	1.609565
33	17	0	-3.040312	0.564183	1.589063
34	17	0	-3.403005	-2.652843	-0.964036
35	6	0	5.590958	-3.117785	-0.280885
36	7	0	6.570688	-3.725658	-0.434195

Frequency Data:
NImag: 1 (-1110.3)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.
Zero-point correction= 0.246714 (Hartree/Particle)
Thermal correction to Energy= 0.271580
Thermal correction to Enthalpy= 0.272524
Thermal correction to Gibbs Free Energy= 0.186172
Sum of electronic and zero-point Energies= -2628.577395
Sum of electronic and thermal Energies= -2628.552529
Sum of electronic and thermal Enthalpies= -2628.551585
Sum of electronic and thermal Free Energies= -2628.637937

Ethyl Glyoxalate

Cartesian Coordinates (Angstroms):

1	6	0	-0.626109	0.266837	-0.000073
2	8	0	-0.756158	1.466790	0.000112
3	8	0	0.539560	-0.402786	-0.000262
4	6	0	1.740790	0.411737	-0.000176
5	1	0	1.717786	1.057408	0.883438
6	1	0	1.718142	1.057050	-0.884066
7	6	0	2.932401	-0.525111	0.000250
8	1	0	3.859403	0.058230	0.000060
9	1	0	2.928359	-1.164560	0.888600
10	1	0	2.928456	-1.165272	-0.887588
11	6	0	-1.787249	-0.739566	-0.000038
12	8	0	-2.936661	-0.379070	0.000146
13	1	0	-1.485083	-1.805708	-0.000189

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.099948 (Hartree/Particle)
Thermal correction to Energy= 0.107689
Thermal correction to Enthalpy= 0.108633
Thermal correction to Gibbs Free Energy= 0.067154
Sum of electronic and zero-point Energies= -381.592786
Sum of electronic and thermal Energies= -381.585046
Sum of electronic and thermal Enthalpies= -381.584101
Sum of electronic and thermal Free Energies= -381.625580

(Ethylglyoxalate)$SnCl_4$ Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	1.727034	1.155088	0.000720
2	8	0	0.996122	0.180520	0.001717
3	1	0	1.343984	2.185620	0.000358
4	50	0	-1.463149	-0.086992	-0.000067
5	17	0	-1.412654	2.253180	0.000853
6	17	0	-3.775435	-0.457576	-0.001837
7	17	0	-0.849186	-1.103179	-2.001778
8	17	0	-0.851934	-1.103706	2.002247
9	6	0	3.248531	1.048683	-0.000221
10	8	0	3.921813	2.057056	-0.001617
11	8	0	3.671274	-0.206749	0.000852
12	6	0	5.116823	-0.397179	0.000272

13	6	0	5.377133	-1.889507	-0.000073
14	1	0	5.523855	0.100759	0.885554
15	1	0	5.523120	0.101121	-0.885151
16	1	0	6.457264	-2.070384	-0.000445
17	1	0	4.947786	-2.362582	0.888237
18	1	0	4.947201	-2.362283	-0.888257

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.106285 (Hartree/Particle)
Thermal correction to Energy= 0.123527
Thermal correction to Enthalpy= 0.124472
Thermal correction to Gibbs Free Energy= 0.055349
Sum of electronic and zero-point Energies= -2225.897780
Sum of electronic and thermal Energies= -2225.880537
Sum of electronic and thermal Enthalpies= -2225.879593
Sum of electronic and thermal Free Energies= -2225.948716

(Ethylglyoxalate)$SnCl_4$(Anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	0.620737	2.279253	0.525213
2	6	0	0.669498	0.875526	-0.088110
3	8	0	-0.134278	-0.053103	0.661480
4	1	0	0.381907	0.927944	-1.141603
5	6	0	2.024254	0.149165	0.064601
6	6	0	2.580395	-0.562934	-1.059942
7	6	0	2.906451	0.419379	1.181724
8	6	0	3.843006	-1.105990	-1.010616
9	1	0	1.948241	-0.727766	-1.927690
10	6	0	4.164780	-0.121655	1.225513
11	1	0	2.518061	1.014877	2.001600
12	6	0	4.648320	-0.888565	0.135000
13	1	0	4.214033	-1.685696	-1.846958
14	1	0	4.821107	0.027859	2.076158
15	1	0	1.247934	-0.688712	0.587441
16	8	0	5.880398	-1.369407	0.282818
17	6	0	6.475851	-2.166140	-0.752121
18	1	0	5.888947	-3.073075	-0.928959
19	1	0	7.463126	-2.432290	-0.376308
20	1	0	6.573984	-1.590257	-1.677824
21	50	0	-1.969144	-0.790486	0.056626
22	17	0	-1.787994	-2.104458	2.008075
23	17	0	-2.716802	1.465560	-0.001780
24	17	0	-0.851117	-1.557547	-1.931760
25	17	0	-4.076586	-1.692426	-0.602654
26	8	0	0.803761	2.517682	1.700245
27	8	0	0.376370	3.196078	-0.416412
28	6	0	0.232777	4.565871	0.044613
29	1	0	1.170885	4.872792	0.518397
30	1	0	-0.552775	4.586873	0.805036
31	6	0	-0.111939	5.416462	-1.162265
32	1	0	-0.234973	6.460188	-0.853490

33	1	0	0.681018	5.371560	-1.915938
34	1	0	-1.046574	5.078598	-1.619846

Frequency Data:

NImag: 1 (-956.3)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.238993 (Hartree/Particle)
Thermal correction to Energy= 0.263165
Thermal correction to Enthalpy= 0.264109
Thermal correction to Gibbs Free Energy= 0.179971
Sum of electronic and zero-point Energies= -2572.485315
Sum of electronic and thermal Energies= -2572.461143
Sum of electronic and thermal Enthalpies= -2572.460199
Sum of electronic and thermal Free Energies= -2572.544336

$PhSnCl_3$

Cartesian Coordinates (Angstroms):

1	50	0	-0.714280	0.000025	-0.004653
2	17	0	-1.661056	-0.005175	2.130387
3	17	0	-1.550639	1.895982	-1.076372
4	17	0	-1.551482	-1.890370	-1.085504
5	6	0	1.388176	-0.000132	-0.003727
6	6	0	2.087627	-1.215771	0.006489
7	6	0	2.087749	1.215428	0.006341
8	6	0	3.483436	-1.210993	0.029696
9	1	0	1.556901	-2.164049	-0.013094
10	6	0	3.483568	1.210501	0.029553
11	1	0	1.557084	2.163733	-0.013337
12	6	0	4.179148	-0.000278	0.042530
13	1	0	4.025031	-2.152656	0.034793
14	1	0	4.025260	2.152109	0.034541
15	1	0	5.265482	-0.000337	0.059771

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.094090 (Hartree/Particle)
Thermal correction to Energy= 0.105646
Thermal correction to Enthalpy= 0.106590
Thermal correction to Gibbs Free Energy= 0.052661
Sum of electronic and zero-point Energies= -1615.634211
Sum of electronic and thermal Energies= -1615.622655
Sum of electronic and thermal Enthalpies= -1615.621711
Sum of electronic and thermal Free Energies= -1615.675640

$PhSnCl_3$(4-Methyl Benzaldehyde) Intermediate

Cartesian Coordinates (Angstroms):

1	6	0	-4.417514	-0.611002	1.268433
2	6	0	-5.777021	-0.483912	1.006372
3	6	0	-6.224590	0.087597	-0.194603

4	6	0	-5.270701	0.525669	-1.134298
5	6	0	-3.913289	0.405626	-0.883275
6	6	0	-3.473435	-0.166548	0.326928
7	1	0	-4.079509	-1.056230	2.201114
8	1	0	-6.503296	-0.831273	1.736014
9	1	0	-5.608581	0.963173	-2.070151
10	1	0	-3.176046	0.742481	-1.604766
11	6	0	-2.061117	-0.308683	0.624176
12	8	0	-1.167812	0.066251	-0.151110
13	1	0	-1.783699	-0.767498	1.583128
14	50	0	1.135838	0.015126	-0.030569
15	17	0	0.770679	-0.950253	2.126946
16	17	0	0.702243	-1.453000	-1.849298
17	17	0	0.692661	2.347181	-0.155764
18	6	0	3.271437	0.041638	-0.081164
19	6	0	3.976835	1.152809	0.400057
20	6	0	3.976939	-1.075726	-0.548467
21	6	0	5.373795	1.145185	0.411401
22	1	0	3.445603	2.031445	0.754792
23	6	0	5.373810	-1.078867	-0.535192
24	1	0	3.446192	-1.940674	-0.936146
25	6	0	6.072417	0.030241	-0.054888
26	1	0	5.914068	2.012501	0.781937
27	1	0	5.913960	-1.947308	-0.903204
28	1	0	7.159304	0.026681	-0.046281
29	6	0	-7.697721	0.253951	-0.471342
30	1	0	-8.305524	-0.378744	0.181369
31	1	0	-7.938848	0.009993	-1.511248
32	1	0	-8.007009	1.294508	-0.306110

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

NImag: 1 (-18.4)

1 imaginary frequencies ignored.

Zero-point correction= 0.233651 (Hartree/Particle)
Thermal correction to Energy= 0.254178
Thermal correction to Enthalpy= 0.255122
Thermal correction to Gibbs Free Energy= 0.178632
Sum of electronic and zero-point Energies= -2000.390711
Sum of electronic and thermal Energies= -2000.370184
Sum of electronic and thermal Enthalpies= -2000.369240
Sum of electronic and thermal Free Energies= -2000.445729

(4-methyl benzaldehyde)PhSnCl$_3$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	-2.604970	2.733091	1.043970
2	6	0	-3.078581	4.012288	0.764677
3	6	0	-2.693643	4.687716	-0.403245
4	6	0	-1.821460	4.033795	-1.282021
5	6	0	-1.344520	2.750364	-1.009735

6	6	0	-1.734031	2.086295	0.157353
7	1	0	-2.908700	2.236592	1.963286
8	1	0	-3.749491	4.499875	1.468405
9	1	0	-1.502734	4.537975	-2.191580
10	1	0	-0.651791	2.265188	-1.689067
11	6	0	-1.265293	0.685100	0.462383
12	8	0	-0.118647	0.293638	-0.341461
13	6	0	-3.177278	6.091465	-0.682910
14	1	0	-2.528572	6.835925	-0.202363
15	1	0	-4.191357	6.251343	-0.300323
16	1	0	-3.180809	6.308320	-1.756317
17	1	0	-1.049528	0.591818	1.531136
18	6	0	-2.223069	-0.457905	0.000165
19	6	0	-2.257896	-1.688218	0.747833
20	6	0	-3.292878	-0.236847	-0.942101
21	6	0	-3.172779	-2.679570	0.467321
22	1	0	-1.488887	-1.865525	1.496238
23	6	0	-4.199203	-1.224712	-1.227639
24	1	0	-3.341870	0.717345	-1.457047
25	6	0	-4.147900	-2.458911	-0.530051
26	1	0	-3.130115	-3.616147	1.009389
27	1	0	-4.978029	-1.089921	-1.970740
28	1	0	-1.199287	-0.696033	-0.712737
29	8	0	-5.070578	-3.353030	-0.889351
30	6	0	-5.097760	-4.641976	-0.261590
31	1	0	-4.155701	-5.174319	-0.428054
32	1	0	-5.915786	-5.178655	-0.741315
33	1	0	-5.294584	-4.549205	0.811553
34	50	0	1.604522	-0.485373	0.390731
35	17	0	0.957997	-2.334166	-1.180620
36	17	0	1.600845	1.444207	1.934548
37	17	0	1.163766	-1.955957	2.238084
38	6	0	3.541722	-0.153938	-0.443385
39	6	0	4.318228	0.931743	-0.010107
40	6	0	4.055882	-1.025231	-1.415626
41	6	0	5.587943	1.145318	-0.551560
42	1	0	3.935880	1.609601	0.745392
43	6	0	5.327847	-0.807341	-1.949695
44	1	0	3.465394	-1.867368	-1.760036
45	6	0	6.094249	0.277351	-1.520233
46	1	0	6.180425	1.991071	-0.212115
47	1	0	5.717445	-1.487722	-2.702611
48	1	0	7.083799	0.444908	-1.938167

Frequency Data:
NImag: 1 (-1035.7)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.365421 (Hartree/Particle)
Thermal correction to Energy= 0.393988
Thermal correction to Enthalpy= 0.394932

Thermal correction to Gibbs Free Energy= 0.300208
Sum of electronic and zero-point Energies= -2346.952815
Sum of electronic and thermal Energies= -2346.924249
Sum of electronic and thermal Enthalpies= -2346.923305
Sum of electronic and thermal Free Energies= -2347.018028

Anisyl(p-tolyl)methanol

Cartesian Coordinates (Angstroms):

1	6	0	3.811104	0.227436	-0.744497
2	6	0	3.951159	-0.997596	-0.086823
3	6	0	2.931676	-1.384587	0.796761
4	6	0	1.820758	-0.575202	1.009972
5	6	0	1.688117	0.652895	0.346963
6	6	0	2.698343	1.046474	-0.532262
7	6	0	0.467550	1.526191	0.611508
8	6	0	-0.845084	0.835818	0.271812
9	6	0	-1.796971	0.565411	1.253823
10	6	0	-3.014118	-0.054052	0.945612
11	6	0	-3.289439	-0.403059	-0.379512
12	6	0	-2.342585	-0.127711	-1.381427
13	6	0	-1.140546	0.480453	-1.056274
14	8	0	0.618891	2.735194	-0.137253
15	1	0	4.585493	0.552718	-1.436312
16	1	0	3.009703	-2.334615	1.321867
17	1	0	1.040050	-0.904758	1.692071
18	1	0	2.613240	1.996416	-1.047240
19	1	0	0.450071	1.761932	1.689532
20	1	0	-1.595154	0.841267	2.287082
21	1	0	-3.728767	-0.249031	1.737055
22	1	0	-2.577116	-0.406418	-2.404224
23	1	0	-0.411507	0.687637	-1.834682
24	1	0	-0.225208	3.208375	-0.079007
25	8	0	-4.437831	-1.006923	-0.803583
26	6	0	-5.427583	-1.319135	0.163116
27	1	0	-6.242190	-1.795927	-0.385119
28	1	0	-5.045497	-2.014534	0.922334
29	1	0	-5.805793	-0.416146	0.660820
30	6	0	5.160821	-1.876643	-0.305224
31	1	0	4.871288	-2.904346	-0.556467
32	1	0	5.788176	-1.497546	-1.118338
33	1	0	5.785497	-1.931353	0.596031

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.274856 (Hartree/Particle)
Thermal correction to Energy= 0.290819
Thermal correction to Enthalpy= 0.291763
Thermal correction to Gibbs Free Energy= 0.229030
Sum of electronic and zero-point Energies= -731.388370
Sum of electronic and thermal Energies= -731.372408
Sum of electronic and thermal Enthalpies= -731.371463
Sum of electronic and thermal Free Energies= -731.434196

(4-methyl benzaldehyde)$AlCl_3$ intermediate

Cartesian Coordinates (Angstroms):

1	6	0	-2.690336	1.387809	-0.001127
2	6	0	-4.053745	1.125095	-0.002453
3	6	0	-4.528721	-0.196505	-0.003099
4	6	0	-3.597517	-1.256693	-0.004442
5	6	0	-2.236629	-1.010011	-0.003069
6	6	0	-1.767482	0.323048	-0.001303
7	1	0	-2.329768	2.413368	-0.001002
8	1	0	-4.762869	1.947728	-0.003376
9	1	0	-3.959388	-2.281348	-0.007102
10	1	0	-1.518409	-1.823345	-0.004378
11	6	0	-0.364996	0.625378	-0.000632
12	8	0	0.522957	-0.261475	-0.000948
13	1	0	-0.054429	1.678178	0.000443
14	17	0	2.656729	2.101067	0.001436
15	17	0	3.008550	-1.056274	1.844727
16	17	0	3.011315	-1.055035	-1.843560
17	13	0	2.429912	-0.076275	0.000462
18	6	0	-6.006230	-0.489428	0.005631
19	1	0	-6.297999	-0.981698	0.942073
20	1	0	-6.601097	0.422238	-0.095955
21	1	0	-6.276717	-1.169795	-0.810406

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.144816 (Hartree/Particle)
Thermal correction to Energy= 0.159775
Thermal correction to Enthalpy= 0.160719
Thermal correction to Gibbs Free Energy= 0.098498
Sum of electronic and zero-point Energies= -1767.545031
Sum of electronic and thermal Energies= -1767.530072
Sum of electronic and thermal Enthalpies= -1767.529128
Sum of electronic and thermal Free Energies= -1767.591349

(4-methyl benzaldehyde)$InCl_3$ intermediate

Cartesian Coordinates (Angstroms):

1	6	0	-3.334791	1.356577	-0.001536
2	6	0	-4.700900	1.103170	-0.002491
3	6	0	-5.185388	-0.214346	-0.002969
4	6	0	-4.261191	-1.279942	-0.004495
5	6	0	-2.898188	-1.041525	-0.003433
6	6	0	-2.419944	0.286857	-0.001850
7	1	0	-2.967701	2.379945	-0.001571

8	1	0	-5.404062	1.931049	-0.003251
9	1	0	-4.629374	-2.302463	-0.007029
10	1	0	-2.185430	-1.859744	-0.004874
11	6	0	-1.008816	0.577792	-0.001494
12	8	0	-0.128581	-0.309622	-0.001766
13	1	0	-0.700689	1.633183	-0.000741
14	17	0	2.017589	2.300376	-0.002751
15	17	0	2.600926	-1.065776	1.993032
16	17	0	2.606306	-1.071876	-1.987381
17	6	0	-6.665346	-0.497389	0.006039
18	1	0	-6.961121	-0.988194	0.941956
19	1	0	-7.253678	0.418708	-0.094614
20	1	0	-6.941363	-1.174506	-0.810862
21	49	0	2.001990	-0.042336	0.000391

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.142922 (Hartree/Particle)
Thermal correction to Energy= 0.158851
Thermal correction to Enthalpy= 0.159795
Thermal correction to Gibbs Free Energy= 0.093942
Sum of electronic and zero-point Energies= -1767.405672
Sum of electronic and thermal Energies= -1767.389744
Sum of electronic and thermal Enthalpies= -1767.388799
Sum of electronic and thermal Free Energies= -1767.454652

(4-methyl benzaldehyde)$ZnCl_2$ intermediate

Cartesian Coordinates (Angstroms):

1	6	0	-2.776687	0.053015	1.414978
2	6	0	-4.142264	0.037614	1.158130
3	6	0	-4.623385	-0.016904	-0.159707
4	6	0	-3.695492	-0.061608	-1.218932
5	6	0	-2.331787	-0.046828	-0.974992
6	6	0	-1.858292	0.011153	0.351055
7	1	0	-2.414071	0.093966	2.439415
8	1	0	-4.847628	0.066538	1.984012
9	1	0	-4.059033	-0.110008	-2.241982
10	1	0	-1.615908	-0.082444	-1.789791
11	6	0	-0.438652	0.024953	0.641463
12	8	0	0.445354	-0.010963	-0.226640
13	1	0	-0.157680	0.071617	1.707200
14	17	0	3.192412	2.104321	-0.040631
15	17	0	3.210477	-2.098668	0.028750
16	30	0	2.532733	-0.001877	-0.104675
17	6	0	-6.103912	-0.004458	-0.442317
18	1	0	-6.442408	1.012879	-0.680141
19	1	0	-6.352403	-0.636330	-1.301310
20	1	0	-6.682001	-0.349932	0.419889

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.141365 (Hartree/Particle)
Thermal correction to Energy= 0.154660
Thermal correction to Enthalpy= 0.155605
Thermal correction to Gibbs Free Energy= 0.096835
Sum of electronic and zero-point Energies= -1370.854698
Sum of electronic and thermal Energies= -1370.841403
Sum of electronic and thermal Enthalpies= -1370.840459
Sum of electronic and thermal Free Energies= -1370.899229

(4-methyl benzaldehyde)BF_3 intermediate

Cartesian Coordinates (Angstroms):

1	6	0	-1.564670	1.370664	-0.001357
2	6	0	-2.941519	1.177510	-0.002223
3	6	0	-3.483513	-0.116575	-0.002473
4	6	0	-2.606143	-1.220078	-0.003746
5	6	0	-1.233257	-1.040551	-0.002695
6	6	0	-0.697420	0.264265	-0.001361
7	1	0	-1.153722	2.377215	-0.001549
8	1	0	-3.607242	2.035989	-0.003020
9	1	0	-3.017368	-2.226236	-0.005958
10	1	0	-0.555859	-1.888371	-0.003803
11	6	0	0.728416	0.493877	-0.000788
12	8	0	1.561493	-0.432304	-0.000623
13	1	0	1.097430	1.525765	-0.000233
14	5	0	3.235831	-0.079304	0.001023
15	9	0	3.652991	-0.673057	-1.163952
16	9	0	3.650231	-0.670935	1.168101
17	9	0	3.285850	1.307294	-0.000138
18	6	0	-4.975076	-0.334948	0.005621
19	1	0	-5.282291	-0.986841	-0.820728
20	1	0	-5.522350	0.607773	-0.081583
21	1	0	-5.292257	-0.825056	0.934773

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.152512 (Hartree/Particle)
Thermal correction to Energy= 0.165053
Thermal correction to Enthalpy= 0.165997
Thermal correction to Gibbs Free Energy= 0.111418
Sum of electronic and zero-point Energies= -709.272029
Sum of electronic and thermal Energies= -709.259488
Sum of electronic and thermal Enthalpies= -709.258544
Sum of electronic and thermal Free Energies= -709.313123

(4-methyl benzaldehyde)$TiCl_4$ intermediate

Cartesian Coordinates (Angstroms):

1	6	0	3.330919	1.441768	0.000606
2	6	0	4.687046	1.134322	0.002666
3	6	0	5.118886	-0.200486	0.003547

4	6	0	4.152244	-1.226223	0.004826
5	6	0	2.798658	-0.932420	0.002906
6	6	0	2.374353	0.412105	0.000623
7	1	0	3.005407	2.479328	0.000382
8	1	0	5.422312	1.934129	0.004071
9	1	0	4.478084	-2.263240	0.008034
10	1	0	2.052824	-1.720806	0.004434
11	6	0	0.966698	0.759773	-0.000267
12	8	0	0.054557	-0.076956	0.000690
13	1	0	0.707492	1.830396	-0.002144
14	17	0	-1.925911	2.145531	-0.005080
15	17	0	-4.353152	-0.082013	-0.001264
16	17	0	-1.856375	-1.136233	-1.903515
17	17	0	-1.858094	-1.127408	1.908227
18	22	0	-2.146552	-0.063692	-0.000231
19	6	0	6.587376	-0.542163	-0.006332
20	1	0	6.834423	-1.246834	0.796306
21	1	0	6.869567	-1.022134	-0.952104
22	1	0	7.210554	0.348102	0.116876

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.145422 (Hartree/Particle)
Thermal correction to Energy= 0.162360
Thermal correction to Enthalpy= 0.163304
Thermal correction to Gibbs Free Energy= 0.096378
Sum of electronic and zero-point Energies= -2283.870707
Sum of electronic and thermal Energies= -2283.853770
Sum of electronic and thermal Enthalpies= -2283.852825
Sum of electronic and thermal Free Energies= -2283.919751

(4-methyl benzaldehyde)$SiCl_4$ intermediate

Cartesian Coordinates (Angstroms):

1	6	0	3.599195	1.407612	-0.001115
2	6	0	4.967949	1.145196	-0.001361
3	6	0	5.445093	-0.172307	-0.001718
4	6	0	4.511477	-1.225940	-0.003799
5	6	0	3.147464	-0.972238	-0.003476
6	6	0	2.678396	0.352578	-0.002010
7	1	0	3.240327	2.434864	-0.001372
8	1	0	5.676408	1.969699	-0.001643
9	1	0	4.869089	-2.253104	-0.006217
10	1	0	2.422569	-1.780543	-0.005469
11	6	0	1.232673	0.636043	-0.002572
12	8	0	0.360036	-0.217183	-0.003558
13	1	0	0.962410	1.713254	-0.001800
14	17	0	-2.158013	1.936990	-0.006964
15	17	0	-4.938669	0.035447	0.003480
16	17	0	-2.258065	-1.060014	-1.727403
17	17	0	-2.253026	-1.048308	1.733849

18	14	0	-2.836695	-0.044285	0.000632
19	6	0	6.925958	-0.465609	0.007475
20	1	0	7.224067	-0.962077	0.939744
21	1	0	7.203276	-1.136012	-0.814872
22	1	0	7.518195	0.449412	-0.087668

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.145238 (Hartree/Particle)
Thermal correction to Energy= 0.162371
Thermal correction to Enthalpy= 0.163315
Thermal correction to Gibbs Free Energy= 0.093194
Sum of electronic and zero-point Energies= -2229.526284
Sum of electronic and thermal Energies= -2229.509150
Sum of electronic and thermal Enthalpies= -2229.508206
Sum of electronic and thermal Free Energies= -2229.578328

(4-methyl benzaldehyde)$AlCl_3$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	-1.623310	-2.246624	1.275112
2	6	0	-2.573614	-3.250360	1.109844
3	6	0	-3.357961	-3.320338	-0.052008
4	6	0	-3.151577	-2.352803	-1.042632
5	6	0	-2.197502	-1.345570	-0.886449
6	6	0	-1.422366	-1.283980	0.275758
7	1	0	-1.037253	-2.207715	2.191444
8	1	0	-2.718055	-3.985473	1.898405
9	1	0	-3.751896	-2.379635	-1.949038
10	1	0	-2.066097	-0.588014	-1.651433
11	6	0	-0.371522	-0.218291	0.464604
12	8	0	-0.509687	0.876411	-0.472531
13	6	0	-4.417228	-4.385911	-0.208940
14	1	0	-4.645153	-4.572032	-1.263510
15	1	0	-5.353925	-4.085623	0.279143
16	1	0	-4.105630	-5.333317	0.244570
17	1	0	-0.381741	0.143905	1.498410
18	6	0	1.087053	-0.628365	0.082279
19	6	0	2.184596	-0.014293	0.786562
20	6	0	1.385095	-1.803611	-0.699662
21	6	0	3.484502	-0.432651	0.603529
22	1	0	1.969328	0.846861	1.416047
23	6	0	2.678270	-2.215106	-0.889978
24	1	0	0.564300	-2.335667	-1.170432
25	6	0	3.742947	-1.536296	-0.241456
26	1	0	4.292093	0.084116	1.107542
27	1	0	2.922557	-3.068126	-1.514174
28	1	0	0.844264	0.292880	-0.745730
29	8	0	4.958709	-2.019680	-0.494152
30	6	0	6.112057	-1.414396	0.107631
31	1	0	6.204996	-0.367468	-0.198562

32	1	0	6.962570	-1.985007	-0.263921
33	1	0	6.064715	-1.487065	1.198931
34	17	0	-2.909379	3.104501	-0.036394
35	17	0	0.176364	2.898283	1.907584
36	17	0	0.346751	3.675154	-1.654967
37	13	0	-0.780571	2.641550	-0.086551

Frequency Data:
NImag: 1 (-1023)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.276104 (Hartree/Particle)
Thermal correction to Energy= 0.298520
Thermal correction to Enthalpy= 0.299464
Thermal correction to Gibbs Free Energy= 0.219313
Sum of electronic and zero-point Energies= -2114.113358
Sum of electronic and thermal Energies= -2114.090943
Sum of electronic and thermal Enthalpies= -2114.089999
Sum of electronic and thermal Free Energies= -2114.170149

(4-methyl benzaldehyde)$InCl_3$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	-1.875349	2.545098	1.256631
2	6	0	-2.418410	3.818285	1.104975
3	6	0	-2.180113	4.573314	-0.053690
4	6	0	-1.383469	4.004975	-1.055287
5	6	0	-0.838420	2.727824	-0.911844
6	6	0	-1.081505	1.983255	0.247003
7	1	0	-2.066023	1.985143	2.170324
8	1	0	-3.028644	4.238547	1.901269
9	1	0	-1.177732	4.572481	-1.960058
10	1	0	-0.202818	2.308501	-1.684374
11	6	0	-0.518705	0.592048	0.416243
12	8	0	0.531643	0.298734	-0.527065
13	6	0	-2.735958	5.970810	-0.197412
14	1	0	-3.699220	6.075308	0.313611
15	1	0	-2.877683	6.239715	-1.249428
16	1	0	-2.054739	6.713320	0.239121
17	1	0	-0.184269	0.449295	1.450772
18	6	0	-1.490235	-0.574204	0.037505
19	6	0	-1.376392	-1.824633	0.750551
20	6	0	-2.700612	-0.365917	-0.724429
21	6	0	-2.296134	-2.836102	0.588753
22	1	0	-0.498617	-1.978585	1.375561
23	6	0	-3.610869	-1.374982	-0.895364
24	1	0	-2.854509	0.598531	-1.198432
25	6	0	-3.420872	-2.621264	-0.241800
26	1	0	-2.152887	-3.781015	1.098529
27	1	0	-4.498983	-1.249763	-1.505724
28	1	0	-0.585866	-0.724226	-0.804542

29	8	0	-4.365485	-3.530856	-0.473570
30	6	0	-4.280458	-4.827571	0.135871
31	1	0	-3.368324	-5.344337	-0.179029
32	1	0	-5.155241	-5.370120	-0.220961
33	1	0	-4.313221	-4.746616	1.227023
34	49	0	2.377093	-0.394536	-0.052530
35	17	0	3.982955	1.283236	-0.236185
36	17	0	2.028057	-1.168263	2.174883
37	17	0	2.586456	-2.205712	-1.535219

Frequency Data:

NImag: 1 (-912.9)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.274311 (Hartree/Particle)
Thermal correction to Energy= 0.297660
Thermal correction to Enthalpy= 0.298604
Thermal correction to Gibbs Free Energy= 0.215061
Sum of electronic and zero-point Energies= -2113.969405
Sum of electronic and thermal Energies= -2113.946055
Sum of electronic and thermal Enthalpies= -2113.945111
Sum of electronic and thermal Free Energies= -2114.028654

(4-methyl benzaldehyde)$ZnCl_2$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	0.568018	2.643197	1.318736
2	6	0	1.052109	3.947538	1.259005
3	6	0	1.819647	4.385447	0.168171
4	6	0	2.079891	3.471585	-0.860143
5	6	0	1.595330	2.163022	-0.807343
6	6	0	0.831568	1.735299	0.283341
7	1	0	-0.015640	2.325699	2.181173
8	1	0	0.840335	4.636053	2.074297
9	1	0	2.677685	3.784671	-1.713348
10	1	0	1.820182	1.452273	-1.595474
11	6	0	0.292293	0.321555	0.341760
12	8	0	0.921583	-0.549118	-0.596576
13	6	0	2.376003	5.789698	0.125967
14	1	0	2.584396	6.107454	-0.900975
15	1	0	3.317999	5.859435	0.686194
16	1	0	1.681938	6.511454	0.570931
17	1	0	0.364940	-0.052731	1.372658
18	6	0	-1.202319	0.173116	-0.117490
19	6	0	-2.013179	-0.837204	0.529363
20	6	0	-1.912304	1.218253	-0.827858
21	6	0	-3.376243	-0.896259	0.350531
22	1	0	-1.497774	-1.598955	1.114375
23	6	0	-3.265693	1.152872	-1.017901
24	1	0	-1.337887	2.038627	-1.247167
25	6	0	-4.014326	0.097841	-0.429018

26	1	0	-3.947725	-1.692821	0.811725
27	1	0	-3.804580	1.901739	-1.588851
28	1	0	-0.648692	-0.491198	-0.968742
29	8	0	-5.323046	0.135132	-0.669209
30	6	0	-6.186880	-0.869158	-0.116189
31	1	0	-5.911676	-1.862588	-0.484322
32	1	0	-7.186611	-0.609882	-0.462969
33	1	0	-6.155742	-0.848531	0.977706
34	30	0	1.757655	-2.231173	-0.039409
35	17	0	0.660199	-2.944283	1.833998
36	17	0	3.330236	-3.184801	-1.288365

Frequency Data:
NImag: 1 (-673.07)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.273407 (Hartree/Particle)
Thermal correction to Energy= 0.294735
Thermal correction to Enthalpy= 0.295679
Thermal correction to Gibbs Free Energy= 0.218444
Sum of electronic and zero-point Energies= -1717.413043
Sum of electronic and thermal Energies= -1717.391715
Sum of electronic and thermal Enthalpies= -1717.390771
Sum of electronic and thermal Free Energies= -1717.468006

(4-methyl benzaldehyde)BF_3(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	-1.941033	-1.179522	1.201640
2	6	0	-3.061156	-1.999974	1.100755
3	6	0	-3.966960	-1.859788	0.037515
4	6	0	-3.706185	-0.872551	-0.919648
5	6	0	-2.583060	-0.047584	-0.826214
6	6	0	-1.687679	-0.194364	0.236697
7	1	0	-1.259936	-1.303747	2.041809
8	1	0	-3.241658	-2.756602	1.861343
9	1	0	-4.395093	-0.739744	-1.750910
10	1	0	-2.399716	0.729755	-1.559694
11	6	0	-0.466723	0.687023	0.352240
12	8	0	-0.452130	1.732668	-0.639773
13	9	0	-0.239623	4.014344	-1.146600
14	9	0	1.077477	3.128319	0.561131
15	9	0	-1.197320	3.391010	0.899523
16	5	0	-0.210879	3.144070	-0.066201
17	6	0	-5.201728	-2.726607	-0.048434
18	1	0	-5.560239	-2.812792	-1.079541
19	1	0	-6.022903	-2.306429	0.547623
20	1	0	-5.011746	-3.736946	0.330734
21	1	0	-0.404273	1.111320	1.358553
22	6	0	0.890447	-0.004009	-0.005836
23	6	0	2.087569	0.403463	0.690066

24	6	0	0.950051	-1.254552	-0.729097
25	6	0	3.271703	-0.288916	0.557535
26	1	0	2.046455	1.333416	1.247584
27	6	0	2.129373	-1.936033	-0.870926
28	1	0	0.042388	-1.628344	-1.192589
29	6	0	3.302744	-1.464530	-0.225140
30	1	0	4.164546	0.072851	1.052985
31	1	0	2.198394	-2.851796	-1.448638
32	1	0	0.842775	0.888812	-0.862747
33	8	0	4.392558	-2.208282	-0.421338
34	6	0	5.634278	-1.834908	0.190424
35	1	0	5.958001	-0.848315	-0.156855
36	1	0	6.350864	-2.591654	-0.127641
37	1	0	5.548474	-1.841166	1.281930

Frequency Data:
NImag: 1 (-840.7)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.284108 (Hartree/Particle)
Thermal correction to Energy= 0.303901
Thermal correction to Enthalpy= 0.304846
Thermal correction to Gibbs Free Energy= 0.232758
Sum of electronic and zero-point Energies= -1055.833332
Sum of electronic and thermal Energies= -1055.813538
Sum of electronic and thermal Enthalpies= -1055.812594
Sum of electronic and thermal Free Energies= -1055.884681

(4-methyl benzaldehyde)$TiCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	0.486554	3.085152	-1.313003
2	6	0	0.449097	4.455828	-1.067424
3	6	0	0.041473	4.957054	0.177172
4	6	0	-0.322115	4.036800	1.169509
5	6	0	-0.283385	2.662570	0.933146
6	6	0	0.123875	2.173031	-0.313932
7	1	0	0.791922	2.722481	-2.292216
8	1	0	0.729022	5.148414	-1.857730
9	1	0	-0.649661	4.399918	2.140906
10	1	0	-0.591227	1.966258	1.706867
11	6	0	0.213410	0.695284	-0.591281
12	8	0	-0.632436	-0.090198	0.290532
13	6	0	-0.040347	6.444492	0.427697
14	1	0	0.162038	6.686811	1.476441
15	1	0	-1.042105	6.828321	0.193471
16	1	0	0.672896	6.996680	-0.193348
17	1	0	-0.030656	0.488201	-1.636385
18	6	0	1.555636	0.006604	-0.185346
19	6	0	1.926776	-1.209922	-0.862331

20	6	0	2.584205	0.671012	0.574592
21	6	0	3.158145	-1.797791	-0.673284
22	1	0	1.181332	-1.708180	-1.477016
23	6	0	3.808435	0.084949	0.769161
24	1	0	2.358585	1.631824	1.026029
25	6	0	4.110302	-1.155840	0.151120
26	1	0	3.383516	-2.741338	-1.154791
27	1	0	4.575833	0.552000	1.377289
28	1	0	0.735084	-0.498741	0.652963
29	8	0	5.326108	-1.637282	0.408115
30	6	0	5.735613	-2.891121	-0.156565
31	1	0	5.078683	-3.700133	0.178784
32	1	0	6.746088	-3.057302	0.215325
33	1	0	5.746646	-2.840445	-1.250161
34	17	0	-1.296450	-2.169356	2.077111
35	17	0	-2.587176	-0.096351	-1.815907
36	17	0	-1.530204	-3.148271	-1.095147
37	17	0	-4.168217	-1.236692	0.807269
38	22	0	-2.081301	-1.331915	0.069203

Frequency Data:

NImag: 1 (-1189.06)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.276644 (Hartree/Particle)
Thermal correction to Energy= 0.301063
Thermal correction to Enthalpy= 0.302007
Thermal correction to Gibbs Free Energy= 0.216936
Sum of electronic and zero-point Energies= -2630.429081
Sum of electronic and thermal Energies= -2630.404663
Sum of electronic and thermal Enthalpies= -2630.403719
Sum of electronic and thermal Free Energies= -2630.488789

(4-methyl benzaldehyde)$SiCl_4$(anisole) TS

Cartesian Coordinates (Angstroms):

1	6	0	-1.911652	-2.284960	1.271623
2	6	0	-2.926425	-3.213630	1.055455
3	6	0	-3.614442	-3.262609	-0.165871
4	6	0	-3.245836	-2.352230	-1.164300
5	6	0	-2.227643	-1.420777	-0.957612
6	6	0	-1.549932	-1.380402	0.265207
7	1	0	-1.403046	-2.258846	2.233005
8	1	0	-3.197182	-3.904011	1.850867
9	1	0	-3.769281	-2.363647	-2.117390
10	1	0	-1.974472	-0.706752	-1.734141
11	6	0	-0.416391	-0.423126	0.514487
12	8	0	-0.400340	0.692839	-0.449086
13	6	0	-4.744074	-4.242056	-0.381815
14	1	0	-4.855885	-4.498826	-1.440439
15	1	0	-5.700551	-3.819560	-0.046583

16	1	0	-4.584948	-5.169479	0.178774
17	1	0	-0.452531	-0.039468	1.535767
18	6	0	1.011465	-0.940764	0.163982
19	6	0	2.140216	-0.422132	0.886716
20	6	0	1.229301	-2.115294	-0.638300
21	6	0	3.408866	-0.931407	0.707196
22	1	0	1.994097	0.444511	1.526493
23	6	0	2.491277	-2.620627	-0.821873
24	1	0	0.378412	-2.575572	-1.130156
25	6	0	3.596229	-2.034062	-0.154939
26	1	0	4.246036	-0.478822	1.224009
27	1	0	2.675921	-3.477269	-1.461261
28	1	0	0.873408	0.041623	-0.678316
29	8	0	4.778191	-2.598754	-0.408060
30	6	0	5.965684	-2.076047	0.202453
31	1	0	6.123459	-1.031908	-0.086653
32	1	0	6.779999	-2.691817	-0.178235
33	1	0	5.914327	-2.163060	1.292795
34	17	0	1.334770	2.504624	-1.541192
35	17	0	-2.203733	2.018917	1.303099
36	17	0	0.813104	3.048161	1.577078
37	17	0	-1.536206	3.862963	-1.207881
38	14	0	-0.446096	2.419406	-0.073900

Frequency Data:

NImag: 1 (-1205.9)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.277713 (Hartree/Particle)

Thermal correction to Energy= 0.301540

Thermal correction to Enthalpy= 0.302484

Thermal correction to Gibbs Free Energy= 0.219904

Sum of electronic and zero-point Energies= -2576.077579

Sum of electronic and thermal Energies= -2576.053752

Sum of electronic and thermal Enthalpies= -2576.052807

Sum of electronic and thermal Free Energies= -2576.135387

Indole

Cartesian Coordinates (Angstroms):

1	6	0	-0.250096	0.752240	0.000021
2	6	0	-0.247903	-0.671857	-0.000055
3	6	0	0.935090	-1.418800	0.000028
4	6	0	2.135894	-0.718715	0.000189
5	6	0	2.159313	0.691541	0.000264
6	6	0	0.982620	1.428929	0.000181
7	6	0	-1.626152	1.166958	-0.000074
8	6	0	-2.390290	0.030290	-0.000314
9	1	0	0.918176	-2.505834	-0.000028
10	1	0	3.073081	-1.268680	0.000262
11	1	0	3.116223	1.206538	0.000393
12	1	0	1.012000	2.515704	0.000247

13	1	0	-1.998732	2.182179	-0.000038
14	1	0	-3.465109	-0.087534	-0.000484
15	1	0	-1.880874	-2.038521	-0.000233
16	7	0	-1.566517	-1.081052	-0.000222

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.129921 (Hartree/Particle)
Thermal correction to Energy= 0.136251
Thermal correction to Enthalpy= 0.137195
Thermal correction to Gibbs Free Energy= 0.099581
Sum of electronic and zero-point Energies= -363.686767
Sum of electronic and thermal Energies= -363.680437
Sum of electronic and thermal Enthalpies= -363.679493
Sum of electronic and thermal Free Energies= -363.717107

Furan

Cartesian Coordinates (Angstroms):

1	6	0	1.095015	-0.347435	0.000511
2	6	0	0.717911	0.959937	-0.000290
3	6	0	-0.718022	0.959859	0.000057
4	6	0	-1.094973	-0.347556	0.000276
5	8	0	0.000065	-1.160967	-0.000523
6	1	0	2.050269	-0.849915	0.000841
7	1	0	1.373597	1.819547	-0.000523
8	1	0	-1.373804	1.819397	0.000095
9	1	0	-2.050176	-0.850134	0.000448

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.070197 (Hartree/Particle)
Thermal correction to Energy= 0.073913
Thermal correction to Enthalpy= 0.074857
Thermal correction to Gibbs Free Energy= 0.043924
Sum of electronic and zero-point Energies= -229.950385
Sum of electronic and thermal Energies= -229.946669
Sum of electronic and thermal Enthalpies= -229.945724
Sum of electronic and thermal Free Energies= -229.976657

Thiophene

Cartesian Coordinates (Angstroms):

1	6	0	0.011594	-1.243610	0.000036
2	6	0	1.272654	-0.715016	0.000117
3	6	0	1.272605	0.715088	0.000052
4	6	0	0.011502	1.243588	-0.000035
5	1	0	-0.280797	-2.285009	0.000045
6	1	0	2.172904	-1.320175	0.000202
7	1	0	2.172811	1.320311	0.000088
8	1	0	-0.280936	2.284975	-0.000083
9	16	0	-1.199632	-0.000025	-0.000080

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.066886 (Hartree/Particle)
Thermal correction to Energy= 0.070962
Thermal correction to Enthalpy= 0.071906
Thermal correction to Gibbs Free Energy= 0.039646
Sum of electronic and zero-point Energies= -552.935742
Sum of electronic and thermal Energies= -552.931666
Sum of electronic and thermal Enthalpies= -552.930722
Sum of electronic and thermal Free Energies= -552.962983

Toluene

Cartesian Coordinates (Angstroms):

1	6	0	-1.201444	1.205289	0.002199
2	6	0	0.194129	1.202402	-0.008985
3	6	0	0.913896	0.000222	-0.011390
4	6	0	0.194385	-1.202271	-0.008983
5	6	0	-1.201060	-1.205493	0.002198
6	6	0	-1.905116	-0.000141	0.008471
7	1	0	-1.739014	2.150176	0.001555
8	1	0	0.734218	2.146899	-0.017836
9	1	0	0.734728	-2.146640	-0.017849
10	1	0	-1.738458	-2.150479	0.001552
11	1	0	-2.991869	-0.000325	0.013921
12	6	0	2.425551	0.000097	0.009375
13	1	0	2.809992	-0.012910	1.038355
14	1	0	2.834300	-0.879700	-0.499566
15	1	0	2.834049	0.892351	-0.477447

Frequency Data:
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.128330 (Hartree/Particle)
Thermal correction to Energy= 0.134525
Thermal correction to Enthalpy= 0.135469
Thermal correction to Gibbs Free Energy= 0.097789
Sum of electronic and zero-point Energies= -271.438320
Sum of electronic and thermal Energies= -271.432125
Sum of electronic and thermal Enthalpies= -271.431181
Sum of electronic and thermal Free Energies= -271.468861

Benzene

Cartesian Coordinates (Angstroms):

1	6	0	1.062830	-0.905897	-0.000005
2	6	0	-0.253256	-1.373251	-0.000068
3	6	0	-1.315989	-0.467462	0.000055
4	6	0	-1.062753	0.905985	-0.000008
5	6	0	0.253140	1.373269	-0.000061
6	6	0	1.316029	0.467357	0.000057
7	1	0	1.889716	-1.610996	0.000066
8	1	0	-0.450131	-2.441986	-0.000077

9	1	0	-2.340030	-0.831097	0.000153
10	1	0	-1.889811	1.610872	-0.000007
11	1	0	0.450262	2.441951	-0.000019
12	1	0	2.339987	0.831246	0.000064

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.100768 (Hartree/Particle)
Thermal correction to Energy= 0.105157
Thermal correction to Enthalpy= 0.106101
Thermal correction to Gibbs Free Energy= 0.073305
Sum of electronic and zero-point Energies= -232.147884
Sum of electronic and thermal Energies= -232.143495
Sum of electronic and thermal Enthalpies= -232.142551
Sum of electronic and thermal Free Energies= -232.175347

Chloro benzene

Cartesian Coordinates (Angstroms):

1	6	0	-1.574431	1.207479	-0.000002
2	6	0	-0.178534	1.216120	-0.000005
3	6	0	0.503667	0.000014	0.000013
4	6	0	-0.178529	-1.216115	0.000005
5	6	0	-1.574407	-1.207495	-0.000011
6	6	0	-2.274914	-0.000002	0.000006
7	1	0	-2.112365	2.151552	-0.000004
8	1	0	0.374577	2.149415	-0.000002
9	1	0	0.374622	-2.149387	0.000009
10	1	0	-2.112359	-2.151557	-0.000015
11	1	0	-3.361070	-0.000024	0.000013
12	17	0	2.264676	0.000000	-0.000002

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.091222 (Hartree/Particle)
Thermal correction to Energy= 0.096717
Thermal correction to Enthalpy= 0.097662
Thermal correction to Gibbs Free Energy= 0.061441
Sum of electronic and zero-point Energies= -691.753753
Sum of electronic and thermal Energies= -691.748257
Sum of electronic and thermal Enthalpies= -691.747313
Sum of electronic and thermal Free Energies= -691.783533

cyano benzene

Cartesian Coordinates (Angstroms):

1	6	0	-1.483966	-1.210933	0.000001
2	6	0	-0.091452	-1.217468	0.000001
3	6	0	0.610245	-0.000001	0.000003
4	6	0	-0.091452	1.217468	0.000002
5	6	0	-1.483966	1.210933	0.000000

6	6	0	-2.180551	-0.000001	0.000001
7	1	0	-2.026187	-2.151985	0.000000
8	1	0	0.458899	-2.152775	0.000001
9	1	0	0.458900	2.152775	0.000002
10	1	0	-2.026188	2.151984	-0.000001
11	1	0	-3.266968	0.000001	0.000001
12	6	0	2.044973	0.000001	0.000002
13	7	0	3.208365	0.000000	-0.000008

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.099441 (Hartree/Particle)
Thermal correction to Energy= 0.105544
Thermal correction to Enthalpy= 0.106488
Thermal correction to Gibbs Free Energy= 0.069163
Sum of electronic and zero-point Energies= -324.392775
Sum of electronic and thermal Energies= -324.386672
Sum of electronic and thermal Enthalpies= -324.385728
Sum of electronic and thermal Free Energies= -324.423053

(4-methyl benzaldehyde)$AlCl_3$(Indole) TS

Cartesian Coordinates (Angstroms):

1	6	0	1.592636	1.766251	-1.440978
2	6	0	2.438552	2.861162	-1.282430
3	6	0	2.461212	3.589841	-0.083992
4	6	0	1.610060	3.179525	0.950212
5	6	0	0.761757	2.081129	0.800504
6	6	0	0.749888	1.361418	-0.397872
7	1	0	1.588900	1.223285	-2.384027
8	1	0	3.085504	3.160599	-2.103748
9	1	0	1.602409	3.732467	1.886645
10	1	0	0.096605	1.785237	1.604204
11	6	0	-0.142742	0.159967	-0.588088
12	8	0	-1.142537	0.024168	0.467679
13	1	0	-0.627347	0.201725	-1.569341
14	1	0	-0.397568	-1.154618	0.562153
15	6	0	0.521534	-1.221492	-0.385191
16	6	0	1.870414	-1.587353	0.092880
17	6	0	2.057074	-2.950685	-0.221667
18	1	0	0.749028	-4.334153	-1.218816
19	17	0	-3.748220	-0.954061	1.988900
20	17	0	-3.634268	2.102231	-0.083856
21	17	0	-3.230713	-1.171623	-1.624213
22	6	0	3.348983	4.802427	0.071027
23	1	0	2.842709	5.709544	-0.284848
24	1	0	3.618187	4.971327	1.118955
25	1	0	4.274378	4.700246	-0.506114
26	6	0	3.196071	-3.672951	0.129115
27	6	0	2.885277	-0.911595	0.781299
28	6	0	4.036860	-1.616356	1.125784

29	6	0	4.191503	-2.977882	0.810027
30	1	0	2.777672	0.135047	1.039831
31	6	0	0.040560	-2.384473	-1.058431
32	7	0	0.915863	-3.381308	-0.919495
33	1	0	-0.915114	-2.508624	-1.555772
34	1	0	5.100066	-3.496110	1.101104
35	1	0	4.834403	-1.102072	1.653650
36	1	0	3.304467	-4.725126	-0.117069
37	13	0	-2.961420	0.054010	0.221608

Frequency Data:

NImag: 1 (-1391.1)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.273253 (Hartree/Particle)
Thermal correction to Energy= 0.294836
Thermal correction to Enthalpy= 0.295780
Thermal correction to Gibbs Free Energy= 0.217859
Sum of electronic and zero-point Energies= -2131.174631
Sum of electronic and thermal Energies= -2131.153048
Sum of electronic and thermal Enthalpies= -2131.152104
Sum of electronic and thermal Free Energies= -2131.230025

(4-methyl benzaldehyde)$AlCl_3$(Furan) TS

Cartesian Coordinates (Angstroms):

1	6	0	2.666142	0.230956	1.172532
2	6	0	3.963973	-0.250569	1.029354
3	6	0	4.320298	-1.059251	-0.061866
4	6	0	3.331863	-1.363241	-1.005589
5	6	0	2.028641	-0.881040	-0.873164
6	6	0	1.686337	-0.077897	0.218929
7	1	0	2.411729	0.842935	2.035723
8	1	0	4.710945	-0.006511	1.781152
9	1	0	3.580246	-1.994997	-1.855043
10	1	0	1.265955	-1.146896	-1.597074
11	6	0	0.289361	0.467630	0.375806
12	8	0	-0.667095	-0.190885	-0.495055
13	1	0	-0.036178	0.440480	1.421544
14	1	0	-0.712034	1.205160	-0.898168
15	6	0	0.076236	1.894161	-0.172952
16	6	0	0.861961	2.725976	-1.016142
17	6	0	0.451738	4.043662	-0.821040
18	1	0	1.599101	2.356831	-1.717207
19	6	0	-0.501916	3.991497	0.187998
20	1	0	0.787700	4.930468	-1.338964
21	1	0	-1.104209	4.765156	0.646727
22	8	0	-0.712626	2.761072	0.614721
23	13	0	-2.239550	-1.017303	-0.003500
24	17	0	-3.747464	0.462246	-0.633569
25	17	0	-2.368931	-2.909857	-1.069103

26	17	0	-2.117416	-1.203824	2.184899
27	6	0	5.719190	-1.614436	-0.189463
28	1	0	5.957448	-1.866136	-1.227882
29	1	0	6.469723	-0.901807	0.169695
30	1	0	5.833334	-2.531545	0.403403

Frequency Data:

NImag: 1 (-1197.5)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.212884 (Hartree/Particle)

Thermal correction to Energy= 0.231911

Thermal correction to Enthalpy= 0.232855

Thermal correction to Gibbs Free Energy= 0.159731

Sum of electronic and zero-point Energies= -1997.427228

Sum of electronic and thermal Energies= -1997.408201

Sum of electronic and thermal Enthalpies= -1997.407257

Sum of electronic and thermal Free Energies= -1997.480381

(4-methyl benzaldehyde)$AlCl_3$(Thiophene) TS

Cartesian Coordinates (Angstroms):

1	6	0	-2.633614	0.112614	-1.218653
2	6	0	-3.952534	-0.314120	-1.090907
3	6	0	-4.373414	-1.039005	0.034951
4	6	0	-3.427746	-1.315834	1.029858
5	6	0	-2.104261	-0.888892	0.911979
6	6	0	-1.696664	-0.168472	-0.215314
7	1	0	-2.330048	0.661943	-2.107660
8	1	0	-4.665421	-0.092079	-1.881582
9	1	0	-3.726485	-1.883640	1.907826
10	1	0	-1.375807	-1.134716	1.677032
11	6	0	-0.277576	0.323612	-0.356305
12	8	0	0.637104	-0.334778	0.559816
13	1	0	0.063837	0.237408	-1.392881
14	1	0	0.700880	1.066726	0.936692
15	6	0	-0.032654	1.767966	0.159657
16	6	0	-0.900028	2.541039	0.985660
17	6	0	-0.570425	3.892250	1.041529
18	1	0	-1.708960	2.076151	1.538886
19	6	0	0.483382	4.206092	0.186081
20	1	0	-1.063084	4.621878	1.673280
21	1	0	0.946139	5.180381	0.074645
22	13	0	2.124581	-1.291804	0.054093
23	17	0	3.423497	-1.191390	1.803438
24	17	0	1.524462	-3.293922	-0.559569
25	17	0	2.878803	-0.088605	-1.655100
26	6	0	-5.794575	-1.537813	0.149067
27	1	0	-6.088894	-1.674483	1.194771
28	1	0	-6.503227	-0.844783	-0.317183
29	1	0	-5.911789	-2.507862	-0.351868

30	16	0	1.098260	2.877795	-0.678023

Frequency Data:
NImag: 1 (-1208.1)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.209578 (Hartree/Particle)
Thermal correction to Energy= 0.228996
Thermal correction to Enthalpy= 0.229941
Thermal correction to Gibbs Free Energy= 0.156706
Sum of electronic and zero-point Energies= -2320.410493
Sum of electronic and thermal Energies= -2320.391074
Sum of electronic and thermal Enthalpies= -2320.390130
Sum of electronic and thermal Free Energies= -2320.463365

(4-methyl benzaldehyde)$AlCl_3$(toluene) TS

Cartesian Coordinates (Angstroms):

1	6	0	2.666379	-0.063248	1.276003
2	6	0	4.009848	-0.384892	1.103378
3	6	0	4.458744	-1.013195	-0.068784
4	6	0	3.514966	-1.301909	-1.062167
5	6	0	2.166748	-0.979563	-0.898099
6	6	0	1.729745	-0.354778	0.274638
7	1	0	2.342453	0.412255	2.199971
8	1	0	4.721150	-0.155592	1.893580
9	1	0	3.835906	-1.795763	-1.976393
10	1	0	1.441417	-1.232277	-1.663888
11	6	0	0.281501	0.023170	0.466987
12	8	0	-0.593482	-0.623409	-0.473279
13	6	0	5.909653	-1.399333	-0.235098
14	1	0	6.195983	-1.437476	-1.291308
15	1	0	6.104040	-2.392709	0.190643
16	1	0	6.575174	-0.693274	0.273335
17	1	0	-0.025536	-0.173447	1.500596
18	6	0	-0.068850	1.511153	0.122230
19	6	0	-1.136948	2.162106	0.844378
20	6	0	0.800448	2.348588	-0.664822
21	6	0	-1.386290	3.508828	0.671200
22	1	0	-1.782722	1.547101	1.467709
23	6	0	0.520486	3.687424	-0.835643
24	1	0	1.656894	1.892264	-1.151865
25	6	0	-0.570073	4.291687	-0.170008
26	1	0	-2.216616	3.974929	1.193908
27	1	0	1.158801	4.297954	-1.468219
28	1	0	-0.753098	0.935641	-0.722877
29	17	0	-1.358790	-3.798354	-0.001989
30	17	0	-2.721727	-0.986028	1.882218
31	17	0	-3.436477	-1.272330	-1.688944
32	13	0	-1.999520	-1.716402	-0.096194
33	6	0	-0.870570	5.748681	-0.377801
34	1	0	0.037440	6.321982	-0.587887

35	1	0	-1.540301	5.870779	-1.240491
36	1	0	-1.375193	6.183926	0.489725

Frequency Data:

NImag: 1 (-732.5)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.270514 (Hartree/Particle)
Thermal correction to Energy= 0.292231
Thermal correction to Enthalpy= 0.293175
Thermal correction to Gibbs Free Energy= 0.214470
Sum of electronic and zero-point Energies= -2038.906962
Sum of electronic and thermal Energies= -2038.885246
Sum of electronic and thermal Enthalpies= -2038.884301
Sum of electronic and thermal Free Energies= -2038.963006

(4-methyl benzaldehyde)$AlCl_3$(benzene) TS

Cartesian Coordinates (Angstroms):

1	6	0	2.737810	0.085101	1.252551
2	6	0	4.070086	-0.282146	1.084258
3	6	0	4.486052	-0.997320	-0.049888
4	6	0	3.521116	-1.325205	-1.010191
5	6	0	2.183861	-0.957650	-0.850554
6	6	0	1.779750	-0.246800	0.284301
7	1	0	2.439457	0.627444	2.147937
8	1	0	4.798324	-0.020465	1.848507
9	1	0	3.816489	-1.885041	-1.894546
10	1	0	1.440683	-1.239745	-1.588378
11	6	0	0.342152	0.172902	0.472699
12	8	0	-0.544660	-0.498323	-0.430912
13	6	0	5.924141	-1.431465	-0.208697
14	1	0	6.195714	-1.541624	-1.263722
15	1	0	6.098152	-2.401929	0.274845
16	1	0	6.614240	-0.713828	0.248039
17	1	0	0.041606	0.021939	1.515750
18	6	0	0.029405	1.655120	0.071808
19	6	0	-1.062310	2.333926	0.731693
20	6	0	0.922325	2.445418	-0.738158
21	6	0	-1.310220	3.672938	0.482399
22	1	0	-1.722511	1.749113	1.368254
23	6	0	0.644350	3.775566	-0.990819
24	1	0	1.785457	1.957925	-1.180667
25	6	0	-0.461466	4.385811	-0.375067
26	1	0	-2.155714	4.166929	0.949859
27	1	0	1.289957	4.355758	-1.642527
28	1	0	-0.645015	1.092946	-0.781218
29	17	0	-2.223785	-3.319883	-0.703733
30	17	0	-2.451844	-0.950958	2.111491
31	17	0	-3.543228	0.084356	-1.173588
32	13	0	-2.161396	-1.243513	-0.069555

33	1	0	-0.663158	5.435907	-0.569514

Frequency Data:
NImag: 1 (-633.7)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.243004 (Hartree/Particle)
Thermal correction to Energy= 0.262884
Thermal correction to Enthalpy= 0.263828
Thermal correction to Gibbs Free Energy= 0.189631
Sum of electronic and zero-point Energies= -1999.612204
Sum of electronic and thermal Energies= -1999.592325
Sum of electronic and thermal Enthalpies= -1999.591380
Sum of electronic and thermal Free Energies= -1999.665577

(4-methyl benzaldehyde)$AlCl_3$(Chlorobenzene) TS

Cartesian Coordinates (Angstroms):

1	6	0	0.882714	2.553763	1.273646
2	6	0	1.484253	3.797168	1.104791
3	6	0	2.183677	4.109138	-0.072432
4	6	0	2.252346	3.133700	-1.074449
5	6	0	1.648551	1.885172	-0.914486
6	6	0	0.956813	1.583651	0.263365
7	1	0	0.359922	2.331768	2.202192
8	1	0	1.422772	4.534568	1.901880
9	1	0	2.796172	3.347518	-1.991459
10	1	0	1.733636	1.127395	-1.685784
11	6	0	0.287388	0.245734	0.453568
12	8	0	0.738198	-0.741196	-0.482690
13	6	0	2.871030	5.444499	-0.232013
14	1	0	3.054809	5.677610	-1.285631
15	1	0	3.842994	5.449491	0.278698
16	1	0	2.276068	6.257619	0.198642
17	1	0	0.409112	-0.091695	1.489716
18	6	0	-1.247896	0.216399	0.111031
19	6	0	-2.095572	-0.710959	0.827390
20	6	0	-1.896134	1.273197	-0.626665
21	6	0	-3.469597	-0.664733	0.701085
22	1	0	-1.614661	-1.496628	1.407989
23	6	0	-3.266414	1.304324	-0.766345
24	1	0	-1.277228	2.025381	-1.106415
25	6	0	-4.044495	0.340845	-0.094052
26	1	0	-4.103030	-1.384551	1.207367
27	1	0	-3.754469	2.069927	-1.359197
28	1	0	-0.841144	-0.546945	-0.747596
29	17	0	3.700159	-2.091897	0.067825
30	17	0	0.623121	-2.912198	1.847996
31	17	0	0.881716	-3.643452	-1.724131
32	13	0	1.540203	-2.330202	-0.102426
33	17	0	-5.764593	0.403392	-0.253098

Frequency Data:
NImag: 1 (-642.9)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.233252 (Hartree/Particle)
Thermal correction to Energy= 0.254359
Thermal correction to Enthalpy= 0.255303
Thermal correction to Gibbs Free Energy= 0.177393
Sum of electronic and zero-point Energies= -2459.212508
Sum of electronic and thermal Energies= -2459.191401
Sum of electronic and thermal Enthalpies= -2459.190457
Sum of electronic and thermal Free Energies= -2459.268367

(4-methyl benzaldehyde)$AlCl_3$(cyanobenzene) TS

Cartesian Coordinates (Angstroms):

1	6	0	2.760907	0.635575	1.277345
2	6	0	4.127033	0.818820	1.087177
3	6	0	4.760178	0.378977	-0.087175
4	6	0	3.974512	-0.245561	-1.063750
5	6	0	2.602741	-0.430127	-0.882542
6	6	0	1.982480	0.010427	0.291916
7	1	0	2.297291	0.973129	2.202527
8	1	0	4.716250	1.300268	1.864195
9	1	0	4.442896	-0.601699	-1.978215
10	1	0	2.008436	-0.938491	-1.633995
11	6	0	0.499567	-0.162083	0.500322
12	8	0	-0.070082	-1.094522	-0.418473
13	6	0	6.249965	0.544604	-0.270233
14	1	0	6.529496	0.520325	-1.328321
15	1	0	6.799409	-0.262905	0.231526
16	1	0	6.605179	1.489569	0.155323
17	1	0	0.296198	-0.440847	1.541095
18	6	0	-0.358692	1.112786	0.159493
19	6	0	-1.603586	1.317246	0.866943
20	6	0	0.166781	2.220778	-0.602156
21	6	0	-2.325117	2.485881	0.711377
22	1	0	-1.993547	0.502574	1.472799
23	6	0	-0.570733	3.373145	-0.773393
24	1	0	1.135988	2.107956	-1.077861
25	6	0	-1.811572	3.511050	-0.108584
26	1	0	-3.275877	2.621685	1.214837
27	1	0	-0.199632	4.187397	-1.386255
28	1	0	-0.785350	0.394751	-0.717908
29	17	0	-0.828623	-4.257110	-0.919344
30	17	0	-1.666074	-2.287237	2.096134
31	17	0	-3.126796	-1.377483	-1.067400
32	13	0	-1.367455	-2.323668	-0.101736
33	6	0	-2.555817	4.724797	-0.268517
34	7	0	-3.152238	5.714768	-0.396907

Frequency Data:
NImag: 1 (-528.8)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.241129 (Hartree/Particle)
Thermal correction to Energy= 0.262862
Thermal correction to Enthalpy= 0.263806
Thermal correction to Gibbs Free Energy= 0.185329
Sum of electronic and zero-point Energies= -2091.842785
Sum of electronic and thermal Energies= -2091.821052
Sum of electronic and thermal Enthalpies= -2091.820108
Sum of electronic and thermal Free Energies= -2091.898585

(4-methyl benzaldehyde)$SnCl_4$(Indole) TS

Cartesian Coordinates (Angstroms):

1	6	0	2.280429	1.794650	-1.499390
2	6	0	3.039705	2.947298	-1.311960
3	6	0	2.968197	3.673777	-0.114346
4	6	0	2.113647	3.200819	0.889849
5	6	0	1.351985	2.045144	0.710320
6	6	0	1.431744	1.329439	-0.487509
7	1	0	2.349586	1.254922	-2.441934
8	1	0	3.692622	3.293318	-2.110066
9	1	0	2.033525	3.749560	1.825431
10	1	0	0.681871	1.699397	1.489726
11	6	0	0.634525	0.064644	-0.702386
12	8	0	-0.357337	-0.173741	0.338512
13	1	0	0.163551	0.077756	-1.691629
14	1	0	0.450850	-1.335547	0.365805
15	6	0	1.413923	-1.259136	-0.507897
16	6	0	2.743233	-1.506019	0.095172
17	6	0	3.120862	-2.814804	-0.272115
18	1	0	2.098713	-4.261706	-1.488749
19	17	0	-2.364475	-0.604909	2.447351
20	17	0	-2.144627	2.131784	-0.717960
21	17	0	-2.250162	-1.803891	-1.494234
22	6	0	3.760350	4.946834	0.070443
23	1	0	4.718504	4.905617	-0.459126
24	1	0	3.210675	5.813457	-0.320332
25	1	0	3.964429	5.142365	1.128385
26	50	0	-2.422929	-0.051265	0.150243
27	17	0	-4.805189	-0.011911	0.035595
28	6	0	4.292830	-3.430480	0.162914
29	6	0	3.592653	-0.772467	0.931574
30	6	0	4.775867	-1.368446	1.363911
31	6	0	5.122084	-2.679138	0.990888
32	1	0	3.337149	0.236245	1.233152
33	6	0	1.150473	-2.419899	-1.296361
34	7	0	2.117828	-3.319672	-1.117685
35	1	0	0.274808	-2.621342	-1.899774

36	1	0	6.049091	-3.112989	1.353092
37	1	0	5.446903	-0.806944	2.007027
38	1	0	4.548724	-4.444771	-0.128921

Frequency Data:

NImag: 1 (-1314.8)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.273013 (Hartree/Particle)
Thermal correction to Energy= 0.297071
Thermal correction to Enthalpy= 0.298015
Thermal correction to Gibbs Free Energy= 0.214006
Sum of electronic and zero-point Energies= -2592.692350
Sum of electronic and thermal Energies= -2592.668293
Sum of electronic and thermal Enthalpies= -2592.667348
Sum of electronic and thermal Free Energies= -2592.751357

(4-methyl benzaldehyde)$SnCl_4$(Furan) TS

Cartesian Coordinates (Angstroms):

1	6	0	-3.209217	-0.289632	-1.255777
2	6	0	-4.339320	-1.092360	-1.123587
3	6	0	-4.539535	-1.876640	0.022408
4	6	0	-3.570647	-1.824678	1.033129
5	6	0	-2.437697	-1.020241	0.911237
6	6	0	-2.249321	-0.244254	-0.237273
7	1	0	-3.069282	0.297501	-2.161257
8	1	0	-5.072274	-1.121185	-1.926460
9	1	0	-3.698778	-2.430865	1.926880
10	1	0	-1.681767	-1.009851	1.689746
11	6	0	-1.052482	0.661934	-0.372911
12	8	0	0.020952	0.331287	0.543821
13	1	0	-0.710101	0.714149	-1.412514
14	1	0	-0.224640	1.766547	0.760924
15	6	0	-1.254343	2.114257	0.119047
16	6	0	-2.148280	2.659521	1.083213
17	6	0	-2.287106	4.020496	0.818228
18	1	0	-2.575442	2.094150	1.901148
19	6	0	-1.550527	4.250384	-0.336632
20	1	0	-2.840264	4.757434	1.382567
21	1	0	-1.354249	5.157986	-0.892989
22	8	0	-0.969927	3.154074	-0.788779
23	17	0	2.374884	1.811211	-0.706928
24	17	0	2.025063	-0.877760	2.344750
25	17	0	0.810246	-1.800929	-1.549014
26	6	0	-5.744125	-2.779933	0.143372
27	1	0	-6.611481	-2.367019	-0.382807
28	1	0	-5.540020	-3.767386	-0.291475
29	1	0	-6.023750	-2.938151	1.190214
30	50	0	1.905994	-0.411448	0.032630
31	17	0	4.083321	-1.246457	-0.458369

Frequency Data:

NImag: 1 (-1140.6)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.212616 (Hartree/Particle)
Thermal correction to Energy= 0.234102
Thermal correction to Enthalpy= 0.235047
Thermal correction to Gibbs Free Energy= 0.156142
Sum of electronic and zero-point Energies= -2458.946313
Sum of electronic and thermal Energies= -2458.924827
Sum of electronic and thermal Enthalpies= -2458.923882
Sum of electronic and thermal Free Energies= -2459.002787

(4-methyl benzaldehyde)$SnCl_4$(Thiophene) TS

Cartesian Coordinates (Angstroms):

1	6	0	-3.129740	-0.545732	-1.277148
2	6	0	-4.234988	-1.384679	-1.160754
3	6	0	-4.430566	-2.168742	-0.013793
4	6	0	-3.482345	-2.079170	1.013424
5	6	0	-2.373565	-1.239048	0.906125
6	6	0	-2.189501	-0.462746	-0.242679
7	1	0	-2.994950	0.042866	-2.182511
8	1	0	-4.952190	-1.441056	-1.976350
9	1	0	-3.606119	-2.684558	1.908321
10	1	0	-1.631166	-1.201452	1.696451
11	6	0	-1.021038	0.484664	-0.366285
12	8	0	0.050796	0.199178	0.567050
13	1	0	-0.662768	0.522146	-1.400488
14	1	0	-0.341530	1.584135	0.880558
15	6	0	-1.305077	1.929030	0.141124
16	6	0	-2.361234	2.319391	1.020138
17	6	0	-2.592433	3.690386	1.055386
18	1	0	-2.886905	1.585577	1.621530
19	6	0	-1.800844	4.374755	0.134734
20	1	0	-3.297166	4.180794	1.716472
21	1	0	-1.768474	5.449760	-0.003953
22	17	0	2.312265	-0.277593	2.385464
23	17	0	0.913372	-2.360216	-0.941793
24	17	0	2.083986	1.453109	-1.354459
25	6	0	-5.607690	-3.109601	0.090636
26	1	0	-5.889516	-3.285809	1.133962
27	1	0	-6.483724	-2.718277	-0.437843
28	1	0	-5.370937	-4.086225	-0.351996
29	50	0	1.950084	-0.485099	0.059189
30	17	0	4.178058	-1.177885	-0.424624
31	16	0	-0.758849	3.376660	-0.762714

Frequency Data:
NImag: 1 (-1117.1)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.

Zero-point correction= 0.209289 (Hartree/Particle)
Thermal correction to Energy= 0.231181
Thermal correction to Enthalpy= 0.232125
Thermal correction to Gibbs Free Energy= 0.152856
Sum of electronic and zero-point Energies= -2781.929655
Sum of electronic and thermal Energies= -2781.907763
Sum of electronic and thermal Enthalpies= -2781.906819
Sum of electronic and thermal Free Energies= -2781.986088

(4-methyl benzaldehyde)$SnCl_4$(toluene) TS

Cartesian Coordinates (Angstroms):

1	6	0	3.029043	-1.238284	1.252166
2	6	0	4.092670	-2.109981	1.036956
3	6	0	4.261559	-2.755644	-0.197817
4	6	0	3.330266	-2.492340	-1.209792
5	6	0	2.262565	-1.617311	-1.002775
6	6	0	2.102866	-0.980379	0.232366
7	1	0	2.911182	-0.763894	2.224243
8	1	0	4.796649	-2.303855	1.842990
9	1	0	3.433966	-2.986412	-2.172965
10	1	0	1.534423	-1.444250	-1.788327
11	6	0	0.976472	-0.009029	0.474717
12	8	0	-0.102874	-0.158634	-0.481704
13	6	0	5.393145	-3.733101	-0.411652
14	1	0	5.140725	-4.721774	-0.006209
15	1	0	6.310125	-3.403398	0.089297
16	1	0	5.614556	-3.863717	-1.475783
17	1	0	0.618382	-0.106349	1.504060
18	6	0	1.304959	1.491064	0.168114
19	6	0	0.598596	2.522288	0.890575
20	6	0	2.467393	1.892598	-0.580524
21	6	0	0.948718	3.849914	0.749903
22	1	0	-0.268985	2.242195	1.483898
23	6	0	2.788441	3.226425	-0.718599
24	1	0	3.061673	1.124670	-1.065884
25	6	0	2.041472	4.226132	-0.056730
26	1	0	0.378245	4.614776	1.268692
27	1	0	3.642097	3.517154	-1.324363
28	1	0	0.445254	1.295105	-0.704076
29	50	0	-2.046793	-0.485535	-0.056231
30	17	0	-2.374415	1.086684	-1.876686
31	17	0	-1.310476	-2.037148	1.659162
32	17	0	-2.843117	1.068608	1.571101
33	17	0	-3.460569	-2.089606	-1.041554
34	6	0	2.391243	5.676222	-0.232951
35	1	0	3.457631	5.812787	-0.435943
36	1	0	1.839534	6.089527	-1.088720
37	1	0	2.116522	6.266658	0.646125

Frequency Data:
Nlmag: 1 (-774.8)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.270157 (Hartree/Particle)
Thermal correction to Energy= 0.294354
Thermal correction to Enthalpy= 0.295298
Thermal correction to Gibbs Free Energy= 0.210087
Sum of electronic and zero-point Energies= -2500.421652
Sum of electronic and thermal Energies= -2500.397456
Sum of electronic and thermal Enthalpies= -2500.396512
Sum of electronic and thermal Free Energies= -2500.481722

(4-methyl benzaldehyde)$SnCl_4$(benzene) TS

Cartesian Coordinates (Angstroms):

1	6	0	3.251221	-0.470831	1.245691
2	6	0	4.437252	-1.170210	1.040506
3	6	0	4.690243	-1.825665	-0.174511
4	6	0	3.715947	-1.749813	-1.177898
5	6	0	2.526012	-1.047514	-0.981479
6	6	0	2.282992	-0.399698	0.234919
7	1	0	3.071807	0.014165	2.203043
8	1	0	5.173732	-1.220725	1.839070
9	1	0	3.884869	-2.255564	-2.125653
10	1	0	1.770338	-1.018396	-1.759554
11	6	0	1.019565	0.389728	0.463748
12	8	0	-0.026611	0.043439	-0.467373
13	6	0	5.958687	-2.620365	-0.376579
14	1	0	5.842514	-3.646827	-0.004321
15	1	0	6.802569	-2.174709	0.161128
16	1	0	6.226113	-2.687295	-1.436217
17	1	0	0.694053	0.273845	1.501947
18	6	0	1.119964	1.916748	0.111075
19	6	0	0.221209	2.836753	0.771164
20	6	0	2.233561	2.472900	-0.615080
21	6	0	0.361103	4.203351	0.600532
22	1	0	-0.619517	2.430167	1.329257
23	6	0	2.344848	3.839504	-0.788596
24	1	0	2.955757	1.791701	-1.053991
25	6	0	1.418118	4.698964	-0.174644
26	1	0	-0.342959	4.885135	1.066344
27	1	0	3.158661	4.251954	-1.376564
28	1	0	0.333297	1.589810	-0.769037
29	50	0	-1.891518	-0.589133	-0.047044
30	17	0	-2.417702	0.666178	-2.051114
31	17	0	-0.968342	-1.777236	1.863717
32	17	0	-3.014246	0.973081	1.368811

33	17	0	-2.962650	-2.529077	-0.843274
34	1	0	1.523182	5.772692	-0.305741

Frequency Data:
NImag: 1 (-630.5)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.242806 (Hartree/Particle)
Thermal correction to Energy= 0.265133
Thermal correction to Enthalpy= 0.266077
Thermal correction to Gibbs Free Energy= 0.185746
Sum of electronic and zero-point Energies= -2461.126411
Sum of electronic and thermal Energies= -2461.104084
Sum of electronic and thermal Enthalpies= -2461.103140
Sum of electronic and thermal Free Energies= -2461.183471

(4-methyl benzaldehyde)$SnCl_4$(chlorobenzene) TS

Cartesian Coordinates (Angstroms):

1	6	0	-2.021145	2.555242	1.254253
2	6	0	-2.591324	3.806916	1.039708
3	6	0	-2.457099	4.461888	-0.194415
4	6	0	-1.737318	3.815520	-1.207510
5	6	0	-1.164866	2.559736	-1.001590
6	6	0	-1.302734	1.916801	0.234198
7	1	0	-2.124451	2.076703	2.225903
8	1	0	-3.138070	4.290957	1.845521
9	1	0	-1.612566	4.305708	-2.170138
10	1	0	-0.586844	2.084199	-1.787204
11	6	0	-0.716270	0.550615	0.473883
12	8	0	0.330286	0.224423	-0.468570
13	6	0	-3.038518	5.839386	-0.407618
14	1	0	-2.339230	6.616448	-0.071646
15	1	0	-3.968131	5.975217	0.155463
16	1	0	-3.249225	6.027031	-1.465509
17	1	0	-0.371059	0.469135	1.508758
18	6	0	-1.671763	-0.654138	0.144384
19	6	0	-1.481317	-1.899051	0.853736
20	6	0	-2.914104	-0.482633	-0.565771
21	6	0	-2.393530	-2.929482	0.747677
22	1	0	-0.558174	-2.045052	1.410781
23	6	0	-3.815266	-1.518737	-0.683878
24	1	0	-3.111820	0.473472	-1.040474
25	6	0	-3.553976	-2.732571	-0.019241
26	1	0	-2.226702	-3.877096	1.247404
27	1	0	-4.729564	-1.405274	-1.255654
28	1	0	-0.824906	-0.829775	-0.730915
29	50	0	2.232548	-0.309677	-0.056252
30	17	0	1.935104	-1.665458	-2.038667
31	17	0	2.161383	1.237806	1.817514
32	17	0	2.240816	-2.203951	1.397723

33	17	0	4.229824	0.638025	-0.867348
34	17	0	-4.700866	-4.018781	-0.151457

Frequency Data:

NImag: 1 (-724.1)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.233024 (Hartree/Particle)
Thermal correction to Energy= 0.256585
Thermal correction to Enthalpy= 0.257529
Thermal correction to Gibbs Free Energy= 0.173450
Sum of electronic and zero-point Energies= -2920.726858
Sum of electronic and thermal Energies= -2920.703297
Sum of electronic and thermal Enthalpies= -2920.702352
Sum of electronic and thermal Free Energies= -2920.786432

(4-methyl benzaldehyde)$SnCl_4$(cyanobenzene) TS

Cartesian Coordinates (Angstroms):

1	6	0	-2.423114	2.160729	1.240886
2	6	0	-3.172579	3.315375	1.038267
3	6	0	-3.128873	4.002015	-0.186118
4	6	0	-2.311353	3.487386	-1.200994
5	6	0	-1.558558	2.328970	-1.007031
6	6	0	-1.608244	1.653204	0.218658
7	1	0	-2.460464	1.657520	2.204829
8	1	0	-3.791727	3.700010	1.845202
9	1	0	-2.253924	4.005885	-2.154994
10	1	0	-0.908639	1.957672	-1.792571
11	6	0	-0.824873	0.388717	0.442999
12	8	0	0.259938	0.239467	-0.486336
13	6	0	-3.910647	5.278086	-0.385656
14	1	0	-3.349950	6.143338	-0.007986
15	1	0	-4.865824	5.253088	0.149979
16	1	0	-4.117198	5.461096	-1.445011
17	1	0	-0.488051	0.340351	1.483430
18	6	0	-1.613330	-0.940655	0.099491
19	6	0	-1.223187	-2.160834	0.772790
20	6	0	-2.897235	-0.927136	-0.559632
21	6	0	-1.997864	-3.301860	0.687120
22	1	0	-0.261821	-2.189610	1.282071
23	6	0	-3.654701	-2.074446	-0.660658
24	1	0	-3.239520	0.001337	-1.005760
25	6	0	-3.212781	-3.259639	-0.027217
26	1	0	-1.683400	-4.222958	1.165472
27	1	0	-4.599355	-2.074686	-1.193580
28	1	0	-0.806053	-0.994755	-0.796523
29	50	0	2.202607	-0.058104	-0.053914
30	17	0	2.111365	-1.422276	-2.051080
31	17	0	1.904454	1.425118	1.853012
32	17	0	2.446780	-1.959376	1.374964

33	17	0	4.053608	1.169388	-0.829047
34	6	0	-4.022422	-4.438225	-0.110531
35	7	0	-4.685837	-5.391067	-0.176547

Frequency Data:

NImag: 1 (-488.3)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.241097 (Hartree/Particle)
Thermal correction to Energy= 0.265258
Thermal correction to Enthalpy= 0.266202
Thermal correction to Gibbs Free Energy= 0.181630
Sum of electronic and zero-point Energies= -2553.356619
Sum of electronic and thermal Energies= -2553.332459
Sum of electronic and thermal Enthalpies= -2553.331515
Sum of electronic and thermal Free Energies= -2553.416087

$AlCl_3$

Cartesian Coordinates (Angstroms):

1	17	0	0.000000	2.127641	0.000000
2	17	0	1.842591	-1.063820	0.000000
3	17	0	-1.842591	-1.063820	0.000000
4	13	0	0.000000	0.000000	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.004467 (Hartree/Particle)
Thermal correction to Energy= 0.009912
Thermal correction to Enthalpy= 0.010856
Thermal correction to Gibbs Free Energy= -0.025048
Sum of electronic and zero-point Energies= -1382.741140
Sum of electronic and thermal Energies= -1382.735695
Sum of electronic and thermal Enthalpies= -1382.734751
Sum of electronic and thermal Free Energies= -1382.770655

$InCl_3$

Cartesian Coordinates (Angstroms):

1	17	0	0.000000	2.288969	0.000000
2	17	0	1.982305	-1.144484	0.000000
3	17	0	-1.982305	-1.144484	0.000000
4	49	0	0.000000	0.000000	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.003111 (Hartree/Particle)
Thermal correction to Energy= 0.009214
Thermal correction to Enthalpy= 0.010158
Thermal correction to Gibbs Free Energy= -0.028470
Sum of electronic and zero-point Energies= -1382.609897
Sum of electronic and thermal Energies= -1382.603794

Sum of electronic and thermal Enthalpies= -1382.602849
Sum of electronic and thermal Free Energies= -1382.641478

$SnCl_4$

Cartesian Coordinates (Angstroms):

1	50	0	0.000000	0.000000	0.000167
2	17	0	0.000000	2.177913	-0.770370
3	17	0	1.886128	-1.088956	-0.770370
4	17	0	-1.886128	-1.088956	-0.770370
5	17	0	0.000000	0.000000	2.310618

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.004654 (Hartree/Particle)
Thermal correction to Energy= 0.012392
Thermal correction to Enthalpy= 0.013336
Thermal correction to Gibbs Free Energy= -0.029815
Sum of electronic and zero-point Energies= -1844.301002
Sum of electronic and thermal Energies= -1844.293263
Sum of electronic and thermal Enthalpies= -1844.292319
Sum of electronic and thermal Free Energies= -1844.335471

$ZnCl_2$

Cartesian Coordinates (Angstroms):

1	17	0	0.000000	0.000000	2.158032
2	17	0	0.000000	0.000000	-2.158032
3	30	0	0.000000	0.000000	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.002138 (Hartree/Particle)
Thermal correction to Energy= 0.006700
Thermal correction to Enthalpy= 0.007644
Thermal correction to Gibbs Free Energy= -0.024469
Sum of electronic and zero-point Energies= -986.073215
Sum of electronic and thermal Energies= -986.068653
Sum of electronic and thermal Enthalpies= -986.067709
Sum of electronic and thermal Free Energies= -986.099823

BF_3

Cartesian Coordinates (Angstroms):

1	5	0	0.000000	0.000000	0.000242
2	9	0	0.000000	1.333901	-0.000045
3	9	0	1.155192	-0.666950	-0.000045
4	9	0	-1.155192	-0.666950	-0.000045

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.012053 (Hartree/Particle)
Thermal correction to Energy= 0.015665
Thermal correction to Enthalpy= 0.016609
Thermal correction to Gibbs Free Energy= -0.013174
Sum of electronic and zero-point Energies= -324.499402
Sum of electronic and thermal Energies= -324.495791
Sum of electronic and thermal Enthalpies= -324.494846
Sum of electronic and thermal Free Energies= -324.524629

$TiCl_4$

Cartesian Coordinates (Angstroms):

1	17	0	0.000000	2.039971	0.721138
2	17	0	0.000000	0.000000	-2.163426
3	17	0	1.766667	-1.019986	0.721138
4	17	0	-1.766667	-1.019986	0.721138
5	22	0	0.000000	0.000000	0.000008

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.005906 (Hartree/Particle)
Thermal correction to Energy= 0.013085
Thermal correction to Enthalpy= 0.014029
Thermal correction to Gibbs Free Energy= -0.027173
Sum of electronic and zero-point Energies= -1899.106682
Sum of electronic and thermal Energies= -1899.099504
Sum of electronic and thermal Enthalpies= -1899.098559
Sum of electronic and thermal Free Energies= -1899.139761

$SiCl_4$

Cartesian Coordinates (Angstroms):

1	17	0	0.000000	1.970156	-0.696613
2	17	0	0.000000	0.000000	2.089716
3	17	0	-1.706205	-0.985078	-0.696613
4	17	0	1.706205	-0.985078	-0.696613
5	14	0	0.000000	0.000000	0.000149

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.006779 (Hartree/Particle)
Thermal correction to Energy= 0.013462
Thermal correction to Enthalpy= 0.014406
Thermal correction to Gibbs Free Energy= -0.025056
Sum of electronic and zero-point Energies= -1844.775988
Sum of electronic and thermal Energies= -1844.769305
Sum of electronic and thermal Enthalpies= -1844.768361
Sum of electronic and thermal Free Energies= -1844.807823

$AlCl_3(OH)$

Cartesian Coordinates (Angstroms):

1	8	0	-0.776750	1.931430	0.000000
2	17	0	2.105584	0.448613	0.000000
3	17	0	-0.776750	-0.855865	1.795413
4	17	0	-0.776750	-0.855865	-1.795413
5	13	0	-0.109961	0.311156	0.000000
6	1	0	-1.741945	1.976531	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.017157 (Hartree/Particle)
Thermal correction to Energy= 0.024047
Thermal correction to Enthalpy= 0.024992
Thermal correction to Gibbs Free Energy= -0.015595
Sum of electronic and zero-point Energies= -1458.712007
Sum of electronic and thermal Energies= -1458.705116
Sum of electronic and thermal Enthalpies= -1458.704172
Sum of electronic and thermal Free Energies= -1458.744758

$InCl_3(OH)$

Cartesian Coordinates (Angstroms):

1	8	0	-0.803865	2.017328	0.000000
2	17	0	2.301931	0.339734	0.000000
3	17	0	-0.803865	-1.024283	1.920446
4	17	0	-0.803865	-1.024283	-1.920446
5	1	0	-1.771361	2.015300	0.000000
6	49	0	-0.073452	0.222372	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.015215 (Hartree/Particle)
Thermal correction to Energy= 0.023001
Thermal correction to Enthalpy= 0.023945
Thermal correction to Gibbs Free Energy= -0.019832
Sum of electronic and zero-point Energies= -1458.564670
Sum of electronic and thermal Energies= -1458.556884
Sum of electronic and thermal Enthalpies= -1458.555939
Sum of electronic and thermal Free Energies= -1458.599717

$SnCl_4(OH)$

Cartesian Coordinates (Angstroms):

1	8	0	0.030667	-0.005206	1.903231
2	17	0	-2.340533	0.000005	0.388179
3	17	0	-0.021605	-1.802480	-0.956380

4	17	0	-0.022513	1.804762	-0.952259
5	17	0	2.400484	0.000876	0.307153
6	14	0	-0.107077	-0.000417	0.234817
7	1	0	0.984563	-0.006297	2.112919

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.020629 (Hartree/Particle)
Thermal correction to Energy= 0.029246
Thermal correction to Enthalpy= 0.030190
Thermal correction to Gibbs Free Energy= -0.014480
Sum of electronic and zero-point Energies= -1920.696745
Sum of electronic and thermal Energies= -1920.688128
Sum of electronic and thermal Enthalpies= -1920.687184
Sum of electronic and thermal Free Energies= -1920.731854

$ZnCl_2(OH)$

Cartesian Coordinates (Angstroms):

1	17	0	-0.012531	-0.889738	1.959578
2	17	0	-0.012531	-0.889738	-1.959578
3	30	0	-0.012531	0.331128	0.000000
4	8	0	-0.011633	2.219646	0.000000
5	1	0	0.895024	2.560093	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.013727 (Hartree/Particle)
Thermal correction to Energy= 0.019746
Thermal correction to Enthalpy= 0.020690
Thermal correction to Gibbs Free Energy= -0.018148
Sum of electronic and zero-point Energies= -1061.988739
Sum of electronic and thermal Energies= -1061.982720
Sum of electronic and thermal Enthalpies= -1061.981776
Sum of electronic and thermal Free Energies= -1062.020613

$BF_3(OH)$

Cartesian Coordinates (Angstroms):

1	8	0	-1.468556	0.071154	0.000000
2	1	0	-1.748728	-0.855622	0.000000
3	5	0	-0.001682	0.026845	0.000000
4	9	0	0.500207	1.356232	0.000000
5	9	0	0.500207	-0.669662	1.155950
6	9	0	0.500207	-0.669662	-1.155950

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.025128 (Hartree/Particle)

Thermal correction to Energy= 0.029625
Thermal correction to Enthalpy= 0.030569
Thermal correction to Gibbs Free Energy= -0.002568
Sum of electronic and zero-point Energies= -400.400814
Sum of electronic and thermal Energies= -400.396317
Sum of electronic and thermal Enthalpies= -400.395373
Sum of electronic and thermal Free Energies= -400.428511

$TiCl_4(OH)$

Cartesian Coordinates (Angstroms):

1	17	0	-2.288855	-0.000001	-0.426200
2	17	0	-0.171103	-0.000007	2.125923
3	17	0	1.192083	-1.935322	-0.146267
4	17	0	1.192079	1.935325	-0.146256
5	8	0	0.132037	0.000006	-2.048504
6	1	0	1.018041	0.000008	-2.445646
7	22	0	-0.035719	0.000001	-0.231305

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.017728 (Hartree/Particle)
Thermal correction to Energy= 0.026483
Thermal correction to Enthalpy= 0.027427
Thermal correction to Gibbs Free Energy= -0.017942
Sum of electronic and zero-point Energies= -1975.034425
Sum of electronic and thermal Energies= -1975.025670
Sum of electronic and thermal Enthalpies= -1975.024726
Sum of electronic and thermal Free Energies= -1975.070094

$SiCl_4(OH)$

Cartesian Coordinates (Angstroms):

1	8	0	0.030667	-0.005206	1.903231
2	17	0	-2.340533	0.000005	0.388179
3	17	0	-0.021605	-1.802480	-0.956380
4	17	0	-0.022513	1.804762	-0.952259
5	17	0	2.400484	0.000876	0.307153
6	14	0	-0.107077	-0.000417	0.234817
7	1	0	0.984563	-0.006297	2.112919

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.020629 (Hartree/Particle)
Thermal correction to Energy= 0.029246
Thermal correction to Enthalpy= 0.030190
Thermal correction to Gibbs Free Energy= -0.014480
Sum of electronic and zero-point Energies= -1920.696745

Sum of electronic and thermal Energies= -1920.688128
Sum of electronic and thermal Enthalpies= -1920.687184
Sum of electronic and thermal Free Energies= -1920.731854

(4-methoxyphenyl)(p-tolyl)methylium

Cartesian Coordinates (Angstroms):

1	6	0	4.613912	0.659204	-0.299926
2	6	0	4.793029	-0.691118	0.023303
3	6	0	3.698890	-1.487720	0.392348
4	6	0	2.421833	-0.951467	0.409989
5	6	0	2.211255	0.409741	0.058153
6	6	0	3.342661	1.210271	-0.260933
7	6	0	0.936465	1.052844	0.038989
8	6	0	-0.366334	0.539601	-0.033273
9	6	0	-1.446683	1.445374	0.219017
10	6	0	-2.758755	1.035152	0.218427
11	6	0	-3.057607	-0.317351	-0.083183
12	6	0	-2.008625	-1.227000	-0.397617
13	6	0	-0.704751	-0.813320	-0.372773
14	1	0	5.466875	1.274832	-0.566271
15	1	0	3.855650	-2.521734	0.682345
16	1	0	1.594765	-1.557583	0.759699
17	1	0	3.197551	2.259512	-0.503012
18	1	0	0.989775	2.140799	0.082641
19	1	0	-1.215803	2.482004	0.448228
20	1	0	-3.549210	1.742256	0.437615
21	1	0	-2.280624	-2.239390	-0.675968
22	1	0	0.073096	-1.505194	-0.671068
23	8	0	-4.276588	-0.826879	-0.125425
24	6	0	-5.431505	-0.007082	0.148283
25	1	0	-6.283678	-0.677167	0.048930
26	1	0	-5.383856	0.390665	1.166109
27	1	0	-5.505023	0.803715	-0.582218
28	1	0	5.790460	-1.120458	0.011552

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.233122 (Hartree/Particle)
Thermal correction to Energy= 0.245690
Thermal correction to Enthalpy= 0.246634
Thermal correction to Gibbs Free Energy= 0.193378
Sum of electronic and zero-point Energies= -616.060321
Sum of electronic and thermal Energies= -616.047753
Sum of electronic and thermal Enthalpies= -616.046809
Sum of electronic and thermal Free Energies= -616.100065