Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Theoretical calculations of stability constants and pK_a values of metal complexes in solution. Application to Pyridoxamine-Copper(II) complexes and their biological implications in AGE inhibition

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Supporting Information.

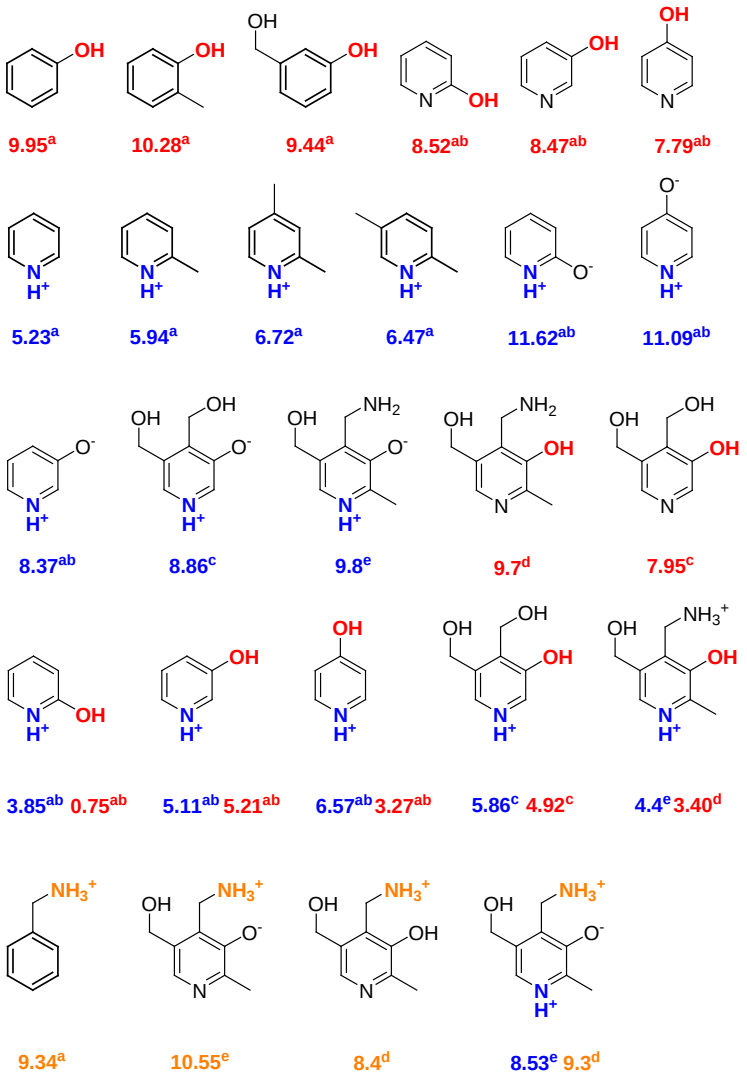

Chart 1-SP. Benchmark set of phenols, pyridines and benzylamines used in the calibration of eqns 10 and 13. Experimental pK_a values taken from references 1(a), 2(b), 3(c), 4(d) and 5(e).

References

1) R. Williams, pKa Data. Available from: <http://www.research.che.edu.psu.edu/brpgroup/pKa_compilation.pdf>.

2) Karelson, M. M.; Katrizky, A. R.; Szafran, M.; Zerner, M. C. *J. Org. Chem*. **1989**, *54*, 6030-6034.

3) Takács-Novák, K.; Tam, K. Y. *J. Pharm. Biomed. Anal*. **2000**, *21*, 1171-1182.

4) Christen, P.; Metzler, D. E. In *Transaminases*; John Wiley: New York, **1985**.

5) Vilanova, B.; Adrover, M.; Muñoz, F.; Donoso, J. *Chem. & Biodiv*. **2004**, *1*, 1073-1090.

Optimized geometries and energetic parameters of the benchmark 1 Cu^{2+} complexes

$[Cu(Gly)(H_2O)_2]^+$

Zero-point correction= 0.121266 (Hartree/Particle)
Thermal correction to Energy= 0.132646
Thermal correction to Enthalpy= 0.133590
Thermal correction to Gibbs Free Energy= 0.083727
Sum of electronic and zero-point Energies= -2076.848192
Sum of electronic and thermal Energies= -2076.836811
Sum of electronic and thermal Enthalpies= -2076.835867
Sum of electronic and thermal Free Energies= -2076.885730

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.237	39.940	104.946
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.351
Rotational	0.889	2.981	29.344
Vibrational	81.459	33.979	32.873

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.948052	0.924724	0.669223
2	6	0	2.214538	2.093786	0.210603
3	6	0	1.078893	2.852560	-0.442115
4	1	0	0.862350	3.720087	0.187206
5	1	0	1.416627	3.233872	-1.408751
6	1	0	-0.960173	2.516741	-0.265176
7	1	0	-0.286855	1.771657	-1.557458
8	8	0	3.322372	2.627040	0.291260
9	7	0	-0.128261	2.024603	-0.583937
10	29	0	0.113736	0.319244	0.439145
11	8	0	-1.840596	-0.175800	0.132255
12	1	0	-2.049352	-1.021573	0.551571
13	8	0	0.548508	-1.381103	1.437187
14	1	0	-0.197881	-1.703429	1.958574
15	1	0	-2.412456	0.471591	0.565785
16	1	0	1.262897	-1.219424	2.067418

Glycine ligand

Zero-point correction= 0.066396 (Hartree/Particle)
Thermal correction to Energy= 0.071703
Thermal correction to Enthalpy= 0.072647
Thermal correction to Gibbs Free Energy= 0.037456
Sum of electronic and zero-point Energies= -283.855877
Sum of electronic and thermal Energies= -283.850570
Sum of electronic and thermal Enthalpies= -283.849626
Sum of electronic and thermal Free Energies= -283.884817

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	44.994	17.085	74.065
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	38.821
Rotational	0.889	2.981	25.280
Vibrational	43.217	11.123	9.964

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.995767	0.859288	-0.649027
2	6	0	-1.954318	0.287355	-0.076201
3	6	0	-1.831695	-1.195080	0.235862
4	1	0	-2.247341	-1.367600	1.233821
5	1	0	-2.514085	-1.699231	-0.467806
6	1	0	-0.478014	-2.703394	0.090422
7	1	0	-0.039723	-1.334504	-0.680772
8	8	0	-3.048609	0.829224	0.232721
9	7	0	-0.464546	-1.690748	0.172034

$[Cu(\beta\text{-Ala})(H_2O)_2]^+$

Zero-point correction= 0.150569 (Hartree/Particle)
Thermal correction to Energy= 0.162824
Thermal correction to Enthalpy= 0.163768
Thermal correction to Gibbs Free Energy= 0.112147
Sum of electronic and zero-point Energies= -2116.111120
Sum of electronic and thermal Energies= -2116.098864
Sum of electronic and thermal Enthalpies= -2116.097920
Sum of electronic and thermal Free Energies= -2116.149541

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.174	44.158	108.646
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.584
Rotational	0.889	2.981	30.010
Vibrational	100.396	38.196	35.675

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.954095	-1.255105	0.253917
2	6	0	-3.067759	1.022546	1.381747
3	6	0	-3.203486	-0.476472	1.525291
4	1	0	-3.501557	1.519327	2.255801
5	1	0	-3.607348	1.379286	0.499618
6	1	0	-2.492633	-0.840196	2.281152
7	1	0	-4.202627	-0.727429	1.889149
8	1	0	0.905552	0.163859	-2.215005
9	1	0	-0.172474	-0.939803	-2.246481
10	8	0	0.943970	1.692997	0.189654
11	8	0	-2.038528	-0.842355	-0.549173
12	8	0	-3.622578	-2.268000	0.016023
13	7	0	-1.655001	1.413148	1.240484
14	29	0	-0.659420	0.468833	-0.193991
15	1	0	-1.575106	2.417280	1.080011
16	1	0	-1.156179	1.218407	2.110112
17	8	0	0.420651	-0.456978	-1.656074
18	1	0	1.713577	1.446604	-0.340305
19	1	0	0.748650	2.608194	-0.052873

β-alanine ligand

Zero-point correction= 0.094953 (Hartree/Particle)
Thermal correction to Energy= 0.101487
Thermal correction to Enthalpy= 0.102432
Thermal correction to Gibbs Free Energy= 0.064143
Sum of electronic and zero-point Energies= -323.118622
Sum of electronic and thermal Energies= -323.112088
Sum of electronic and thermal Enthalpies= -323.111144
Sum of electronic and thermal Free Energies= -323.149433

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	63.684	21.782	80.586
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.338
Rotational	0.889	2.981	26.637
Vibrational	61.907	15.821	14.611

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.771997	0.152694	0.389832
2	1	0	-0.391769	-0.871871	0.315229
3	1	0	-1.869960	0.084794	0.357096
4	6	0	-0.297595	0.957052	-0.802584
5	1	0	-0.693834	0.503335	-1.719432
6	1	0	-0.692819	1.978121	-0.740469
7	7	0	-0.275034	0.742714	1.632398
8	1	0	-0.662120	1.680261	1.723575
9	1	0	-0.629728	0.215991	2.425948
10	6	0	1.221017	0.999869	-0.909019
11	8	0	1.786161	2.124616	-0.876497
12	8	0	1.818894	-0.102170	-1.027185

[Cu(Adp)(H_2O)$_2$]

Zero-point correction= 0.191101 (Hartree/Particle)
Thermal correction to Energy= 0.207119
Thermal correction to Enthalpy= 0.208063
Thermal correction to Gibbs Free Energy= 0.146766
Sum of electronic and zero-point Energies= -2327.401275
Sum of electronic and thermal Energies= -2327.385257
Sum of electronic and thermal Enthalpies= -2327.384313
Sum of electronic and thermal Free Energies= -2327.445610

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	129.969	57.230	129.011
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.365
Rotational	0.889	2.981	31.929
Vibrational	128.192	51.269	53.340

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.931144	1.642471	0.029752
2	6	0	-2.534226	2.043396	-0.964136
3	6	0	0.415243	2.663967	1.016274
4	6	0	-1.646502	3.172511	-0.412381
5	6	0	-1.090883	2.887846	0.992366
6	1	0	0.754408	2.358546	2.014595
7	1	0	-2.209214	1.087575	-0.551075
8	1	0	-2.222472	4.104422	-0.416890
9	1	0	-3.577426	2.210582	-0.677763
10	1	0	0.946044	3.599409	0.798348
11	1	0	-0.808235	3.345745	-1.101484
12	1	0	-1.601605	2.016191	1.419340
13	1	0	-1.313198	3.722647	1.666111
14	6	0	-2.449120	1.978219	-2.466047
15	8	0	-3.263376	2.606934	-3.161200
16	8	0	-1.506649	1.286193	-3.003123
17	8	0	0.064024	0.849163	-0.472562
18	8	0	2.145660	1.618912	-0.253063
19	29	0	0.114427	0.385920	-2.366627
20	8	0	1.949377	-0.430681	-2.027532
21	1	0	2.500284	-0.372252	-2.818632
22	8	0	0.331369	-0.053189	-4.347939
23	1	0	0.656456	-0.950606	-4.496760
24	1	0	-0.545610	-0.013354	-4.752719
25	1	0	2.296508	0.242720	-1.392197

Adipic acid ligand

Zero-point correction= 0.136117 (Hartree/Particle)
Thermal correction to Energy= 0.146615
Thermal correction to Enthalpy= 0.147559
Thermal correction to Gibbs Free Energy= 0.096630
Sum of electronic and zero-point Energies= -534.416976
Sum of electronic and thermal Energies= -534.406479
Sum of electronic and thermal Enthalpies= -534.405534
Sum of electronic and thermal Free Energies= -534.456463

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.002	34.770	107.189
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.806
Rotational	0.889	2.981	30.514
Vibrational	90.225	28.809	35.869

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.696718	-0.249563	0.755321
2	6	0	2.650651	4.540917	-0.778185
3	6	0	1.963521	1.076944	0.860804
4	6	0	1.923833	3.464093	0.020042
5	6	0	2.654210	2.134257	0.006386
6	1	0	0.926579	0.955284	0.525400
7	1	0	3.632940	4.726270	-0.326328
8	1	0	0.911502	3.327610	-0.388199
9	1	0	2.807860	4.191629	-1.805709
10	1	0	1.947705	1.409226	1.906147
11	1	0	1.797516	3.802092	1.058695
12	1	0	3.683770	2.277937	0.364746
13	1	0	2.732728	1.772542	-1.029501
14	6	0	1.841168	5.826604	-0.790699
15	8	0	1.088009	6.035632	-1.778764
16	8	0	1.940828	6.584953	0.210659
17	8	0	2.273818	-1.087937	-0.084622
18	8	0	3.710788	-0.411879	1.485423

$[Cu(Ala)(H_2O)_2]^+$

Zero-point correction= 0.149235 (Hartree/Particle)
Thermal correction to Energy= 0.162064
Thermal correction to Enthalpy= 0.163008
Thermal correction to Gibbs Free Energy= 0.109409
Sum of electronic and zero-point Energies= -2116.114339
Sum of electronic and thermal Energies= -2116.101510
Sum of electronic and thermal Enthalpies= -2116.100565
Sum of electronic and thermal Free Energies= -2116.154165

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.697	45.148	112.809
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.584
Rotational	0.889	2.981	29.963
Vibrational	99.919	39.187	39.885

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.586576	-1.307488	-0.183612
2	6	0	1.739456	-0.743105	-0.231507
3	6	0	1.754629	0.778528	-0.219148
4	1	0	2.518085	1.120642	-0.925481
5	1	0	0.240208	2.197107	-0.199392
6	1	0	0.378296	1.404509	-1.628815
7	8	0	2.806374	-1.357866	-0.240229
8	7	0	0.426228	1.286024	-0.617702
9	29	0	-0.937664	-0.092840	-0.131080
10	8	0	-2.492645	1.208039	-0.206184
11	1	0	-3.262509	0.877290	0.276211
12	8	0	-2.186100	-1.610328	0.400633
13	1	0	-2.789251	-1.334618	1.103418
14	1	0	-2.274669	2.056223	0.203136
15	1	0	-1.669509	-2.337889	0.771754
16	6	0	2.091791	1.252988	1.180499
17	1	0	3.067905	0.870798	1.487331
18	1	0	2.124046	2.345854	1.214128
19	1	0	1.338967	0.902721	1.896344

Alanine ligand

Zero-point correction= 0.094060 (Hartree/Particle)
Thermal correction to Energy= 0.100715
Thermal correction to Enthalpy= 0.101660
Thermal correction to Gibbs Free Energy= 0.062770
Sum of electronic and zero-point Energies= -323.120786
Sum of electronic and thermal Energies= -323.114130
Sum of electronic and thermal Enthalpies= -323.113186
Sum of electronic and thermal Free Energies= -323.152076

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	63.200	22.610	81.850
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.338
Rotational	0.889	2.981	26.502
Vibrational	61.422	16.648	16.010

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.977520	-0.944506	-0.436018
2	6	0	1.981408	-0.273136	-0.094670
3	6	0	1.813419	1.221780	0.191372
4	1	0	2.437826	1.721203	-0.570591
5	1	0	0.389574	2.660255	0.080153
6	1	0	0.016124	1.310844	-0.759942
7	8	0	3.152114	-0.724812	0.012127
8	7	0	0.418110	1.644124	0.111847
9	6	0	2.368656	1.582534	1.556883
10	1	0	3.440840	1.381913	1.621199
11	1	0	2.211335	2.647732	1.759630
12	1	0	1.860094	1.012357	2.343214

[Cu(Cys)(H_2O)$_2$]

Zero-point correction= 0.139966 (Hartree/Particle)
Thermal correction to Energy= 0.153943
Thermal correction to Enthalpy= 0.154887
Thermal correction to Gibbs Free Energy= 0.098319
Sum of electronic and zero-point Energies= -2513.859293
Sum of electronic and thermal Energies= -2513.845316
Sum of electronic and thermal Enthalpies= -2513.844371
Sum of electronic and thermal Free Energies= -2513.900940

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	96.601	48.392	119.059
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.040
Rotational	0.889	2.981	31.246
Vibrational	94.823	42.431	44.395

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.378701	-3.780694	0.218832
2	1	0	1.102909	-3.769905	0.941373
3	6	0	-0.066375	-2.392748	0.006809
4	1	0	-0.712190	-2.376222	-0.877528
5	6	0	-0.863457	-1.967725	1.224327
6	6	0	1.099637	-1.418773	-0.212148
7	1	0	-0.194619	-1.913037	2.093455
8	1	0	-1.294075	-0.975548	1.066848
9	16	0	-2.225056	-3.148837	1.560042
10	8	0	2.240676	-1.781354	0.157738
11	29	0	-1.116951	-4.981112	0.793943
12	1	0	0.834612	-4.134768	-0.622481
13	8	0	0.795096	-0.312151	-0.717470
14	8	0	-2.590859	-6.223191	1.530469
15	1	0	-2.312026	-7.147492	1.564497
16	8	0	-0.249208	-6.608033	-0.210532
17	1	0	-0.420652	-7.453832	0.221793
18	1	0	0.710545	-6.563467	-0.303857
19	1	0	-2.824647	-5.994463	2.439272

Cysteine ligand

Zero-point correction= 0.085097 (Hartree/Particle)
Thermal correction to Energy= 0.092474
Thermal correction to Enthalpy= 0.093418
Thermal correction to Gibbs Free Energy= 0.052458
Sum of electronic and zero-point Energies= -720.837098
Sum of electronic and thermal Energies= -720.829721
Sum of electronic and thermal Enthalpies= -720.828777
Sum of electronic and thermal Free Energies= -720.869737

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	58.028	25.113	86.207
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.237
Rotational	0.889	2.981	28.415
Vibrational	56.251	19.152	17.555

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.129714	1.867726	-0.046913
2	1	0	-0.090584	1.598113	-1.005763
3	6	0	0.361641	0.634318	0.697619
4	1	0	0.827815	0.883538	1.660268
5	6	0	-0.925755	-0.145012	0.994404
6	6	0	1.307886	-0.300475	-0.048779
7	1	0	-1.347126	-0.478343	0.033279
8	1	0	-0.665323	-1.047089	1.562653
9	16	0	-2.180069	0.834026	1.915256
10	8	0	2.009963	-1.078215	0.651487
11	8	0	1.290214	-0.281844	-1.306316
12	1	0	-0.732767	2.261141	0.340015

$[Cu(DmgH)(H_2O)_2]^+$

Zero-point correction= 0.166548 (Hartree/Particle)
Thermal correction to Energy= 0.182199
Thermal correction to Enthalpy= 0.183143
Thermal correction to Gibbs Free Energy= 0.123965
Sum of electronic and zero-point Energies= -2209.368740
Sum of electronic and thermal Energies= -2209.353090
Sum of electronic and thermal Enthalpies= -2209.352146
Sum of electronic and thermal Free Energies= -2209.411324

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.332	55.049	124.552
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.986
Rotational	0.889	2.981	30.997
Vibrational	112.554	49.087	50.191

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.128484	-0.026504	-0.037753
2	6	0	1.570123	0.758757	-0.009785
3	6	0	1.604046	-0.711426	0.003934
4	6	0	2.820604	1.546017	0.032794
5	1	0	2.628540	2.617150	0.028117
6	1	0	3.388719	1.288313	0.932764
7	1	0	3.448443	1.290300	-0.827172
8	6	0	2.849407	-1.514043	0.040878
9	1	0	2.836360	-2.192830	0.901126
10	1	0	2.925095	-2.140705	-0.855368
11	1	0	3.741047	-0.890450	0.103104
12	7	0	0.435354	-1.280319	-0.013737
13	7	0	0.388438	1.265614	-0.055760
14	8	0	0.268984	2.628950	-0.055844
15	1	0	-0.693575	2.773600	-0.060477
16	8	0	0.267757	-2.551277	-0.002686
17	8	0	-2.442352	1.555014	0.096155
18	1	0	-2.916125	1.557464	0.938260
19	8	0	-2.301644	-1.664166	-0.089845
20	1	0	-2.889189	-1.746526	0.671038
21	1	0	-3.126118	1.536664	-0.586369
22	1	0	-1.618677	-2.365213	0.002553

Dimethylglyoxime ligand

Zero-point correction= 0.112706 (Hartree/Particle)
Thermal correction to Energy= 0.121791
Thermal correction to Enthalpy= 0.122735
Thermal correction to Gibbs Free Energy= 0.078860
Sum of electronic and zero-point Energies= -416.368783
Sum of electronic and thermal Energies= -416.359698
Sum of electronic and thermal Enthalpies= -416.358754
Sum of electronic and thermal Free Energies= -416.402629

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.425	31.850	92.342
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.136
Rotational	0.889	2.981	28.447
Vibrational	74.647	25.888	23.758

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.378050	-1.559385	0.042034
2	6	0	1.580980	-2.779080	0.129041
3	6	0	3.847321	-1.617332	-0.209515
4	1	0	4.393362	-1.181578	0.633938
5	1	0	4.181206	-2.642255	-0.354938
6	1	0	4.104883	-1.022382	-1.091427
7	6	0	0.112752	-2.728089	0.387985
8	1	0	-0.137363	-3.256084	1.316334
9	1	0	-0.251822	-1.704083	0.465410
10	1	0	-0.439973	-3.236450	-0.410989
11	7	0	2.214585	-3.909893	-0.024183
12	7	0	1.752873	-0.439748	0.197452
13	8	0	2.632673	0.655253	0.098799
14	1	0	2.055096	1.417647	0.221600
15	8	0	1.491805	-5.011159	0.062866

$[Cu(Hst)(H_2O)_2]^{2+}$

Zero-point correction= 0.199723 (Hartree/Particle)
Thermal correction to Energy= 0.213577
Thermal correction to Enthalpy= 0.214521
Thermal correction to Gibbs Free Energy= 0.159578
Sum of electronic and zero-point Energies= -2152.905690
Sum of electronic and thermal Energies= -2152.891836
Sum of electronic and thermal Enthalpies= -2152.890891
Sum of electronic and thermal Free Energies= -2152.945834

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.021	51.407	115.637
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.930
Rotational	0.889	2.981	30.904
Vibrational	132.244	45.445	41.426

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.067585	-0.647606	0.161139
2	6	0	-1.479166	1.716888	-0.317494
3	6	0	-2.215090	0.761055	0.602078
4	1	0	-1.785125	2.747935	-0.112970
5	1	0	-1.715818	1.498574	-1.362796
6	1	0	-1.840262	0.888243	1.627365
7	1	0	-3.278296	1.016413	0.619761
8	1	0	2.673555	-1.992189	-0.341485
9	1	0	1.564414	-2.709136	0.450696
10	8	0	2.614140	0.837204	0.021668
11	7	0	-0.020746	1.597140	-0.140290
12	29	0	0.869066	-0.209411	-0.037068
13	1	0	0.467458	2.125029	-0.863845
14	1	0	0.244335	2.025671	0.748897
15	8	0	2.010238	-1.858900	0.348674
16	1	0	3.374570	0.283363	0.242460
17	1	0	2.827077	1.243584	-0.828841
18	7	0	-0.832217	-1.197681	-0.124911
19	6	0	-3.018741	-1.590133	-0.077607
20	1	0	-4.092202	-1.558123	0.018453
21	1	0	-2.767852	-3.594970	-0.778170
22	6	0	-1.041768	-2.439656	-0.529080
23	1	0	-0.291185	-3.146916	-0.848430
24	7	0	-2.350066	-2.712506	-0.507290

Histamine ligand

Zero-point correction= 0.144566 (Hartree/Particle)
Thermal correction to Energy= 0.152151
Thermal correction to Enthalpy= 0.153095
Thermal correction to Gibbs Free Energy= 0.112259
Sum of electronic and zero-point Energies= -359.913591
Sum of electronic and thermal Energies= -359.906005
Sum of electronic and thermal Enthalpies= -359.905061
Sum of electronic and thermal Free Energies= -359.945898

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.476	28.348	85.947
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.031
Rotational	0.889	2.981	28.119
Vibrational	93.699	22.387	17.797

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.140659	-0.590211	-0.306978
2	6	0	-1.398867	1.750549	0.242414
3	6	0	-2.463502	0.861446	-0.380275
4	1	0	-1.254226	1.434187	1.288737
5	1	0	-1.770672	2.780622	0.275732
6	1	0	-3.409735	1.034684	0.145205
7	1	0	-2.615029	1.159949	-1.426359
8	7	0	-0.161583	1.728494	-0.533967
9	1	0	0.566921	2.214788	-0.018580
10	1	0	0.148433	0.762861	-0.625670
11	7	0	-1.213796	-1.196543	-1.134744
12	6	0	-2.649182	-1.510997	0.565073
13	1	0	-3.386160	-1.428690	1.349415
14	1	0	-2.172056	-3.590260	0.719724
15	6	0	-1.175917	-2.454943	-0.755319
16	1	0	-0.557981	-3.229956	-1.186688
17	7	0	-2.023672	-2.697638	0.266931

$[Cu(His)(H_2O)_2]^+$

Zero-point correction= 0.202823 (Hartree/Particle)
Thermal correction to Energy= 0.218747
Thermal correction to Enthalpy= 0.219691
Thermal correction to Gibbs Free Energy= 0.159352
Sum of electronic and zero-point Energies= -2341.006986
Sum of electronic and thermal Energies= -2340.991062
Sum of electronic and thermal Enthalpies= -2340.990118
Sum of electronic and thermal Free Energies= -2341.050457

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	137.266	59.061	126.995
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.485
Rotational	0.889	2.981	32.544
Vibrational	135.488	53.099	50.588

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.086280	-0.650499	0.161198
2	6	0	-1.497651	1.720794	-0.386187
3	6	0	-2.257474	0.773600	0.536218
4	1	0	-1.707594	1.469002	-1.430641
5	1	0	-1.916670	0.950456	1.567324
6	1	0	-3.323862	1.014854	0.504434
7	1	0	2.696406	-1.879543	-0.557490
8	1	0	1.670395	-2.724464	0.219281
9	8	0	2.582890	0.880283	0.036232
10	7	0	-0.050722	1.584896	-0.159456
11	29	0	0.857908	-0.201047	-0.021798
12	1	0	0.453752	2.103101	-0.880815
13	1	0	0.165884	2.072771	0.715254
14	8	0	2.063094	-1.844560	0.171597
15	1	0	3.354006	0.336902	0.246854
16	1	0	2.778070	1.285631	-0.819467
17	7	0	-0.847194	-1.212222	-0.088047
18	6	0	-3.034188	-1.610027	-0.013291
19	1	0	-4.107492	-1.574943	0.082137
20	1	0	-2.774457	-3.655544	-0.580959
21	6	0	-1.054905	-2.479576	-0.404647
22	1	0	-0.308654	-3.207877	-0.681355
23	7	0	-2.361740	-2.755778	-0.365593
24	6	0	-1.978121	3.158745	-0.118029
25	8	0	-1.266963	3.873214	0.624157
26	8	0	-3.070390	3.473984	-0.642355

Histidine ligand

Zero-point correction= 0.146989 (Hartree/Particle)
Thermal correction to Energy= 0.157046
Thermal correction to Enthalpy= 0.157990
Thermal correction to Gibbs Free Energy= 0.109869
Sum of electronic and zero-point Energies= -548.013563
Sum of electronic and thermal Energies= -548.003506
Sum of electronic and thermal Enthalpies= -548.002562
Sum of electronic and thermal Free Energies= -548.050683

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	98.548	36.569	101.281
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	41.006
Rotational	0.889	2.981	30.294
Vibrational	96.770	30.608	29.981

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.181354	0.856797	1.849593
2	6	0	-1.303633	1.411067	-0.460184
3	6	0	-2.412410	0.773924	0.381399
4	1	0	-0.350066	0.941723	-0.184758
5	1	0	-3.361053	1.272468	0.137833
6	1	0	-2.517971	-0.274262	0.076547
7	7	0	-1.217112	2.835386	-0.168837
8	1	0	-0.522453	3.253603	-0.783736
9	1	0	-2.102759	3.263431	-0.436046
10	7	0	-2.980006	1.606573	2.688200
11	6	0	-1.191955	0.253171	2.573424
12	1	0	-0.384122	-0.402897	2.286457
13	1	0	-0.838465	0.364755	4.678052
14	6	0	-2.473258	1.447743	3.892162
15	1	0	-2.847073	1.892273	4.803522
16	7	0	-1.390105	0.642304	3.876356
17	6	0	-1.578388	1.050733	-1.927698
18	8	0	-2.182974	1.888184	-2.641905
19	8	0	-1.205960	-0.091768	-2.302360

$[Cu(i\text{-}Val)(H_2O)_3]^+$

Zero-point correction= 0.185694 (Hartree/Particle)
Thermal correction to Energy= 0.200649
Thermal correction to Enthalpy= 0.201593
Thermal correction to Gibbs Free Energy= 0.142369
Sum of electronic and zero-point Energies= -2139.299551
Sum of electronic and thermal Energies= -2139.284596
Sum of electronic and thermal Enthalpies= -2139.283652
Sum of electronic and thermal Free Energies= -2139.342877

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	125.909	52.004	124.649
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.784
Rotational	0.889	2.981	30.974
Vibrational	124.132	46.042	50.513

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.110706	-0.306760	-0.860070
2	1	0	-2.347329	-1.374109	-0.943915
3	1	0	-2.276211	0.151392	-1.844060
4	6	0	-3.016257	0.354450	0.179755
5	1	0	-2.752860	1.420290	0.229633
6	6	0	-4.464637	0.226753	-0.256398
7	1	0	-4.750451	-0.830412	-0.332701
8	1	0	-5.136444	0.702533	0.465647
9	1	0	-4.634136	0.690944	-1.234092
10	6	0	-2.804321	-0.272151	1.547557
11	1	0	-1.771316	-0.159766	1.897728
12	1	0	-3.459131	0.185364	2.296516
13	1	0	-3.032198	-1.345825	1.514240
14	6	0	-0.663101	-0.159737	-0.550466
15	8	0	-0.139800	0.978845	-0.353792
16	8	0	0.108179	-1.168686	-0.485864
17	29	0	1.652234	0.029627	-0.100637
18	8	0	2.878894	1.608464	0.157779
19	1	0	3.583310	1.398453	0.785327
20	8	0	3.088523	-1.338138	0.237300
21	1	0	2.867563	-2.157068	-0.226267
22	1	0	2.379498	2.332789	0.558139
23	1	0	3.941840	-1.055507	-0.118011

i-Valeric acid ligand

Zero-point correction= 0.132834 (Hartree/Particle)
Thermal correction to Energy= 0.140698
Thermal correction to Enthalpy= 0.141642
Thermal correction to Gibbs Free Energy= 0.100485
Sum of electronic and zero-point Energies= -346.325072
Sum of electronic and thermal Energies= -346.317207
Sum of electronic and thermal Enthalpies= -346.316263
Sum of electronic and thermal Free Energies= -346.357420

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.289	27.859	86.623
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.749
Rotational	0.889	2.981	27.718
Vibrational	86.512	21.898	19.155

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.530323	0.303110	0.027114
2	1	0	0.913484	-0.724061	-0.037373
3	1	0	0.874243	0.842358	-0.865770
4	6	0	-0.997169	0.267264	0.035340
5	1	0	-1.359668	1.305185	0.070355
6	6	0	-1.512748	-0.384590	-1.235926
7	1	0	-1.165213	-1.424301	-1.302532
8	1	0	-2.608162	-0.399518	-1.261606
9	1	0	-1.160398	0.141513	-2.130285
10	6	0	-1.513058	-0.468280	1.261801
11	1	0	-1.196735	0.014228	2.194196
12	1	0	-2.607760	-0.514314	1.267094
13	1	0	-1.135364	-1.499904	1.275569
14	6	0	1.110547	0.993446	1.251544
15	8	0	0.806825	2.204200	1.424385
16	8	0	1.848152	0.323107	2.021784

$[Cu(Lct)(H_2O)_2]^+$

Zero-point correction= 0.135499 (Hartree/Particle)
Thermal correction to Energy= 0.148466
Thermal correction to Enthalpy= 0.149410
Thermal correction to Gibbs Free Energy= 0.095809
Sum of electronic and zero-point Energies= -2135.990478
Sum of electronic and thermal Energies= -2135.977511
Sum of electronic and thermal Enthalpies= -2135.976567
Sum of electronic and thermal Free Energies= -2136.030168

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.164	45.289	112.813
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.599
Rotational	0.889	2.981	30.004
Vibrational	91.387	39.327	39.833

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.689882	-1.210107	0.750917
2	1	0	3.676149	-0.741025	0.740114
3	1	0	2.227370	-1.032050	1.727262
4	1	0	2.816917	-2.286617	0.612518
5	6	0	1.828526	-0.644887	-0.351185
6	1	0	2.283997	-0.821803	-1.331626
7	6	0	1.642426	0.859411	-0.210771
8	8	0	2.642662	1.574626	-0.197129
9	8	0	0.442201	1.305713	-0.115458
10	8	0	0.541180	-1.297045	-0.322985
11	1	0	0.417532	-1.822227	-1.124474
12	29	0	-0.970910	0.006234	-0.105759
13	8	0	-2.375191	1.424447	0.295801
14	8	0	-2.366620	-1.417539	-0.153090
15	1	0	-2.056187	-2.223825	0.280498
16	1	0	-3.159508	1.312972	-0.257712
17	1	0	-3.166337	-1.153452	0.321611
18	1	0	-2.022962	2.298007	0.078051

Lactic acid ligand

Zero-point correction= 0.081822 (Hartree/Particle)
Thermal correction to Energy= 0.088182
Thermal correction to Enthalpy= 0.089127
Thermal correction to Gibbs Free Energy= 0.051652
Sum of electronic and zero-point Energies= -343.012942
Sum of electronic and thermal Energies= -343.006581
Sum of electronic and thermal Enthalpies= -343.005637
Sum of electronic and thermal Free Energies= -343.043111

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	55.335	21.730	78.871
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.371
Rotational	0.889	2.981	26.460
Vibrational	53.558	15.768	13.040

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.883515	1.061457	-1.464609
2	1	0	-0.675812	2.043855	-1.031479
3	1	0	-0.245918	0.923155	-2.345585
4	1	0	-1.929090	1.047653	-1.790616
5	6	0	-0.629624	-0.043449	-0.456740
6	1	0	-1.226386	0.137381	0.448729
7	6	0	0.844200	-0.023863	-0.046185
8	8	0	1.619805	-0.871501	-0.544443
9	8	0	1.165920	0.895806	0.748222
10	8	0	-0.962176	-1.312977	-1.004476
11	1	0	-1.880446	-1.274301	-1.294557

$[Cu(Leu)(H_2O)_2]^+$

Zero-point correction= 0.233908 (Hartree/Particle)
Thermal correction to Energy= 0.250165
Thermal correction to Enthalpy= 0.251109
Thermal correction to Gibbs Free Energy= 0.191215
Sum of electronic and zero-point Energies= -2233.900448
Sum of electronic and thermal Energies= -2233.884191
Sum of electronic and thermal Enthalpies= -2233.883247
Sum of electronic and thermal Free Energies= -2233.943141

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.981	60.229	126.058
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.188
Rotational	0.889	2.981	31.856
Vibrational	155.203	54.267	50.636

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.048022	-1.025050	-0.224797
2	6	0	2.093958	-0.320496	-0.478686
3	6	0	1.962261	1.172833	-0.211233
4	1	0	2.631584	1.709830	-0.892610
5	1	0	0.323094	2.420928	0.023127
6	1	0	0.390325	1.697027	-1.450800
7	8	0	3.155788	-0.790541	-0.886309
8	7	0	0.555652	1.550514	-0.455214
9	29	0	-0.578926	0.016307	0.118551
10	8	0	-2.200671	1.194225	0.446678
11	1	0	-2.935477	0.711573	0.848983
12	8	0	-1.690692	-1.665057	0.398314
13	1	0	-2.286410	-1.586284	1.154883
14	1	0	-1.998852	1.916674	1.056231
15	1	0	-1.115201	-2.415837	0.596037
16	6	0	2.310846	1.536362	1.229942
17	1	0	2.161385	2.621797	1.309582
18	1	0	1.572430	1.070685	1.901822
19	6	0	3.724695	1.177036	1.692419
20	1	0	4.391485	1.190488	0.817016
21	6	0	4.223520	2.213601	2.686865
22	1	0	3.546932	2.271687	3.550037
23	1	0	5.219673	1.956094	3.063027
24	1	0	4.276735	3.211102	2.237658
25	6	0	3.774774	-0.205647	2.327842
26	1	0	3.384615	-0.991321	1.672930
27	1	0	4.801551	-0.478379	2.595591
28	1	0	3.177037	-0.214157	3.249058

Leucine ligand

Zero-point correction= 0.178556 (Hartree/Particle)
Thermal correction to Energy= 0.189027
Thermal correction to Enthalpy= 0.189971
Thermal correction to Gibbs Free Energy= 0.142294
Sum of electronic and zero-point Energies= -440.911144
Sum of electronic and thermal Energies= -440.900673
Sum of electronic and thermal Enthalpies= -440.899729
Sum of electronic and thermal Free Energies= -440.947406

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	118.616	37.662	100.346
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.502
Rotational	0.889	2.981	29.470
Vibrational	116.839	31.700	30.374

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.983803	-1.038065	0.087464
2	6	0	2.057780	-0.391335	0.168191
3	6	0	1.994959	1.140746	0.087878
4	1	0	2.895474	1.461305	-0.452734
5	1	0	0.715006	1.184627	-1.484372
6	1	0	0.002175	1.436247	-0.056332
7	8	0	3.197427	-0.897833	0.345467
8	7	0	0.828027	1.679223	-0.602334
9	6	0	2.056419	1.671541	1.517012
10	1	0	1.181090	1.280040	2.061249
11	1	0	2.943931	1.245068	2.007971
12	6	0	2.101237	3.188003	1.677476
13	1	0	1.185300	3.612987	1.243195
14	6	0	2.132517	3.538370	3.156690
15	1	0	3.048104	3.151167	3.623851
16	1	0	2.113560	4.622995	3.311835
17	1	0	1.278760	3.107248	3.692026
18	6	0	3.298944	3.797277	0.968201
19	1	0	3.264499	3.648193	-0.116146
20	1	0	3.355453	4.876736	1.149309
21	1	0	4.232192	3.349303	1.336968

[Cu(ox)(H_2O)$_2$]

Zero-point correction= 0.077244 (Hartree/Particle)
Thermal correction to Energy= 0.088822
Thermal correction to Enthalpy= 0.089767
Thermal correction to Gibbs Free Energy= 0.039098
Sum of electronic and zero-point Energies= -2170.354359
Sum of electronic and thermal Energies= -2170.342780
Sum of electronic and thermal Enthalpies= -2170.341836
Sum of electronic and thermal Free Energies= -2170.392504

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	55.737	39.185	106.642
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.583
Rotational	0.889	2.981	29.838
Vibrational	53.959	33.224	33.843

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.989901	1.472882	0.019614
2	8	0	3.207974	1.337959	0.002953
3	8	0	1.366412	2.590718	0.017699
4	6	0	1.076169	0.216532	0.046403
5	8	0	-0.179524	0.464480	0.033894
6	8	0	1.580088	-0.900330	0.076397
7	29	0	-0.564450	2.370118	0.016583
8	8	0	-2.563659	2.086310	0.032764
9	8	0	-0.862742	4.358530	-0.017082
10	1	0	-0.050251	4.827748	0.214599
11	1	0	-1.519602	4.629981	0.637136
12	1	0	-2.760920	1.140016	0.023999
13	1	0	-2.963470	2.441464	-0.772037

Oxalic acid ligand

Zero-point correction= 0.023771 (Hartree/Particle)
Thermal correction to Energy= 0.028690
Thermal correction to Enthalpy= 0.029634
Thermal correction to Gibbs Free Energy= -0.005430
Sum of electronic and zero-point Energies= -377.361692
Sum of electronic and thermal Energies= -377.356773
Sum of electronic and thermal Enthalpies= -377.355829
Sum of electronic and thermal Free Energies= -377.390893

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	18.003	15.313	73.798
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.336
Rotational	0.889	2.981	26.126
Vibrational	16.226	9.351	8.336

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.840862	1.537159	-0.000022
2	8	0	3.076996	1.389192	-0.141596
3	8	0	1.241136	2.628234	0.141543
4	6	0	0.962010	0.235488	0.000031
5	8	0	-0.274131	0.383453	-0.141452
6	8	0	1.561724	-0.855562	0.141835

$[Cu(Slh)(H_2O)_2]^+$

Zero-point correction= 0.155567 (Hartree/Particle)
Thermal correction to Energy= 0.168590
Thermal correction to Enthalpy= 0.169534
Thermal correction to Gibbs Free Energy= 0.116764
Sum of electronic and zero-point Energies= -2213.068917
Sum of electronic and thermal Energies= -2213.055893
Sum of electronic and thermal Enthalpies= -2213.054949
Sum of electronic and thermal Free Energies= -2213.107720

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	105.792	49.811	111.065
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.068
Rotational	0.889	2.981	31.362
Vibrational	104.014	43.850	36.258

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.307079	-0.492752	0.446474
2	6	0	1.521333	-0.600725	-0.184730
3	6	0	2.245784	0.547429	-0.587922
4	6	0	1.651476	1.817916	-0.310869
5	6	0	0.398622	1.888967	0.343847
6	6	0	-0.273325	0.758863	0.722120
7	1	0	-0.217068	-1.398559	0.739129
8	1	0	1.960351	-1.571940	-0.392595
9	1	0	-0.019018	2.874036	0.538564
10	1	0	-1.232953	0.820725	1.222551
11	8	0	3.387822	0.387190	-1.174717
12	6	0	2.257354	3.048026	-0.669863
13	8	0	3.343966	3.226102	-1.254327
14	1	0	1.693409	3.953970	-0.398013
15	29	0	4.543383	1.776394	-1.808784
16	8	0	5.828761	0.338245	-2.424613
17	1	0	6.751075	0.615136	-2.352430
18	8	0	5.860031	3.153420	-2.523645
19	1	0	6.201419	3.658781	-1.773501
20	1	0	5.369820	3.797851	-3.052313
21	1	0	5.742995	-0.454615	-1.879578

Salicylaldehyde ligand

Zero-point correction= 0.100334 (Hartree/Particle)
Thermal correction to Energy= 0.107526
Thermal correction to Enthalpy= 0.108470
Thermal correction to Gibbs Free Energy= 0.068445
Sum of electronic and zero-point Energies= -420.081665
Sum of electronic and thermal Energies= -420.074474
Sum of electronic and thermal Enthalpies= -420.073529
Sum of electronic and thermal Free Energies= -420.113554

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.473	27.018	84.239
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.287
Rotational	0.889	2.981	28.716
Vibrational	65.696	21.057	15.236

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.506932	-0.473805	0.004641
2	6	0	1.876218	-0.490101	0.047104
3	6	0	2.655253	0.714317	0.044768
4	6	0	1.897391	1.940466	-0.005238
5	6	0	0.487951	1.915480	-0.048083
6	6	0	-0.214489	0.737859	-0.043992
7	1	0	-0.035917	-1.416483	0.008615
8	1	0	2.418230	-1.432477	0.084289
9	1	0	-0.037307	2.867386	-0.084848
10	1	0	-1.298995	0.730845	-0.077465
11	8	0	3.928475	0.674377	0.083723
12	6	0	2.587606	3.198176	-0.011441
13	8	0	2.058663	4.313446	-0.052717
14	1	0	3.690987	3.130017	0.024855

$[Cu(Src)(H_2O)_2]^+$

Zero-point correction= 0.149489 (Hartree/Particle)
Thermal correction to Energy= 0.162034
Thermal correction to Enthalpy= 0.162978
Thermal correction to Gibbs Free Energy= 0.110902
Sum of electronic and zero-point Energies= -2116.099438
Sum of electronic and thermal Energies= -2116.086893
Sum of electronic and thermal Enthalpies= -2116.085948
Sum of electronic and thermal Free Energies= -2116.138025

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.678	44.713	109.604
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.584
Rotational	0.889	2.981	30.014
Vibrational	99.900	38.751	36.629

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.921326	-1.024619	-0.314626
2	6	0	1.994268	-0.348072	-0.117126
3	6	0	1.802551	1.096084	0.284800
4	1	0	1.912830	1.138483	1.375100
5	1	0	2.584437	1.726992	-0.149201
6	1	0	0.472173	1.866776	-1.044286
7	8	0	3.130309	-0.816470	-0.196590
8	7	0	0.458765	1.581058	-0.064343
9	29	0	-0.741401	-0.038327	-0.048744
10	8	0	-2.438845	1.061570	0.224814
11	1	0	-3.218231	0.493622	0.156384
12	8	0	-1.804020	-1.783405	-0.097520
13	1	0	-2.500259	-1.779709	0.572347
14	1	0	-2.465388	1.424197	1.120526
15	1	0	-1.224239	-2.521564	0.132448
16	6	0	0.059406	2.740137	0.745562
17	1	0	0.838206	3.510865	0.724681
18	1	0	-0.866794	3.162548	0.354335
19	1	0	-0.095644	2.423834	1.780179

Sarcosine ligand

Zero-point correction= 0.094651 (Hartree/Particle)
Thermal correction to Energy= 0.101027
Thermal correction to Enthalpy= 0.101971
Thermal correction to Gibbs Free Energy= 0.064410
Sum of electronic and zero-point Energies= -323.109018
Sum of electronic and thermal Energies= -323.102642
Sum of electronic and thermal Enthalpies= -323.101698
Sum of electronic and thermal Free Energies= -323.139258

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	63.395	21.500	79.052
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.338
Rotational	0.889	2.981	26.683
Vibrational	61.618	15.538	13.031

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.655133	1.309933	-0.053258
2	6	0	0.670071	0.055538	-0.024155
3	6	0	-0.648559	-0.684966	0.126012
4	1	0	-0.629898	-1.568793	-0.522272
5	1	0	-0.657287	-1.075661	1.162459
6	1	0	-1.716226	0.997878	0.321990
7	8	0	1.701202	-0.665469	-0.063754
8	7	0	-1.825640	0.111402	-0.164967
9	6	0	-3.025598	-0.550812	0.316918
10	1	0	-3.901655	0.083578	0.160937
11	1	0	-3.187737	-1.479514	-0.240856
12	1	0	-2.976734	-0.814821	1.386376

[Cu(Suc)(H_2O)$_2$]

Zero-point correction= 0.132754 (Hartree/Particle)
Thermal correction to Energy= 0.147211
Thermal correction to Enthalpy= 0.148155
Thermal correction to Gibbs Free Energy= 0.089987
Sum of electronic and zero-point Energies= -2248.869006
Sum of electronic and thermal Energies= -2248.854549
Sum of electronic and thermal Enthalpies= -2248.853605
Sum of electronic and thermal Free Energies= -2248.911773

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.376	49.314	122.426
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	41.999
Rotational	0.889	2.981	31.689
Vibrational	90.599	43.353	47.360

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.679680	-0.504053	-0.732851
2	1	0	-2.095687	-1.110398	0.078793
3	1	0	-1.696504	-1.148226	-1.622188
4	6	0	-2.481709	0.759557	-0.961475
5	1	0	-2.059239	1.336611	-1.793061
6	6	0	-0.244434	-0.263661	-0.423157
7	8	0	0.330905	0.835301	-0.684401
8	8	0	0.465692	-1.174990	0.109136
9	29	0	2.042750	0.063093	0.055029
10	8	0	3.349832	1.492675	-0.410756
11	1	0	4.076307	1.539068	0.225077
12	8	0	3.420686	-1.094059	0.945033
13	1	0	3.204706	-2.022246	0.782624
14	1	0	2.918673	2.357240	-0.382165
15	1	0	4.297451	-0.956175	0.561555
16	1	0	-2.419688	1.416182	-0.085613
17	6	0	-3.956842	0.546118	-1.276334
18	8	0	-4.661456	1.588889	-1.330369
19	8	0	-4.376209	-0.620389	-1.473552

Succinic acid

Zero-point correction= 0.079707 (Hartree/Particle)
Thermal correction to Energy= 0.086398
Thermal correction to Enthalpy= 0.087342
Thermal correction to Gibbs Free Energy= 0.047528
Sum of electronic and zero-point Energies= -455.894485
Sum of electronic and thermal Energies= -455.887794
Sum of electronic and thermal Enthalpies= -455.886850
Sum of electronic and thermal Free Energies= -455.926664

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	54.215	23.154	83.797
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.161
Rotational	0.889	2.981	28.260
Vibrational	52.438	17.193	15.376

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.060072	1.861237	-0.130871
2	1	0	-0.309803	2.681884	0.499594
3	1	0	-0.339861	2.048803	-1.132559
4	6	0	-0.436569	0.539901	0.412162
5	1	0	-0.106198	0.390790	1.445710
6	1	0	-1.534731	0.541169	0.449655
7	6	0	1.575077	2.008967	-0.180391
8	8	0	2.271273	1.316579	0.605768
9	8	0	2.037660	2.855003	-0.993389
10	6	0	-0.037563	-0.688640	-0.395362
11	8	0	0.356827	-0.533940	-1.579545
12	8	0	-0.161623	-1.804945	0.178585

[Cu(Asp)(H_2O)$_2$]

Zero-point correction= 0.152334 (Hartree/Particle)
Thermal correction to Energy= 0.167421
Thermal correction to Enthalpy= 0.168365
Thermal correction to Gibbs Free Energy= 0.109041
Sum of electronic and zero-point Energies= -2304.213027
Sum of electronic and thermal Energies= -2304.197940
Sum of electronic and thermal Enthalpies= -2304.196996
Sum of electronic and thermal Free Energies= -2304.256320

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	105.058	52.734	124.858
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.200
Rotational	0.889	2.981	31.838
Vibrational	103.281	46.773	49.443

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.980093	-0.657489	0.137976
2	6	0	-1.367084	1.766201	-0.434363
3	6	0	-2.193067	0.813484	0.416451
4	1	0	-1.444500	1.488784	-1.490525
5	1	0	-1.961061	0.990828	1.477222
6	1	0	-3.255466	1.031153	0.281519
7	1	0	2.626698	-1.937065	-0.437597
8	1	0	1.217260	-2.564930	-0.444556
9	8	0	2.691211	0.842546	0.254760
10	8	0	-0.792767	-1.074542	-0.114031
11	8	0	-2.949651	-1.424672	0.175858
12	7	0	0.050834	1.702210	-0.048628
13	29	0	0.883376	-0.096221	0.014091
14	1	0	0.601174	2.282463	-0.683682
15	1	0	0.145248	2.142574	0.870886
16	8	0	1.778939	-1.934432	0.025000
17	1	0	3.427825	0.218335	0.220277
18	1	0	2.874581	1.490669	-0.438094
19	6	0	-1.938788	3.183907	-0.252845
20	8	0	-2.936378	3.468385	-0.953814
21	8	0	-1.389493	3.913557	0.603598

Aspartic acid ligand

Zero-point correction= 0.097056 (Hartree/Particle)
Thermal correction to Energy= 0.105930
Thermal correction to Enthalpy= 0.106874
Thermal correction to Gibbs Free Energy= 0.061859
Sum of electronic and zero-point Energies= -511.217363
Sum of electronic and thermal Energies= -511.208489
Sum of electronic and thermal Enthalpies= -511.207545
Sum of electronic and thermal Free Energies= -511.252560

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.472	30.132	94.742
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.523
Rotational	0.889	2.981	29.190
Vibrational	64.694	24.170	25.029

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.910588	-0.665079	0.095329
2	6	0	-1.360251	1.791323	-0.431289
3	6	0	-2.237418	0.806587	0.321569
4	1	0	-1.473344	1.589197	-1.509804
5	1	0	-2.188313	1.015800	1.398071
6	1	0	-3.285555	0.936733	0.022909
7	8	0	-1.298910	-0.994388	-0.952111
8	8	0	-2.317693	-1.470762	0.974585
9	7	0	0.023995	1.649711	0.010129
10	1	0	0.407468	0.803111	-0.402520
11	1	0	0.569746	2.429502	-0.345626
12	6	0	-1.884506	3.216804	-0.238434
13	8	0	-3.052221	3.434878	-0.656577
14	8	0	-1.136692	4.073021	0.292673

$[Cu(AspH)(H_2O)_2]^+$

Zero-point correction= 0.165646 (Hartree/Particle)
Thermal correction to Energy= 0.180793
Thermal correction to Enthalpy= 0.181737
Thermal correction to Gibbs Free Energy= 0.122715
Sum of electronic and zero-point Energies= -2304.649425
Sum of electronic and thermal Energies= -2304.634277
Sum of electronic and thermal Enthalpies= -2304.633333
Sum of electronic and thermal Free Energies= -2304.692355

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	113.449	53.911	124.223
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.213
Rotational	0.889	2.981	31.890
Vibrational	111.672	47.950	48.742

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.978617	-0.636913	0.228571
2	6	0	-1.296966	1.788408	-0.281792
3	6	0	-2.238358	0.839655	0.445995
4	1	0	-1.251118	1.526230	-1.344581
5	1	0	-2.170835	1.030141	1.527211
6	1	0	-3.272066	1.041187	0.156825
7	1	0	2.570270	-1.929251	-0.638782
8	1	0	1.157101	-2.540298	-0.525659
9	8	0	2.746760	0.849169	0.067430
10	8	0	-0.793908	-1.034813	-0.055582
11	8	0	-2.927305	-1.418386	0.351798
12	7	0	0.052312	1.703229	0.279590
13	29	0	0.907594	-0.087748	0.018488
14	1	0	0.655713	2.410012	-0.143513
15	1	0	0.017873	1.916387	1.278953
16	8	0	1.767270	-1.921959	-0.102225
17	1	0	3.462149	0.211908	-0.058554
18	1	0	2.833985	1.477969	-0.661571
19	6	0	-1.833349	3.198457	-0.173987
20	8	0	-2.879924	3.385110	-0.971004
21	8	0	-1.377818	4.046042	0.555539
22	1	0	-3.221994	4.286554	-0.847475

Aspartic acid-H ligand

Zero-point correction= 0.109776 (Hartree/Particle)
Thermal correction to Energy= 0.118494
Thermal correction to Enthalpy= 0.119438
Thermal correction to Gibbs Free Energy= 0.074858
Sum of electronic and zero-point Energies= -511.669768
Sum of electronic and thermal Energies= -511.661050
Sum of electronic and thermal Enthalpies= -511.660106
Sum of electronic and thermal Free Energies= -511.704685

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.356	30.400	93.825
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.546
Rotational	0.889	2.981	29.199
Vibrational	72.578	24.438	24.080

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.968532	-0.662780	0.199622
2	6	0	-1.413711	1.758603	-0.420639
3	6	0	-2.272531	0.797527	0.403563
4	1	0	-1.558718	1.541103	-1.484980
5	1	0	-2.108101	1.005172	1.472382
6	1	0	-3.334584	0.953111	0.203123
7	8	0	-0.701285	-0.976931	-0.023553
8	8	0	-2.819666	-1.529377	0.261300
9	7	0	-0.002142	1.532971	-0.098624
10	6	0	-1.911695	3.187039	-0.153729
11	8	0	-2.966782	3.524810	-0.743970
12	8	0	-1.255613	3.887319	0.651892
13	1	0	0.191887	1.992269	0.791311
14	1	0	0.583790	1.993075	-0.790519
15	1	0	-0.164400	-0.112850	-0.049896

$[Cu(Asp)_2(H_2O)_2]^{2-}$

Zero-point correction= 0.202112 (Hartree/Particle)
Thermal correction to Energy= 0.221352
Thermal correction to Enthalpy= 0.222296
Thermal correction to Gibbs Free Energy= 0.151336
Sum of electronic and zero-point Energies= -2662.640311
Sum of electronic and thermal Energies= -2662.621071
Sum of electronic and thermal Enthalpies= -2662.620127
Sum of electronic and thermal Free Energies= -2662.691087

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.900	67.946	149.348
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.231
Rotational	0.889	2.981	34.347
Vibrational	137.123	61.984	70.392

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.836120	-0.603543	0.428000
2	6	0	-2.354994	1.791007	-0.388696
3	6	0	-3.079968	0.883009	0.591759
4	1	0	-2.496898	1.418896	-1.409758
5	1	0	-2.783454	1.155301	1.616407
6	1	0	-4.157759	1.050729	0.524763
7	6	0	2.302057	-1.708859	-0.865091
8	1	0	0.347648	-2.253988	-1.175057
9	1	0	0.807501	-2.329652	0.376969
10	6	0	2.863460	0.524588	0.287937
11	6	0	3.110084	-0.967104	0.187606
12	1	0	2.363054	-1.175115	-1.820367
13	1	0	2.896198	-1.404186	1.175117
14	1	0	4.177767	-1.114269	0.006867
15	8	0	1.706059	0.992215	0.006735
16	8	0	-1.708212	-1.011726	-0.017624
17	8	0	3.800905	1.249637	0.655575
18	8	0	-3.745798	-1.384768	0.747039
19	7	0	0.890900	-1.759577	-0.467293
20	7	0	-0.915938	1.785539	-0.103774
21	29	0	-0.007396	0.002668	-0.159721
22	1	0	-0.428348	2.391683	-0.763585
23	1	0	-0.760271	2.211431	0.812255
24	6	0	-2.971031	3.198367	-0.311014
25	8	0	-4.087041	3.335575	-0.866891
26	8	0	-2.336671	4.079946	0.312256
27	6	0	2.913268	-3.105990	-1.066876
28	8	0	2.325898	-4.081224	-0.545342
29	8	0	3.979475	-3.143704	-1.726452

$[Cu(Asp)(AspH)(H_2O)_2]^-$

Zero-point correction= 0.214530 (Hartree/Particle)
Thermal correction to Energy= 0.234054
Thermal correction to Enthalpy= 0.234999
Thermal correction to Gibbs Free Energy= 0.163123
Sum of electronic and zero-point Energies= -2663.081443
Sum of electronic and thermal Energies= -2663.061919
Sum of electronic and thermal Enthalpies= -2663.060975
Sum of electronic and thermal Free Energies= -2663.132850

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	146.871	69.505	151.275
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.240
Rotational	0.889	2.981	34.059
Vibrational	145.094	63.543	72.598

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.834570	-0.657870	-0.058705
2	6	0	-2.345357	1.825339	-0.386484
3	6	0	-3.067306	0.756589	0.424889
4	1	0	-2.485226	1.636257	-1.455824
5	1	0	-2.733277	0.820213	1.471308
6	1	0	-4.143591	0.946913	0.418067
7	6	0	2.317031	-1.734107	0.480921
8	1	0	0.925143	-2.195575	-0.938881
9	1	0	0.362043	-2.367582	0.589394
10	6	0	2.895303	0.668374	-0.163418
11	6	0	3.166687	-0.807773	-0.374533
12	1	0	2.766750	-2.737246	0.449732
13	1	0	4.227415	-0.996684	-0.199051
14	1	0	2.976455	-1.040307	-1.430080
15	8	0	1.714182	1.026168	0.177641
16	8	0	-1.652596	-0.995810	-0.420566
17	8	0	3.824538	1.471148	-0.321294
18	8	0	-3.787226	-1.450330	-0.086503
19	7	0	0.939587	-1.777183	-0.009024
20	7	0	-0.906266	1.789488	-0.100041
21	29	0	0.011427	0.013980	-0.093901
22	1	0	-0.406251	2.393391	-0.752291
23	1	0	-0.760777	2.211133	0.821183
24	6	0	-2.968886	3.188337	-0.044786
25	8	0	-3.998355	3.501822	-0.687204
26	8	0	-2.426503	3.852316	0.868850
27	6	0	2.305832	-1.348988	1.940439
28	8	0	1.320629	-1.345469	2.638887
29	8	0	3.525252	-1.046023	2.376766
30	1	0	3.483314	-0.832723	3.323947

$[Cu(AspH)_2(H_2O)_2]$

Zero-point correction= 0.227306 (Hartree/Particle)
Thermal correction to Energy= 0.247111
Thermal correction to Enthalpy= 0.248055
Thermal correction to Gibbs Free Energy= 0.175705
Sum of electronic and zero-point Energies= -2663.519769
Sum of electronic and thermal Energies= -2663.499964
Sum of electronic and thermal Enthalpies= -2663.499020
Sum of electronic and thermal Free Energies= -2663.571370

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	155.065	71.025	152.275
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.250
Rotational	0.889	2.981	34.078
Vibrational	153.287	65.064	73.570

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.818518	-0.642298	0.001075
2	6	0	-2.317431	1.842610	-0.255421
3	6	0	-3.032785	0.756004	0.544431
4	1	0	-2.490471	1.688663	-1.325695
5	1	0	-2.669186	0.784218	1.581651
6	1	0	-4.106873	0.950855	0.572092
7	6	0	2.322449	-1.748984	0.432640
8	1	0	0.937552	-2.170731	-1.007124
9	1	0	0.367119	-2.387675	0.513818
10	6	0	2.907431	0.666460	-0.153887
11	6	0	3.177164	-0.804561	-0.397522
12	1	0	2.770228	-2.752038	0.380268
13	1	0	4.236876	-0.999479	-0.223114
14	1	0	2.990117	-1.011509	-1.458987
15	8	0	1.721711	1.019450	0.179201
16	8	0	-1.653604	-0.962566	-0.422347
17	8	0	3.838674	1.471448	-0.279694
18	8	0	-3.773045	-1.429686	-0.008457
19	7	0	0.946721	-1.779915	-0.065207
20	7	0	-0.879580	1.808319	-0.002431
21	29	0	0.026807	0.012504	-0.094797
22	1	0	-0.388991	2.438097	-0.637316
23	1	0	-0.695711	2.161173	0.939876
24	6	0	-2.899419	3.184245	0.129420
25	8	0	-4.071350	3.399766	-0.459245
26	8	0	-2.378381	3.953920	0.901023
27	6	0	2.303564	-1.397194	1.900687
28	8	0	1.315220	-1.415277	2.594504
29	8	0	3.518731	-1.095056	2.348343
30	1	0	-4.437339	4.245472	-0.150369
31	1	0	3.471478	-0.901305	3.299503

[Cu(Glu)(H_2O)$_2$]

Zero-point correction= 0.181482 (Hartree/Particle)
Thermal correction to Energy= 0.197531
Thermal correction to Enthalpy= 0.198475
Thermal correction to Gibbs Free Energy= 0.137113
Sum of electronic and zero-point Energies= -2343.472892
Sum of electronic and thermal Energies= -2343.456844
Sum of electronic and thermal Enthalpies= -2343.455899
Sum of electronic and thermal Free Energies= -2343.517261

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	123.952	57.013	129.147
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.377
Rotational	0.889	2.981	32.151
Vibrational	122.175	51.051	53.242

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.342774	-0.864837	-1.098928
2	6	0	-3.019835	-0.494285	0.052607
3	6	0	-1.541400	-0.155639	0.312347
4	1	0	-1.227161	-0.725225	1.198340
5	1	0	-0.997290	-1.470965	-1.157196
6	1	0	-0.785805	0.088557	-1.582482
7	8	0	-3.787415	-0.360914	1.034670
8	7	0	-0.674234	-0.567767	-0.807971
9	29	0	1.253598	-0.698983	-0.260182
10	8	0	1.047903	-2.685183	0.117650
11	1	0	1.772503	-3.046874	0.644806
12	8	0	3.113580	-0.689580	0.575745
13	1	0	3.665360	-0.032565	0.131458
14	1	0	0.243722	-2.881565	0.617422
15	1	0	3.590525	-1.526563	0.503807
16	6	0	-1.401928	1.333310	0.602937
17	1	0	-1.751258	1.901285	-0.273149
18	1	0	-2.094140	1.564062	1.416696
19	6	0	-0.002131	1.810933	1.007805
20	1	0	-0.098675	2.728447	1.593631
21	1	0	0.481518	1.053899	1.639198
22	6	0	0.874421	2.128159	-0.185388
23	8	0	1.523144	1.169737	-0.748199
24	8	0	0.932864	3.290834	-0.606640

Glutamic acid ligand

Zero-point correction= 0.126269 (Hartree/Particle)
Thermal correction to Energy= 0.136234
Thermal correction to Enthalpy= 0.137179
Thermal correction to Gibbs Free Energy= 0.089481
Sum of electronic and zero-point Energies= -550.479299
Sum of electronic and thermal Energies= -550.469334
Sum of electronic and thermal Enthalpies= -550.468390
Sum of electronic and thermal Free Energies= -550.516087

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.488	34.501	100.388
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.826
Rotational	0.889	2.981	30.129
Vibrational	83.711	28.539	29.432

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.014209	-1.845634	0.049217
2	1	0	0.606764	-1.957480	-0.771076
3	6	0	-0.616615	-0.526652	0.000149
4	1	0	-1.249884	-0.483463	-0.894546
5	6	0	-1.495921	-0.353235	1.230259
6	6	0	0.384455	0.633415	-0.082657
7	1	0	-2.240251	-1.160893	1.234573
8	1	0	-0.874354	-0.487537	2.128477
9	6	0	-2.207436	0.993701	1.299667
10	8	0	1.351832	0.613834	0.721048
11	1	0	-1.473623	1.802026	1.405186
12	1	0	-2.770044	1.160065	0.373153
13	6	0	-3.152447	1.011629	2.489548
14	8	0	-2.665802	1.308346	3.612775
15	8	0	-4.352525	0.686705	2.288324
16	8	0	0.161011	1.539680	-0.926691
17	1	0	0.652370	-1.849377	0.844247

$[Cu(GluH)(H_2O)_2]^+$

Zero-point correction= 0.194106 (Hartree/Particle)
Thermal correction to Energy= 0.210309
Thermal correction to Enthalpy= 0.211254
Thermal correction to Gibbs Free Energy= 0.149651
Sum of electronic and zero-point Energies= -2343.910348
Sum of electronic and thermal Energies= -2343.894144
Sum of electronic and thermal Enthalpies= -2343.893200
Sum of electronic and thermal Free Energies= -2343.954803

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	131.971	58.577	129.655
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.389
Rotational	0.889	2.981	32.177
Vibrational	130.194	52.615	53.711

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.223103	3.520290	-0.007652
2	6	0	2.560193	2.410219	0.328530
3	6	0	1.754337	1.156841	0.069526
4	1	0	1.747634	0.568410	0.996481
5	1	0	0.030066	2.235131	0.347482
6	1	0	0.329266	1.869537	-1.223123
7	8	0	3.697073	2.140055	0.962389
8	7	0	0.368555	1.497847	-0.272251
9	29	0	-0.877442	-0.083292	-0.064705
10	8	0	-1.089786	0.408797	1.891574
11	1	0	-1.704730	-0.187111	2.340289
12	8	0	-2.128016	-1.669478	0.125506
13	1	0	-1.923707	-2.176422	0.922607
14	1	0	-0.251595	0.320133	2.365854
15	1	0	-1.969729	-2.269164	-0.616068
16	6	0	2.430260	0.348113	-1.036545
17	1	0	2.483372	0.966164	-1.944816
18	1	0	3.460942	0.166271	-0.721464
19	6	0	1.770302	-0.998219	-1.349706
20	1	0	2.522135	-1.657335	-1.790070
21	1	0	1.415094	-1.462562	-0.420684
22	6	0	0.634690	-0.882340	-2.346141
23	8	0	-0.547118	-0.616295	-1.912450
24	8	0	0.869946	-1.034952	-3.550878
25	1	0	4.201370	2.962793	1.078922

Glutamic acid-H ligand

Zero-point correction= 0.139896 (Hartree/Particle)
Thermal correction to Energy= 0.150287
Thermal correction to Enthalpy= 0.151231
Thermal correction to Gibbs Free Energy= 0.102140
Sum of electronic and zero-point Energies= -550.930184
Sum of electronic and thermal Energies= -550.919793
Sum of electronic and thermal Enthalpies= -550.918849
Sum of electronic and thermal Free Energies= -550.967940

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.307	35.267	103.322
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.847
Rotational	0.889	2.981	30.176
Vibrational	92.529	29.305	32.298

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.049435	-1.786402	-0.004684
2	1	0	0.511751	-1.997169	-0.893062
3	6	0	-0.631117	-0.455533	-0.044789
4	1	0	-1.236109	-0.423673	-0.953598
5	6	0	-1.498677	-0.335443	1.196527
6	6	0	0.453257	0.632382	-0.084552
7	1	0	-2.222951	-1.162068	1.188015
8	1	0	-0.863698	-0.469455	2.083609
9	6	0	-2.239661	0.991791	1.283128
10	8	0	1.494213	0.391784	0.569259
11	1	0	-1.524421	1.810583	1.421385
12	1	0	-2.790932	1.170919	0.353205
13	6	0	-3.200460	0.959253	2.464121
14	8	0	-2.699738	1.099323	3.610162
15	8	0	-4.418787	0.759120	2.223578
16	8	0	0.183296	1.663298	-0.733574
17	1	0	0.775939	-1.753828	0.721508
18	1	0	-0.607284	-2.542407	0.208876

$[Cu(Glu)_2(H_2O)_2]^{2-}$

Zero-point correction= 0.258265 (Hartree/Particle)
Thermal correction to Energy= 0.279789
Thermal correction to Enthalpy= 0.280733
Thermal correction to Gibbs Free Energy= 0.203842
Sum of electronic and zero-point Energies= -2741.166811
Sum of electronic and thermal Energies= -2741.145287
Sum of electronic and thermal Enthalpies= -2741.144343
Sum of electronic and thermal Free Energies= -2741.221234

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	175.570	77.401	161.832
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.478
Rotational	0.889	2.981	34.987
Vibrational	173.793	71.440	81.989

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.682840	1.006984	0.076405
2	6	0	2.746892	0.295045	0.034897
3	6	0	2.580512	-1.221990	0.051424
4	1	0	2.980843	-1.554022	1.018619
5	1	0	0.940927	-2.038640	-0.894875
6	1	0	0.930989	-2.274829	0.721683
7	8	0	3.887026	0.770129	0.005113
8	7	0	1.148716	-1.586275	0.004727
9	29	0	-0.014591	0.017016	0.181979
10	1	0	-1.233053	1.919006	1.315814
11	1	0	-0.807923	2.371943	-0.230867
12	6	0	-2.768433	-0.247748	0.110927
13	6	0	-2.537125	1.238972	-0.135606
14	7	0	-1.197497	1.615981	0.345143
15	8	0	-1.724872	-0.977358	0.253892
16	8	0	-3.925087	-0.682078	0.124544
17	1	0	-3.313135	1.794053	0.406618
18	6	0	3.394856	-1.875466	-1.060289
19	1	0	4.433613	-1.558653	-0.927174
20	1	0	3.069703	-1.474425	-2.029357
21	6	0	3.334535	-3.394198	-1.069258
22	1	0	4.217008	-3.791121	-1.586197
23	1	0	3.399249	-3.787498	-0.045426
24	6	0	2.135507	-4.057698	-1.742738
25	8	0	1.279846	-3.338735	-2.323541
26	8	0	2.095198	-5.312853	-1.683477
27	6	0	-2.688319	1.515380	-1.629631
28	1	0	-3.598666	1.002612	-1.958522
29	1	0	-1.852425	1.044379	-2.165536
30	6	0	-2.811192	2.986230	-2.001554
31	1	0	-3.301492	3.071475	-2.978624
32	1	0	-3.485452	3.494497	-1.298352
33	6	0	-1.543835	3.830432	-2.098041
34	8	0	-0.429598	3.311363	-1.820989
35	8	0	-1.706522	5.021660	-2.463785

Glutamic acid(b) ligand

Zero-point correction= 0.126316 (Hartree/Particle)
Thermal correction to Energy= 0.136071
Thermal correction to Enthalpy= 0.137015
Thermal correction to Gibbs Free Energy= 0.090092
Sum of electronic and zero-point Energies= -550.478782
Sum of electronic and thermal Energies= -550.469027
Sum of electronic and thermal Enthalpies= -550.468083
Sum of electronic and thermal Free Energies= -550.515007

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.386	34.409	98.759
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.826
Rotational	0.889	2.981	29.865
Vibrational	83.608	28.447	28.067

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.265574	1.603165	-0.308899
2	1	0	-3.182860	1.273941	-0.601331
3	6	0	-1.310097	0.508835	-0.438351
4	1	0	-1.161922	0.314002	-1.509610
5	6	0	0.036441	0.900240	0.161694
6	6	0	-1.734710	-0.817732	0.205750
7	1	0	-0.088349	1.057956	1.242931
8	1	0	0.717750	0.048705	0.047540
9	6	0	0.656750	2.132782	-0.474157
10	8	0	-2.467814	-0.774743	1.225485
11	1	0	1.724056	2.171665	-0.214434
12	1	0	0.605851	2.058919	-1.567216
13	6	0	0.085704	3.475763	-0.039373
14	8	0	-0.182939	3.641356	1.178861
15	8	0	-0.023767	4.369730	-0.922469
16	8	0	-1.279698	-1.869114	-0.318007
17	1	0	-2.359847	1.830017	0.680185

$[Cu(Glu)(GluH)(H_2O)_2]^-$

Zero-point correction= 0.271540 (Hartree/Particle)
Thermal correction to Energy= 0.293258
Thermal correction to Enthalpy= 0.294202
Thermal correction to Gibbs Free Energy= 0.217433
Sum of electronic and zero-point Energies= -2741.610530
Sum of electronic and thermal Energies= -2741.588812
Sum of electronic and thermal Enthalpies= -2741.587868
Sum of electronic and thermal Free Energies= -2741.664637

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	184.022	78.788	161.575
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.486
Rotational	0.889	2.981	35.069
Vibrational	182.245	72.827	81.642

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.608805	1.028463	-0.232036
2	6	0	2.663442	0.302131	-0.265784
3	6	0	2.453853	-1.207816	-0.145386
4	1	0	2.598255	-1.431217	0.921271
5	1	0	0.953324	-1.713562	-1.457918
6	1	0	0.758254	-2.386616	0.018134
7	8	0	3.808103	0.755082	-0.344419
8	7	0	1.048550	-1.533250	-0.457195
9	29	0	-0.093142	0.056279	-0.010447
10	1	0	-1.152652	1.914597	1.358552
11	1	0	-0.819300	2.455979	-0.184059
12	6	0	-2.840971	-0.119807	0.176747
13	6	0	-2.572349	1.365280	-0.038420
14	7	0	-1.191924	1.675443	0.370559
15	8	0	-1.816326	-0.891030	0.197042
16	8	0	-4.006700	-0.514410	0.278130
17	1	0	-3.293772	1.932262	0.563097
18	6	0	3.464105	-2.003826	-0.954337
19	1	0	4.461249	-1.682979	-0.642921
20	1	0	3.369938	-1.745234	-2.016761
21	6	0	3.358225	-3.506177	-0.765651
22	1	0	4.316906	-3.988197	-0.995629
23	1	0	3.147432	-3.769475	0.278891
24	6	0	2.353893	-4.197351	-1.632007
25	8	0	1.735759	-3.702984	-2.548687
26	8	0	2.227072	-5.487947	-1.297965
27	6	0	-2.799540	1.684862	-1.514819
28	1	0	-3.736917	1.197870	-1.805428
29	1	0	-2.004324	1.211205	-2.107464
30	6	0	-2.916142	3.165903	-1.846750
31	1	0	-3.460223	3.281711	-2.791647
32	1	0	-3.538683	3.669748	-1.094428
33	6	0	-1.641842	3.990189	-1.996489
34	8	0	-0.525671	3.456012	-1.760727
35	8	0	-1.801446	5.182525	-2.360162
36	1	0	1.594149	-5.908782	-1.902654

Glutamic acid-H(b) ligand

Zero-point correction= 0.139244 (Hartree/Particle)
Thermal correction to Energy= 0.149420
Thermal correction to Enthalpy= 0.150364
Thermal correction to Gibbs Free Energy= 0.102400
Sum of electronic and zero-point Energies= -550.924668
Sum of electronic and thermal Energies= -550.914492
Sum of electronic and thermal Enthalpies= -550.913548
Sum of electronic and thermal Free Energies= -550.961512

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.762	35.934	100.949
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.847
Rotational	0.889	2.981	30.158
Vibrational	91.985	29.972	29.945

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.013028	-1.845105	0.082531
2	6	0	-0.615812	-0.528100	0.008694
3	1	0	-1.245725	-0.497349	-0.888455
4	6	0	-1.500647	-0.342744	1.232833
5	6	0	0.383851	0.634689	-0.081572
6	1	0	-2.243905	-1.149683	1.247597
7	1	0	-0.885295	-0.452851	2.136985
8	6	0	-2.215010	1.008516	1.257462
9	8	0	1.353805	0.617495	0.718087
10	1	0	-1.491711	1.824748	1.358657
11	1	0	-2.781913	1.151887	0.332603
12	6	0	-3.170738	1.050607	2.401525
13	8	0	-2.572915	1.361138	3.558186
14	8	0	-4.353811	0.795746	2.331609
15	8	0	0.151479	1.538480	-0.924787
16	1	0	0.662520	-1.830279	0.868294
17	1	0	0.593261	-1.977651	-0.743363
18	1	0	-3.230857	1.327226	4.272061

$[Cu(GluH)_2(H_2O)_2]$

Zero-point correction= 0.284490 (Hartree/Particle)
Thermal correction to Energy= 0.306425
Thermal correction to Enthalpy= 0.307369
Thermal correction to Gibbs Free Energy= 0.230729
Sum of electronic and zero-point Energies= -2742.053127
Sum of electronic and thermal Energies= -2742.031192
Sum of electronic and thermal Enthalpies= -2742.030248
Sum of electronic and thermal Free Energies= -2742.106888

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.285	80.378	161.303
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.495
Rotational	0.889	2.981	35.082
Vibrational	190.507	74.416	81.348

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.639654	0.995964	-0.206239
2	6	0	2.690239	0.262974	-0.244094
3	6	0	2.470958	-1.245261	-0.124242
4	1	0	2.616302	-1.471136	0.941743
5	1	0	0.960767	-1.731778	-1.433818
6	1	0	0.763367	-2.409047	0.041555
7	8	0	3.836552	0.710038	-0.326333
8	7	0	1.062672	-1.558153	-0.432600
9	29	0	-0.065155	0.037760	0.024613
10	1	0	-1.195211	1.806655	1.461395
11	1	0	-0.804692	2.472877	0.000688
12	6	0	-2.818124	-0.149928	0.171365
13	6	0	-2.551217	1.340944	-0.021891
14	7	0	-1.191004	1.645593	0.456234
15	8	0	-1.788769	-0.910898	0.228973
16	8	0	-3.983714	-0.551399	0.220885
17	1	0	-3.300557	1.900375	0.551179
18	6	0	3.471735	-2.049663	-0.937221
19	1	0	4.472758	-1.745309	-0.621626
20	1	0	3.383434	-1.783082	-1.998091
21	6	0	3.342133	-3.551639	-0.758675
22	1	0	4.293415	-4.046895	-0.991693
23	1	0	3.126252	-3.819157	0.283627
24	6	0	2.329172	-4.221024	-1.632301
25	8	0	1.733693	-3.715419	-2.557879
26	8	0	2.166333	-5.506261	-1.294134
27	6	0	-2.717198	1.663278	-1.504547
28	1	0	-3.645126	1.185851	-1.833759
29	1	0	-1.902325	1.192432	-2.071110
30	6	0	-2.818247	3.142999	-1.838926
31	1	0	-3.363688	3.283841	-2.779166
32	1	0	-3.406456	3.680514	-1.083146
33	6	0	-1.523569	3.872525	-1.995502
34	8	0	-0.416929	3.414949	-1.803615
35	8	0	-1.715805	5.134346	-2.389178
36	1	0	1.530037	-5.913890	-1.904254
37	1	0	-0.854088	5.575242	-2.468695

Glutamic acid-H(c) ligand

Zero-point correction= 0.138299 (Hartree/Particle)
Thermal correction to Energy= 0.148329
Thermal correction to Enthalpy= 0.149273
Thermal correction to Gibbs Free Energy= 0.101390
Sum of electronic and zero-point Energies= -550.927580
Sum of electronic and thermal Energies= -550.917550
Sum of electronic and thermal Enthalpies= -550.916606
Sum of electronic and thermal Free Energies= -550.964488

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.078	35.668	100.778
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.847
Rotational	0.889	2.981	29.909
Vibrational	91.300	29.706	30.021

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.035134	1.603247	-0.529339
2	6	0	-1.225700	0.385536	-0.566267
3	1	0	-1.232638	-0.049099	-1.575164
4	6	0	0.228014	0.585692	-0.144508
5	6	0	-1.864421	-0.663632	0.330594
6	1	0	0.256611	0.978529	0.880218
7	1	0	0.698250	-0.402397	-0.113712
8	6	0	1.018258	1.483781	-1.080268
9	8	0	-2.946559	-0.246378	0.969678
10	1	0	2.089245	1.270241	-0.971815
11	1	0	0.781859	1.246977	-2.126193
12	6	0	0.887828	2.994213	-0.903990
13	8	0	0.254071	3.447402	0.084178
14	8	0	1.462090	3.699225	-1.773331
15	8	0	-1.436790	-1.791098	0.465116
16	1	0	-1.466210	2.399886	-0.241432
17	1	0	-2.424499	1.808495	-1.442790
18	1	0	-3.056277	0.693031	0.653670

Optimized geometries and energetic parameters of the benchmark 2 (pyridoxamine) Cu^{2+} complexes

Complex A

Zero-point correction= 0.268910 (Hartree/Particle)
Thermal correction to Energy= 0.286980
Thermal correction to Enthalpy= 0.287924
Thermal correction to Gibbs Free Energy= 0.223515
Sum of electronic and zero-point Energies= -2365.025988
Sum of electronic and thermal Energies= -2365.007917
Sum of electronic and thermal Enthalpies= -2365.006973
Sum of electronic and thermal Free Energies= -2365.071383

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.083	68.286	135.562
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.657
Rotational	0.889	2.981	32.934
Vibrational	178.305	62.324	58.593

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	2.091736	-0.278158	0.112397
2	8	0	0.646483	1.083072	0.997440
3	6	0	-0.627391	1.003372	0.533370
4	6	0	-1.230339	-0.248208	0.569528
5	6	0	-1.291609	2.120945	0.043013
6	6	0	-2.521514	-0.390778	0.048861
7	6	0	-3.155765	0.727228	-0.438613
8	1	0	-4.153811	0.710336	-0.857581
9	7	0	-2.539120	1.918807	-0.410439
10	6	0	-0.468393	-1.380464	1.184005
11	1	0	-0.138865	-1.082174	2.183602
12	1	0	-1.099436	-2.264198	1.286311
13	6	0	-3.211458	-1.716752	-0.016870
14	1	0	-3.298412	-2.149054	0.988648
15	1	0	-4.227326	-1.576333	-0.404310
16	6	0	-0.703346	3.476092	0.010110
17	1	0	-0.467299	3.812384	1.026043
18	1	0	0.231131	3.470800	-0.562421
19	1	0	-1.387882	4.194708	-0.442151
20	8	0	-2.450601	-2.560927	-0.865510
21	1	0	-2.820298	-3.449879	-0.816205
22	8	0	3.407956	1.221049	-0.020571
23	1	0	2.961471	2.029056	-0.309565
24	1	0	4.087397	1.046799	-0.686209
25	7	0	0.730648	-1.708721	0.390140
26	1	0	1.227440	-2.477701	0.842779
27	1	0	0.446767	-2.056727	-0.528750
28	1	0	4.112359	-1.273420	-1.050574
29	8	0	3.265164	-1.661756	-0.792631
30	1	0	2.858520	-1.957309	-1.619210
31	1	0	-3.043746	2.727695	-0.774183
32	1	0	0.983192	1.992039	1.050509

Complex B(acid)

Zero-point correction= 0.294782 (Hartree/Particle)
Thermal correction to Energy= 0.315866
Thermal correction to Enthalpy= 0.316810
Thermal correction to Gibbs Free Energy= 0.245585
Sum of electronic and zero-point Energies= -2441.448047
Sum of electronic and thermal Energies= -2441.426963
Sum of electronic and thermal Enthalpies= -2441.426018
Sum of electronic and thermal Free Energies= -2441.497244

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.209	77.833	149.907
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.851
Rotational	0.889	2.981	33.657
Vibrational	196.432	71.871	72.022

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-2.691207	-0.283562	-0.133858
2	8	0	1.645785	-2.196328	0.234070
3	6	0	2.264881	-1.004068	0.177596
4	6	0	1.496032	0.138139	0.398424
5	6	0	3.630011	-0.896163	-0.092530
6	6	0	2.093615	1.400576	0.295022
7	6	0	3.436577	1.471709	0.015354
8	1	0	3.979575	2.402636	-0.084728
9	7	0	4.142426	0.342333	-0.152795
10	6	0	0.034636	-0.021599	0.690316
11	1	0	-0.140561	-0.929739	1.270587
12	1	0	-0.340052	0.822175	1.273217
13	6	0	1.304231	2.662755	0.444147
14	1	0	0.841102	2.704624	1.438915
15	1	0	1.975031	3.524818	0.352936
16	6	0	4.512406	-2.060968	-0.312608
17	1	0	4.498872	-2.720405	0.562290
18	1	0	4.165905	-2.645948	-1.172093
19	1	0	5.542103	-1.750875	-0.496751
20	8	0	0.309369	2.681531	-0.570528
21	1	0	-0.289243	3.416039	-0.392398
22	8	0	-4.669813	-0.397924	0.174130
23	1	0	-4.992680	0.299512	0.760547
24	1	0	-4.945828	-1.228880	0.583292
25	7	0	-0.756630	-0.103633	-0.555047
26	1	0	-0.585487	0.748803	-1.096546
27	1	0	-0.448201	-0.900253	-1.115419
28	1	0	-3.193203	-2.762900	0.338873
29	8	0	-2.468187	-2.315824	-0.118481
30	1	0	-1.663327	-2.594843	0.340827
31	1	0	5.137724	0.429339	-0.358566
32	8	0	-2.837703	1.754618	-0.084078
33	1	0	-3.742120	2.071272	-0.211679
34	1	0	-2.312674	2.205816	-0.759079
35	1	0	2.246829	-2.930070	0.043964

Complex B(base)

Zero-point correction= 0.281110 (Hartree/Particle)
Thermal correction to Energy= 0.301426
Thermal correction to Enthalpy= 0.302371
Thermal correction to Gibbs Free Energy= 0.233470
Sum of electronic and zero-point Energies= -2441.016900
Sum of electronic and thermal Energies= -2440.996583
Sum of electronic and thermal Enthalpies= -2440.995639
Sum of electronic and thermal Free Energies= -2441.064540

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.148	76.245	145.014
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.840
Rotational	0.889	2.981	33.597
Vibrational	187.371	70.284	67.199

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.757131	-3.170520	0.999994
2	8	0	1.412034	0.732426	-2.154108
3	6	0	0.433311	1.099689	-1.428138
4	6	0	0.172338	0.569957	-0.132366
5	6	0	-0.475440	2.104699	-1.885345
6	6	0	-0.956217	0.951473	0.599930
7	6	0	-1.809060	1.897231	0.078129
8	1	0	-2.704409	2.249591	0.572649
9	7	0	-1.523518	2.436213	-1.124611
10	6	0	1.122897	-0.453038	0.394405
11	1	0	2.132740	-0.253985	0.027644
12	1	0	1.160241	-0.444084	1.485950
13	6	0	-1.271923	0.353308	1.941323
14	1	0	-0.448379	0.521102	2.642065
15	1	0	-2.163576	0.831534	2.361230
16	6	0	-0.287025	2.776448	-3.186855
17	1	0	0.694015	3.262853	-3.224091
18	1	0	-0.303906	2.044725	-4.001977
19	1	0	-1.060475	3.526101	-3.367832
20	8	0	-1.451517	-1.061058	1.884127
21	1	0	-2.249057	-1.260739	1.378559
22	8	0	2.695934	-4.684838	1.973725
23	1	0	2.462848	-4.698694	2.911624
24	1	0	3.657080	-4.588572	1.946967
25	7	0	0.750370	-1.822898	-0.041097
26	1	0	-0.248324	-1.962158	0.126666
27	1	0	0.917090	-1.921211	-1.043441
28	1	0	4.071847	-3.496189	-0.093965
29	8	0	3.272263	-3.036131	-0.381675
30	1	0	3.542167	-2.119519	-0.529432
31	1	0	-2.157047	3.148010	-1.486245
32	8	0	0.523014	-2.878784	2.587178
33	1	0	0.190463	-3.717101	2.932074
34	1	0	-0.261658	-2.315571	2.408803

Complex C(acid)

Zero-point correction= 0.295685 (Hartree/Particle)
Thermal correction to Energy= 0.316080
Thermal correction to Enthalpy= 0.317024
Thermal correction to Gibbs Free Energy= 0.248392
Sum of electronic and zero-point Energies= -2441.454572
Sum of electronic and thermal Energies= -2441.434177
Sum of electronic and thermal Enthalpies= -2441.433233
Sum of electronic and thermal Free Energies= -2441.501865

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.343	76.811	144.449
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.851
Rotational	0.889	2.981	33.215
Vibrational	196.566	70.850	67.006

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.843674	0.007011	1.609197
2	8	0	0.225546	1.075182	1.555774
3	6	0	-0.788943	0.894867	0.761553
4	6	0	-1.477819	-0.327117	0.616749
5	6	0	-1.250006	2.005294	0.014049
6	6	0	-2.580918	-0.425460	-0.245633
7	6	0	-2.983776	0.688914	-0.939485
8	1	0	-3.820163	0.701608	-1.625652
9	7	0	-2.314288	1.845552	-0.778307
10	6	0	-1.002753	-1.509042	1.400481
11	1	0	-0.394269	-1.192020	2.247233
12	1	0	-1.833760	-2.109171	1.774395
13	6	0	-3.339696	-1.702796	-0.432762
14	1	0	-3.721499	-2.060212	0.532950
15	1	0	-4.200437	-1.525132	-1.086677
16	6	0	-0.584453	3.320447	0.087393
17	1	0	-0.618392	3.706733	1.111193
18	1	0	0.473527	3.217158	-0.177280
19	1	0	-1.051962	4.043749	-0.583257
20	8	0	-2.468924	-2.674292	-1.007245
21	1	0	-2.933029	-3.519350	-1.037833
22	8	0	1.791910	0.160772	3.618129
23	1	0	1.229849	0.908808	3.862331
24	1	0	2.661636	0.350725	3.994736
25	7	0	-0.160279	-2.400777	0.547299
26	1	0	0.225681	-3.172004	1.096683
27	1	0	-0.763101	-2.783469	-0.202696
28	1	0	4.043781	-0.898026	2.516938
29	8	0	3.536837	-1.064746	1.710508
30	1	0	4.140917	-0.870400	0.981372
31	1	0	-2.630896	2.656520	-1.309902
32	8	0	1.777092	-0.356140	-0.402944
33	1	0	2.628164	-0.580640	-0.803529
34	1	0	1.440943	0.402896	-0.900623
35	1	0	0.616221	-1.870792	0.121048

Complex C(base)

Zero-point correction= 0.279703 (Hartree/Particle)
Thermal correction to Energy= 0.300656
Thermal correction to Enthalpy= 0.301601
Thermal correction to Gibbs Free Energy= 0.231594
Sum of electronic and zero-point Energies= -2441.011707
Sum of electronic and thermal Energies= -2440.990753
Sum of electronic and thermal Enthalpies= -2440.989809
Sum of electronic and thermal Free Energies= -2441.059816

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.665	77.729	147.341
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.840
Rotational	0.889	2.981	33.283
Vibrational	186.887	71.767	69.841

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.921417	-0.033159	1.486161
2	8	0	0.786854	0.636197	0.074993
3	6	0	-0.522080	0.648996	0.120785
4	6	0	-1.300831	-0.518782	0.275644
5	6	0	-1.180992	1.885252	-0.019974
6	6	0	-2.700412	-0.429613	0.238070
7	6	0	-3.290705	0.799371	0.064252
8	1	0	-4.361732	0.948921	0.015781
9	7	0	-2.522189	1.896749	-0.048458
10	6	0	-0.594922	-1.835844	0.414171
11	1	0	0.168667	-1.762078	1.197007
12	1	0	-1.290316	-2.606608	0.748756
13	6	0	-3.579134	-1.637125	0.348419
14	1	0	-3.332042	-2.208555	1.252651
15	1	0	-4.625594	-1.319618	0.437108
16	6	0	-0.440373	3.156729	-0.151432
17	1	0	0.242501	3.283562	0.695657
18	1	0	0.175906	3.146994	-1.056506
19	1	0	-1.116770	4.012646	-0.195734
20	8	0	-3.390144	-2.435512	-0.811806
21	1	0	-3.843740	-3.274715	-0.675213
22	8	0	0.764215	0.746758	2.957197
23	1	0	0.375330	1.581244	2.659245
24	1	0	1.305905	0.979133	3.723757
25	7	0	0.047330	-2.284215	-0.821653
26	1	0	-0.658791	-2.335811	-1.553480
27	1	0	2.999665	-0.661282	3.732167
28	8	0	3.149425	-0.945252	2.820726
29	1	0	4.078022	-0.750825	2.634497
30	1	0	-2.985852	2.797025	-0.163083
31	8	0	3.112218	-0.839748	0.057973
32	1	0	4.043801	-0.630302	0.207671
33	1	0	2.886516	-0.456204	-0.800179
34	1	0	0.715869	-1.574917	-1.117275

Complex D

Zero-point correction= 0.254437 (Hartree/Particle)
Thermal correction to Energy= 0.272627
Thermal correction to Enthalpy= 0.273571
Thermal correction to Gibbs Free Energy= 0.209167
Sum of electronic and zero-point Energies= -2364.613642
Sum of electronic and thermal Energies= -2364.595452
Sum of electronic and thermal Enthalpies= -2364.594507
Sum of electronic and thermal Free Energies= -2364.658912

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.076	67.969	135.550
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.646
Rotational	0.889	2.981	32.902
Vibrational	169.298	62.007	58.624

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	2.017540	-0.171946	0.182752
2	8	0	0.660225	1.089730	0.735621
3	6	0	-0.585833	0.935558	0.383791
4	6	0	-1.253901	-0.302097	0.449502
5	6	0	-1.304878	2.062818	-0.063411
6	6	0	-2.590574	-0.405238	0.048030
7	6	0	-3.244487	0.726150	-0.379161
8	1	0	-4.275664	0.736493	-0.706641
9	7	0	-2.589130	1.901052	-0.406156
10	6	0	-0.476434	-1.466584	0.973734
11	1	0	-0.132558	-1.240064	1.988968
12	1	0	-1.087812	-2.368866	1.020183
13	6	0	-3.322627	-1.711070	0.041309
14	1	0	-3.269466	-2.184130	1.030568
15	1	0	-4.381537	-1.535135	-0.183842
16	6	0	-0.682128	3.398077	-0.161974
17	1	0	-0.357621	3.742553	0.825547
18	1	0	0.214080	3.346677	-0.789745
19	1	0	-1.372484	4.130743	-0.584458
20	8	0	-2.726787	-2.543685	-0.944098
21	1	0	-3.136741	-3.414169	-0.889066
22	8	0	3.264161	1.464931	0.081486
23	1	0	2.682564	2.229807	-0.027200
24	1	0	3.809541	1.434476	-0.715291
25	7	0	0.722955	-1.705867	0.143454
26	1	0	1.210310	-2.535730	0.482355
27	1	0	0.437464	-1.908045	-0.816448
28	1	0	4.378465	-0.901830	-0.473695
29	8	0	3.602603	-1.406080	-0.194761
30	1	0	3.436382	-2.036395	-0.907948
31	1	0	-3.099142	2.724129	-0.724971

Complex E

Zero-point correction= 0.240499 (Hartree/Particle)
Thermal correction to Energy= 0.258621
Thermal correction to Enthalpy= 0.259566
Thermal correction to Gibbs Free Energy= 0.195164
Sum of electronic and zero-point Energies= -2364.170580
Sum of electronic and thermal Energies= -2364.152458
Sum of electronic and thermal Enthalpies= -2364.151514
Sum of electronic and thermal Free Energies= -2364.215915

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.287	67.306	135.544
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.635
Rotational	0.889	2.981	32.877
Vibrational	160.510	61.344	58.655

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	2.011835	-0.165017	0.192301
2	8	0	0.661303	1.080085	0.757472
3	6	0	-0.596555	0.922890	0.390640
4	6	0	-1.245108	-0.318089	0.467898
5	6	0	-1.331516	2.037312	-0.080574
6	6	0	-2.578611	-0.409110	0.061094
7	6	0	-3.204845	0.745711	-0.379424
8	1	0	-4.243555	0.700311	-0.703084
9	7	0	-2.607636	1.939685	-0.444368
10	6	0	-0.460575	-1.480967	0.984881
11	1	0	-0.102807	-1.269603	1.998705
12	1	0	-1.067486	-2.387679	1.029972
13	6	0	-3.327901	-1.702683	0.055805
14	1	0	-3.248487	-2.208401	1.027506
15	1	0	-4.392287	-1.506399	-0.126562
16	6	0	-0.655684	3.362447	-0.171722
17	1	0	-0.348697	3.724674	0.816688
18	1	0	0.258408	3.297895	-0.774403
19	1	0	-1.322544	4.101035	-0.621308
20	8	0	-2.794436	-2.535221	-0.973154
21	1	0	-3.240971	-3.388049	-0.927099
22	8	0	3.242274	1.487178	0.081643
23	1	0	2.636618	2.233186	-0.028028
24	1	0	3.782275	1.467197	-0.718950
25	7	0	0.734389	-1.712194	0.141128
26	1	0	1.225815	-2.547286	0.460228
27	1	0	0.437598	-1.897069	-0.818491
28	1	0	4.387289	-0.862054	-0.485814
29	8	0	3.625891	-1.376886	-0.187878
30	1	0	3.464997	-2.024187	-0.886590

Complex E(base)

Zero-point correction= 0.224886 (Hartree/Particle)
Thermal correction to Energy= 0.243498
Thermal correction to Enthalpy= 0.244443
Thermal correction to Gibbs Free Energy= 0.178613
Sum of electronic and zero-point Energies= -2363.692931
Sum of electronic and thermal Energies= -2363.674319
Sum of electronic and thermal Enthalpies= -2363.673375
Sum of electronic and thermal Free Energies= -2363.739205

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.798	67.809	138.551
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.623
Rotational	0.889	2.981	32.892
Vibrational	151.020	61.847	61.658

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.960816	-0.305735	0.050680
2	8	0	0.738213	1.117208	0.607820
3	6	0	-0.547164	0.999912	0.338733
4	6	0	-1.227221	-0.227489	0.450070
5	6	0	-1.283691	2.141693	-0.056841
6	6	0	-2.579632	-0.270537	0.098634
7	6	0	-3.196996	0.903917	-0.308008
8	1	0	-4.249277	0.887004	-0.590079
9	7	0	-2.578744	2.085795	-0.369520
10	6	0	-0.451106	-1.408255	0.966815
11	1	0	-0.129327	-1.172192	1.992169
12	1	0	-1.121059	-2.273651	1.060293
13	6	0	-3.372796	-1.537919	0.117722
14	1	0	-3.258340	-2.065886	1.073765
15	1	0	-4.438627	-1.302751	-0.002030
16	6	0	-0.592287	3.461391	-0.132697
17	1	0	-0.155093	3.743203	0.832604
18	1	0	0.237268	3.437510	-0.850600
19	1	0	-1.293839	4.241308	-0.437024
20	8	0	-2.931398	-2.373768	-0.954042
21	1	0	-3.413722	-3.206251	-0.899908
22	8	0	3.404270	1.220400	-0.102434
23	1	0	2.930018	2.025461	-0.346393
24	1	0	4.026449	1.058049	-0.822077
25	7	0	0.734292	-1.772906	0.197951
26	1	0	0.412441	-1.963715	-0.755615
27	1	0	4.010069	-1.317825	-1.297718
28	8	0	3.535380	-1.622157	-0.514141
29	1	0	3.121227	-2.456432	-0.769093

Complex F

Zero-point correction= 0.405381 (Hartree/Particle)
Thermal correction to Energy= 0.431422
Thermal correction to Enthalpy= 0.432366
Thermal correction to Gibbs Free Energy= 0.348184
Sum of electronic and zero-point Energies= -2783.446609
Sum of electronic and thermal Energies= -2783.420568
Sum of electronic and thermal Enthalpies= -2783.419624
Sum of electronic and thermal Free Energies= -2783.503806

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	270.721	98.842	177.175
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.844
Rotational	0.889	2.981	35.734
Vibrational	268.944	92.881	96.219

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.003406	-0.063563	0.051777
2	8	0	-1.387685	-1.275910	-0.672111
3	6	0	-2.641534	-1.028026	-0.430798
4	6	0	-3.211688	0.254537	-0.569928
5	6	0	-3.484228	-2.088118	-0.030432
6	6	0	-4.557523	0.471497	-0.254932
7	6	0	-5.324700	-0.593706	0.154398
8	1	0	-6.370775	-0.515827	0.419911
9	7	0	-4.769077	-1.816418	0.233486
10	6	0	-2.315392	1.339649	-1.071933
11	1	0	-1.892475	1.030875	-2.034743
12	1	0	-2.859651	2.272093	-1.232006
13	6	0	-5.187234	1.828160	-0.321463
14	1	0	-5.030123	2.277564	-1.310753
15	1	0	-6.269458	1.732824	-0.171048
16	6	0	-2.989235	-3.472986	0.101184
17	1	0	-2.604356	-3.833048	-0.858717
18	1	0	-2.155517	-3.511370	0.810745
19	1	0	-3.777490	-4.148396	0.440023
20	8	0	-4.605710	2.636061	0.693407
21	1	0	-4.954819	3.529935	0.603072
22	7	0	1.252992	-1.652441	0.120205
23	1	0	1.551027	-1.895818	-0.825708
24	1	0	0.698942	-2.439178	0.456768
25	7	0	-1.188927	1.545238	-0.142908
26	1	0	-0.589761	2.296578	-0.483503
27	1	0	-1.543830	1.849984	0.764729
28	6	0	2.435860	-1.470014	0.981560
29	1	0	2.073765	-1.277803	1.997892
30	1	0	3.035221	-2.382398	1.010082
31	6	0	3.249107	-0.297484	0.533480
32	6	0	4.590334	-0.413736	0.151511
33	6	0	2.615983	0.963203	0.533692
34	6	0	5.290763	0.722217	-0.179193
35	6	0	3.386756	2.095397	0.190887
36	1	0	6.328821	0.722605	-0.483995
37	7	0	4.674158	1.916985	-0.131804
38	8	0	1.364995	1.128848	0.849297
39	6	0	2.813550	3.456508	0.189052
40	1	0	1.920424	3.488603	-0.444595
41	1	0	2.493770	3.736334	1.198698
42	1	0	3.533249	4.195124	-0.169816
43	6	0	5.283581	-1.737619	0.062444
44	1	0	6.349390	-1.576307	-0.140162
45	1	0	5.207171	-2.276763	1.015543
46	8	0	4.677242	-2.485004	-0.983609
47	1	0	5.065667	-3.367194	-0.985167
48	1	0	-5.363110	-2.590296	0.528036
49	1	0	5.218856	2.743534	-0.375051

Complex G

Zero-point correction= 0.390788 (Hartree/Particle)
Thermal correction to Energy= 0.417041
Thermal correction to Enthalpy= 0.417985
Thermal correction to Gibbs Free Energy= 0.332229
Sum of electronic and zero-point Energies= -2783.002641
Sum of electronic and thermal Energies= -2782.976388
Sum of electronic and thermal Enthalpies= -2782.975443
Sum of electronic and thermal Free Energies= -2783.061200

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	261.697	98.399	180.490
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.836
Rotational	0.889	2.981	35.715
Vibrational	259.920	92.437	99.561

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.007819	-0.048461	0.013407
2	8	0	-1.391246	-1.263527	-0.725418
3	6	0	-2.639177	-1.023917	-0.454326
4	6	0	-3.219219	0.257188	-0.574092
5	6	0	-3.468307	-2.089497	-0.037899
6	6	0	-4.557729	0.466072	-0.224704
7	6	0	-5.310514	-0.604518	0.197186
8	1	0	-6.350021	-0.533024	0.488846
9	7	0	-4.747781	-1.825097	0.257487
10	6	0	-2.341335	1.347786	-1.096673
11	1	0	-1.940927	1.040479	-2.069574
12	1	0	-2.895600	2.276485	-1.245095
13	6	0	-5.195168	1.820159	-0.265349
14	1	0	-5.062669	2.280391	-1.253063
15	1	0	-6.273453	1.717573	-0.092586
16	6	0	-2.962707	-3.472601	0.074574
17	1	0	-2.607619	-3.828408	-0.898495
18	1	0	-2.105032	-3.508431	0.755295
19	1	0	-3.735072	-4.153846	0.437652
20	8	0	-4.595988	2.621706	0.744411
21	1	0	-4.950874	3.514678	0.669468
22	7	0	1.235442	-1.648596	0.131126
23	1	0	1.557514	-1.898417	-0.805061
24	1	0	0.670336	-2.431498	0.458256
25	7	0	-1.193550	1.560032	-0.196877
26	1	0	-0.598493	2.303406	-0.560650
27	1	0	-1.525075	1.879109	0.714455
28	6	0	2.400123	-1.452873	1.018283
29	1	0	2.008124	-1.247221	2.020913
30	1	0	2.992515	-2.369541	1.078594
31	6	0	3.228475	-0.295637	0.558264
32	6	0	4.573193	-0.410674	0.194891
33	6	0	2.617143	0.967929	0.506735
34	6	0	5.253421	0.740074	-0.168998
35	6	0	3.412942	2.078047	0.128226
36	1	0	6.301150	0.675237	-0.458952
37	7	0	4.698475	1.956168	-0.191942
38	8	0	1.347157	1.147237	0.809405
39	6	0	2.791886	3.432786	0.091895
40	1	0	1.916917	3.452441	-0.569767
41	1	0	2.433903	3.735322	1.083403
42	1	0	3.513748	4.174039	-0.257494
43	6	0	5.281507	-1.726476	0.156596
44	1	0	6.354961	-1.556596	0.001988
45	1	0	5.167373	-2.266072	1.106452
46	8	0	4.743426	-2.504081	-0.912762
47	1	0	5.164724	-3.370528	-0.892635
48	1	0	-5.331802	-2.602929	0.561493

Complex H

Zero-point correction= 0.377609 (Hartree/Particle)
Thermal correction to Energy= 0.403338
Thermal correction to Enthalpy= 0.404282
Thermal correction to Gibbs Free Energy= 0.320706
Sum of electronic and zero-point Energies= -2782.556296
Sum of electronic and thermal Energies= -2782.530567
Sum of electronic and thermal Enthalpies= -2782.529623
Sum of electronic and thermal Free Energies= -2782.613199

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	253.098	97.279	175.900
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.829
Rotational	0.889	2.981	35.689
Vibrational	251.321	91.317	95.005

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000861	0.000613	-0.003390
2	8	0	-1.358065	-1.180342	-0.816280
3	6	0	-2.622447	-0.971578	-0.513351
4	6	0	-3.208715	0.303356	-0.585185
5	6	0	-3.440196	-2.057437	-0.110341
6	6	0	-4.547828	0.454000	-0.214407
7	6	0	-5.249240	-0.674885	0.177757
8	1	0	-6.292785	-0.582058	0.475366
9	7	0	-4.719991	-1.902147	0.218743
10	6	0	-2.355672	1.432081	-1.069375
11	1	0	-1.962870	1.192283	-2.064130
12	1	0	-2.927906	2.359179	-1.157288
13	6	0	-5.228556	1.784821	-0.196358
14	1	0	-5.102465	2.308831	-1.153343
15	1	0	-6.305558	1.639429	-0.041370
16	6	0	-2.845834	-3.423640	-0.056622
17	1	0	-2.511625	-3.752930	-1.048060
18	1	0	-1.958637	-3.446541	0.588536
19	1	0	-3.574728	-4.144662	0.319460
20	8	0	-4.676505	2.566547	0.863121
21	1	0	-5.084091	3.439231	0.833727
22	7	0	1.194001	-1.621177	0.173608
23	1	0	1.513986	-1.907898	-0.752523
24	1	0	0.604221	-2.377445	0.518889
25	7	0	-1.192180	1.622422	-0.180638
26	1	0	-0.602301	2.378599	-0.525948
27	1	0	-1.512221	1.909266	0.745435
28	6	0	2.357559	-1.430870	1.062270
29	1	0	1.964821	-1.191298	2.057105
30	1	0	2.929897	-2.357928	1.149960
31	6	0	3.210467	-0.301980	0.578228
32	6	0	4.549580	-0.452438	0.207372
33	6	0	2.624091	0.972923	0.506663
34	6	0	5.250887	0.676582	-0.184584
35	6	0	3.441734	2.058926	0.103833
36	1	0	6.294430	0.583901	-0.482244
37	7	0	4.721533	1.903807	-0.225315
38	8	0	1.359705	1.181519	0.809692
39	6	0	2.847279	3.425101	0.050408
40	1	0	1.960004	3.448073	-0.594638
41	1	0	2.513174	3.754201	1.041945
42	1	0	3.576098	4.146217	-0.325636
43	6	0	5.230405	-1.783203	0.189029
44	1	0	6.307380	-1.637710	0.033951
45	1	0	5.104449	-2.307384	1.145939
46	8	0	4.678295	-2.564792	-0.870522
47	1	0	5.086044	-3.437408	-0.841392