Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Theoretical Investigations of the Reactivities of Lattice–Framework Carbene Analogues of the Group 14 Elements

Jun Hsiao and Ming-Der Su*

Department of Applied Chemistry, National Chiayi University, Chiayi 60004, Taiwan

Email: midesu@mail.ncyu.edu.tw

(All geometries were calculated B3LYP/LANL2DZ)

Rea-C (Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.211603	0.056699	-0.094005
6	-0.860040	0.734272	-0.542149
6	0.787297	0.077098	1.042660
6	1.995366	-0.323672	0.122092
6	-2.024591	-1.301008	0.001472
6	1.637329	-1.305635	-0.773916
6	3.319924	0.378246	0.275382
1	4.068522	0.008056	-0.434063
1	3.193085	1.460063	0.124515
1	3.717497	0.245690	1.291185
6	2.430730	-1.962270	-1.868070
1	1.992159	-1.761416	-2.856260
1	3.471568	-1.612422	-1.888296
1	2.448722	-3.053798	-1.742733
6	1.119183	-0.021064	2.536935
1	1.607194	-0.974431	2.786805
1	1.785694	0.802365	2.841731
1	0.207423	0.062525	3.140838
6	-0.988816	1.699167	-1.723674
1	-1.539949	1.244326	-2.560428
1	-1.511586	2.620989	-1.417850
1	-0.000262	1.996668	-2.095655
6	-3.429025	0.874809	0.242076
1	-4.258895	0.259091	0.606745
1	-3.169589	1.618269	1.009436
1	-3.778444	1.435383	-0.636680
6	-2.958694	-2.390319	0.445879
1	-2.566231	-2.914194	1.329317
1	-3.951946	-1.998590	0.702697
1	-3.092707	-3.146656	-0.340036
6	-0.088552	1.305924	0.692525
14	-0.163518	-1.039318	-0.282590

Zero-point correction= 0.268194

(Hartree/Particle)

Thermal correction to Energy= 0.284746

Thermal correction to Enthalpy= 0.285690

Thermal correction to Gibbs Free Energy= 0.226018

Sum of electronic and zero-point Energies= -509.511051

Sum of electronic and thermal Energies= -509.494499

Sum of electronic and thermal Enthalpies= -509.493555

Sum of electronic and thermal Free Energies= -509.553227

Rea-C (Triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.221324	0.106889	-0.085567
6	-0.910253	0.802633	-0.581017
6	0.833942	0.074464	1.044933
6	2.063051	-0.315392	0.159328
6	-1.999323	-1.249788	-0.000999
6	1.663944	-1.257852	-0.762600
6	3.403014	0.358341	0.307791
1	4.138370	-0.000916	-0.421436
1	3.293428	1.444933	0.184339
1	3.811542	0.191611	1.314774
6	2.430632	-1.923461	-1.872377
1	2.002331	-1.684656	-2.856448
1	3.484289	-1.613699	-1.881380
1	2.407070	-3.017471	-1.769538
6	1.027449	-0.079537	2.549850
1	1.472125	-1.052537	2.799390
1	1.691004	0.704229	2.947345
1	0.069390	0.007023	3.077086
6	-1.054600	1.678237	-1.821340
1	-1.611945	1.161076	-2.614142
1	-1.591316	2.611095	-1.587987
1	-0.071032	1.958741	-2.217856
6	-3.445320	0.894545	0.306138
1	-4.254927	0.257046	0.679809
1	-3.188644	1.623864	1.087300

1	-3.829367	1.466921	-0.550420
6	-2.898546	-2.358378	0.472292
1	-2.493381	-2.848408	1.369502
1	-3.903990	-1.990295	0.716865
1	-3.007763	-3.136629	-0.296011
6	0.025615	1.255231	0.529269
14	-0.148221	-0.993014	-0.291010

Zero-point correction= 0.269562
(Hartree/Particle)
Thermal correction to Energy= 0.286547
Thermal correction to Enthalpy= 0.287491
Thermal correction to Gibbs Free Energy= 0.225735
Sum of electronic and zero-point Energies= -509.524633
Sum of electronic and thermal Energies= -509.507648
Sum of electronic and thermal Enthalpies= -509.506704
Sum of electronic and thermal Free Energies= -509.568461

Rea-Si (Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-2.221753	-0.089526	-0.030566
14	0.605106	0.020582	0.010329
6	-0.209048	1.596163	1.527902
6	-0.801190	0.172567	1.340436
6	-0.744252	-0.223299	-1.360650
6	-0.047224	-1.600361	-1.538789
6	0.947303	1.710276	0.782341
6	1.088473	-1.638207	-0.754707
6	-0.617101	-2.681261	-2.424136
1	0.010719	-3.579468	-2.445825
1	-1.623694	-2.968176	-2.084272
1	-0.726272	-2.317477	-3.455502
6	2.071857	-2.751115	-0.518823
1	2.110509	-3.033363	0.543718
1	1.820509	-3.652846	-1.094190
1	3.089621	-2.448195	-0.803661

6	-0.973836	0.547720	-2.671054
1	-0.047787	0.614606	-3.263017
1	-1.737417	0.064851	-3.300875
1	-1.313785	1.576552	-2.486539
6	-1.013054	-0.602168	2.651835
1	-0.098982	-0.605645	3.265781
1	-1.820224	-0.163233	3.258985
1	-1.283452	-1.651682	2.469185
6	-0.885080	2.639369	2.383411
1	-0.326425	3.581830	2.414886
1	-1.898538	2.847696	2.008482
1	-1.000502	2.277620	3.414780
6	1.855904	2.889818	0.570682
1	1.905660	3.172238	-0.491032
1	1.524726	3.772275	1.134862
1	2.883492	2.660591	0.886227

Zero-point correction= 0.265928
(Hartree/Particle)
Thermal correction to Energy= 0.283987
Thermal correction to Enthalpy= 0.284931
Thermal correction to Gibbs Free Energy= 0.220952
Sum of electronic and zero-point Energies= -475.396777
Sum of electronic and thermal Energies= -475.378718
Sum of electronic and thermal Enthalpies= -475.377774
Sum of electronic and thermal Free Energies= -475.441752

Rea-Si (Triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-2.161406	-0.071638	-0.033796
14	0.544727	0.022473	0.006584
6	-0.241895	1.616543	1.570185
6	-0.809934	0.189455	1.406799
6	-0.752587	-0.236717	-1.433202
6	-0.081030	-1.620247	-1.578851

6	0.888165	1.714326	0.784505
6	1.028599	-1.640133	-0.758997
6	-0.630816	-2.713066	-2.458259
1	-0.022851	-3.624365	-2.426944
1	-1.654493	-2.968139	-2.148799
1	-0.688552	-2.376145	-3.503116
6	2.027282	-2.732575	-0.494518
1	2.016819	-3.037644	0.562062
1	1.826328	-3.624887	-1.102411
1	3.050689	-2.401093	-0.720059
6	-0.912164	0.563777	-2.727271
1	0.030545	0.590450	-3.296667
1	-1.677780	0.123161	-3.383800
1	-1.215794	1.597632	-2.521406
6	-0.950742	-0.621670	2.696395
1	-0.025629	-0.581939	3.293222
1	-1.764625	-0.237208	3.329738
1	-1.174227	-1.674171	2.482504
6	-0.896519	2.667766	2.428202
1	-0.358629	3.622427	2.409226
1	-1.927227	2.842869	2.087904
1	-0.958852	2.330874	3.472830
6	1.815291	2.874439	0.549226
1	1.820989	3.174743	-0.508688
1	1.529602	3.751870	1.144747
1	2.850978	2.617561	0.812857

Zero-point correction= 0.266399
(Hartree/Particle)
Thermal correction to Energy= 0.284202
Thermal correction to Enthalpy= 0.285146
Thermal correction to Gibbs Free Energy= 0.221398
Sum of electronic and zero-point Energies= -475.374320
Sum of electronic and thermal Energies= -475.356517
Sum of electronic and thermal Enthalpies= -475.355573
Sum of electronic and thermal Free Energies= -475.419322

Rea-Ge (Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-2.330448	-0.087229	-0.033838
14	0.559156	0.020890	0.008054
6	-0.210568	1.602076	1.551191
6	-0.803836	0.185355	1.374076
6	-0.746773	-0.234550	-1.397544
6	-0.049389	-1.604843	-1.561394
6	0.922102	1.714272	0.766598
6	1.062475	-1.640856	-0.740513
6	-0.580900	-2.686856	-2.470230
1	0.051962	-3.581863	-2.471012
1	-1.598116	-2.981372	-2.170443
1	-0.652621	-2.320568	-3.504214
6	2.036567	-2.754764	-0.470665
1	2.035460	-3.040264	0.591773
1	1.808014	-3.655148	-1.057455
1	3.064504	-2.451356	-0.715469
6	-0.960827	0.553841	-2.699565
1	-0.024548	0.642799	-3.273950
1	-1.703942	0.071894	-3.354358
1	-1.316298	1.576689	-2.507863
6	-0.998081	-0.610673	2.674702
1	-0.073102	-0.633678	3.273363
1	-1.788655	-0.176973	3.307252
1	-1.278892	-1.655974	2.480345
6	-0.848438	2.646431	2.435452
1	-0.284117	3.586022	2.449275
1	-1.874733	2.862756	2.101711
1	-0.925624	2.281055	3.469381
6	1.823199	2.893814	0.523440
1	1.840408	3.173373	-0.540290
1	1.509820	3.778262	1.095026
1	2.860504	2.666169	0.807367

Zero-point correction= 0.264996
(Hartree/Particle)
Thermal correction to Energy= 0.283454
Thermal correction to Enthalpy= 0.284398

Thermal correction to Gibbs Free Energy= 0.218905
Sum of electronic and zero-point Energies= -475.306686
Sum of electronic and thermal Energies= -475.288228
Sum of electronic and thermal Enthalpies= -475.287284
Sum of electronic and thermal Free Energies= -475.352776

Rea-Ge (Triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-2.291540	-0.074638	-0.037516
14	0.487573	0.022367	0.004055
6	-0.236351	1.622812	1.597949
6	-0.803977	0.203029	1.448624
6	-0.743364	-0.248473	-1.478746
6	-0.074195	-1.625348	-1.606837
6	0.860274	1.720707	0.764219
6	1.000815	-1.645937	-0.740062
6	-0.577480	-2.713303	-2.519482
1	0.036383	-3.619770	-2.470064
1	-1.611084	-2.980039	-2.256292
1	-0.593063	-2.367324	-3.562872
6	1.993144	-2.734173	-0.439964
1	1.940950	-3.043054	0.614464
1	1.822360	-3.625334	-1.058756
1	3.023626	-2.396941	-0.621244
6	-0.912135	0.559461	-2.764400
1	0.033358	0.609602	-3.329656
1	-1.664058	0.109544	-3.430211
1	-1.236250	1.585417	-2.552124
6	-0.952392	-0.618987	2.727990
1	-0.023418	-0.601632	3.321858
1	-1.755162	-0.227579	3.370997
1	-1.193973	-1.665258	2.505004
6	-0.843483	2.669808	2.495226
1	-0.298347	3.619871	2.461504
1	-1.886620	2.857918	2.203183
1	-0.861845	2.322803	3.538249

6	1.782960	2.876358	0.495804
1	1.739176	3.186650	-0.558586
1	1.533619	3.750090	1.112773
1	2.828763	2.610084	0.705114

Zero-point correction= 0.264993
(Hartree/Particle)
Thermal correction to Energy= 0.283415
Thermal correction to Enthalpy= 0.284359
Thermal correction to Gibbs Free Energy= 0.218710
Sum of electronic and zero-point Energies= -475.278923
Sum of electronic and thermal Energies= -475.260500
Sum of electronic and thermal Enthalpies= -475.259556
Sum of electronic and thermal Free Energies= -475.325205

Rea-Sn (Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.455889	0.020492	0.003760
6	-0.231269	1.615584	1.581726
6	-0.849862	0.213842	1.423488
6	-0.791573	-0.263474	-1.452758
6	-0.071296	-1.617916	-1.591101
6	0.861402	1.714856	0.737890
6	1.000499	-1.640617	-0.715439
6	-0.533513	-2.703700	-2.533453
1	0.110932	-3.589962	-2.500843
1	-1.562330	-3.014124	-2.294949
1	-0.550005	-2.334075	-3.568776
6	1.975473	-2.742952	-0.402536
1	1.932347	-3.028130	0.659407
1	1.784002	-3.646870	-0.997811
1	3.009693	-2.427419	-0.602581
6	-0.940805	0.542310	-2.755050
1	0.028055	0.661843	-3.268790
1	-1.628078	0.055847	-3.464958
1	-1.330399	1.555497	-2.574310

6	-0.977113	-0.602017	2.722003
1	-0.016624	-0.651980	3.262302
1	-1.716865	-0.167042	3.412421
1	-1.287441	-1.640507	2.531737
6	-0.797642	2.664111	2.509233
1	-0.209864	3.589506	2.506068
1	-1.833854	2.910510	2.230822
1	-0.832049	2.286909	3.541311
6	1.765413	2.883502	0.453807
1	1.738548	3.162952	-0.609869
1	1.489619	3.772275	1.038249
1	2.811839	2.643297	0.690269
50	-2.559597	-0.085877	-0.039332

Zero-point correction= 0.264562
(Hartree/Particle)
Thermal correction to Energy= 0.283133
Thermal correction to Enthalpy= 0.284078
Thermal correction to Gibbs Free Energy= 0.217991
Sum of electronic and zero-point Energies= -474.927691
Sum of electronic and thermal Energies= -474.909119
Sum of electronic and thermal Enthalpies= -474.908175
Sum of electronic and thermal Free Energies= -474.974261

Rea-Sn (Triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.409262	0.019781	0.002517
6	-0.263161	1.634966	1.615670
6	-0.831608	0.219173	1.494223
6	-0.769675	-0.265917	-1.524958
6	-0.100836	-1.638833	-1.625602
6	0.806051	1.724712	0.744902
6	0.946567	-1.652749	-0.724241
6	-0.563000	-2.723886	-2.563563
1	0.049073	-3.630718	-2.491997
1	-1.607071	-2.992767	-2.344836

1	-0.535339	-2.373415	-3.605734
6	1.943852	-2.730419	-0.404347
1	1.882367	-3.032687	0.651590
1	1.788663	-3.626803	-1.020259
1	2.973524	-2.384285	-0.575901
6	-0.870646	0.544016	-2.818907
1	0.104742	0.587434	-3.334734
1	-1.588085	0.098787	-3.524870
1	-1.196922	1.573495	-2.626682
6	-0.912376	-0.599889	2.783911
1	0.047361	-0.573142	3.329093
1	-1.681566	-0.211106	3.468374
1	-1.155875	-1.650055	2.581070
6	-0.827567	2.680832	2.541979
1	-0.278442	3.628684	2.491846
1	-1.881118	2.877049	2.292480
1	-0.807070	2.327568	3.583564
6	1.734630	2.870231	0.455437
1	1.681912	3.171758	-0.601357
1	1.500234	3.751196	1.068794
1	2.780817	2.595652	0.655331
50	-2.535167	-0.081991	-0.040856

Zero-point correction= 0.263751
(Hartree/Particle)
Thermal correction to Energy= 0.281810
Thermal correction to Enthalpy= 0.282754
Thermal correction to Gibbs Free Energy= 0.217396
Sum of electronic and zero-point Energies= -474.898060
Sum of electronic and thermal Energies= -474.880001
Sum of electronic and thermal Enthalpies= -474.879056
Sum of electronic and thermal Free Energies= -474.944415

Rea-Pb (Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.421380	0.020114	0.002577

6	-0.225400	1.618768	1.599292
6	-0.851198	0.226059	1.445422
6	-0.790559	-0.275030	-1.476628
6	-0.064301	-1.620459	-1.608129
6	0.846930	1.715329	0.726992
6	0.986526	-1.640742	-0.705016
6	-0.493499	-2.705599	-2.567444
1	0.154355	-3.588703	-2.519230
1	-1.526930	-3.022457	-2.359667
1	-0.481709	-2.332814	-3.601775
6	1.955683	-2.742003	-0.369810
1	1.894131	-3.022205	0.692438
1	1.774927	-3.648975	-0.963722
1	2.993535	-2.428280	-0.552731
6	-0.947637	0.541151	-2.769977
1	0.022264	0.690194	-3.275921
1	-1.616770	0.047804	-3.492613
1	-1.360923	1.543973	-2.581618
6	-0.987508	-0.602318	2.733509
1	-0.024214	-0.684206	3.266694
1	-1.709639	-0.158824	3.437282
1	-1.323769	-1.631313	2.533466
6	-0.757603	2.667325	2.547528
1	-0.168275	3.591462	2.525374
1	-1.802131	2.916582	2.305564
1	-0.756614	2.289132	3.579910
6	1.745772	2.882779	0.421020
1	1.692790	3.163119	-0.641763
1	1.486699	3.772117	1.012664
1	2.797847	2.641004	0.630502
82	-2.640627	-0.086315	-0.042254

Zero-point correction= 0.264158
(Hartree/Particle)
Thermal correction to Energy= 0.282894
Thermal correction to Enthalpy= 0.283838
Thermal correction to Gibbs Free Energy= 0.216689
Sum of electronic and zero-point Energies= -475.024775
Sum of electronic and thermal Energies= -475.006038
Sum of electronic and thermal Enthalpies= -475.005094

Sum of electronic and thermal Free Energies= -475.072243

Rea-Pb (Triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.367732	0.019174	0.001026
6	-0.254166	1.637829	1.641955
6	-0.816694	0.229946	1.532418
6	-0.751712	-0.275185	-1.565022
6	-0.090373	-1.641076	-1.651969
6	0.785333	1.729800	0.732980
6	0.926580	-1.657943	-0.713412
6	-0.516033	-2.723062	-2.611470
1	0.092099	-3.630828	-2.517644
1	-1.568201	-2.991949	-2.433503
1	-0.447476	-2.370919	-3.651658
6	1.921154	-2.730106	-0.371390
1	1.833679	-3.037553	0.681555
1	1.789759	-3.624547	-0.996321
1	2.953053	-2.375452	-0.513256
6	-0.879225	0.533981	-2.853654
1	0.093079	0.604257	-3.375623
1	-1.585462	0.070121	-3.559407
1	-1.230987	1.554424	-2.659498
6	-0.924253	-0.591232	2.815490
1	0.033553	-0.590344	3.368322
1	-1.685540	-0.184318	3.499034
1	-1.191773	-1.634824	2.609290
6	-0.780014	2.681638	2.594074
1	-0.233518	3.629847	2.522131
1	-1.843290	2.878529	2.388728
1	-0.715872	2.327289	3.634028
6	1.712070	2.870081	0.422218
1	1.630552	3.178033	-0.631147
1	1.503501	3.749137	1.048116
1	2.762011	2.586189	0.589059
82	-2.646035	-0.084267	-0.043512

Zero-point correction= 0.262980
(Hartree/Particle)
Thermal correction to Energy= 0.281301
Thermal correction to Enthalpy= 0.282245
Thermal correction to Gibbs Free Energy= 0.215561
Sum of electronic and zero-point Energies= -474.992814
Sum of electronic and thermal Energies= -474.974493
Sum of electronic and thermal Enthalpies= -474.973549
Sum of electronic and thermal Free Energies= -475.040232

C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.044764	0.523063	0.000000
1	-1.529213	-0.435595	0.000000
1	-3.132755	0.489690	0.000000
6	-1.370870	1.690875	0.000000
1	-1.886422	2.649534	0.000000
1	-0.282880	1.724248	0.000000

Zero-point correction= 0.051324
(Hartree/Particle)
Thermal correction to Energy= 0.054355
Thermal correction to Enthalpy= 0.055299
Thermal correction to Gibbs Free Energy= 0.029777
Sum of electronic and zero-point Energies= -78.526885
Sum of electronic and thermal Energies= -78.523854
Sum of electronic and thermal Enthalpies= -78.522910
Sum of electronic and thermal Free Energies= -78.548432

CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	-2.402400	-2.045453	-0.031449
1	-2.037298	-3.078116	-0.031449
1	-2.037281	-1.529132	0.862857
1	-2.037281	-1.529132	-0.925755
1	-3.497697	-2.045440	-0.031449

Zero-point correction= 0.045240
(Hartree/Particle)
Thermal correction to Energy= 0.048103
Thermal correction to Enthalpy= 0.049047
Thermal correction to Gibbs Free Energy= 0.025565
Sum of electronic and zero-point Energies= -40.469232
Sum of electronic and thermal Energies= -40.466369
Sum of electronic and thermal Enthalpies= -40.465425
Sum of electronic and thermal Free Energies= -40.488907

H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z

8	2.757322	0.126781	-0.036124
1	3.734006	0.121936	-0.036124
1	2.426729	1.045829	-0.036124

Zero-point correction= 0.020772
(Hartree/Particle)
Thermal correction to Energy= 0.023609
Thermal correction to Enthalpy= 0.024553
Thermal correction to Gibbs Free Energy= 0.002456
Sum of electronic and zero-point Energies= -76.393544
Sum of electronic and thermal Energies= -76.390708
Sum of electronic and thermal Enthalpies= -76.389764
Sum of electronic and thermal Free Energies= -76.411860

TS-C-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.317084	0.046208	-0.366125
6	0.164824	-0.035948	2.433460
6	1.329539	-0.042968	1.708500
1	-0.345220	-0.956440	2.706806
1	-0.319633	0.896270	2.717005
1	1.883502	0.871822	1.518267
1	1.865333	-0.968084	1.507061
6	-0.349405	-1.219330	-0.916230
6	-0.271389	1.302961	-0.758201
14	-0.970268	-0.116011	-2.332540
6	-1.777731	1.622253	-0.877211
6	-2.383059	1.043632	-1.970956
6	-2.439636	2.455036	0.199868
1	-3.516319	2.576690	0.036388
1	-2.291146	1.990125	1.183747
1	-1.988326	3.456405	0.247344
6	-3.828114	1.070682	-2.401500
1	-4.290340	0.074296	-2.347938
1	-4.422278	1.745818	-1.772419
1	-3.925963	1.416219	-3.439872
6	0.689455	-1.730594	-1.993997
6	0.365764	-1.132281	-3.192630
6	1.881049	-2.575884	-1.635325
1	2.550003	-2.745636	-2.486645
1	2.452299	-2.079687	-0.839684
1	1.563353	-3.555162	-1.248420
6	1.077996	-1.136916	-4.514900
1	1.450733	-0.133353	-4.766666
1	1.938305	-1.819517	-4.504646
1	0.414269	-1.449489	-5.332333
6	0.617111	2.543440	-0.719468
1	0.341207	3.259312	-1.507864
1	0.539646	3.075454	0.244682
1	1.664068	2.251025	-0.863252
6	-1.045258	-2.273677	-0.068267
1	-1.437271	-3.085682	-0.697690

1	-0.353014	-2.722216	0.660966
1	-1.880682	-1.839342	0.494885
-1	-0.10	-0.43	0.12
-2	0.03	0.26	-0.01
-3	0.09	0.52	-0.05
-4	0.05	0.23	-0.02
-5	0.03	0.15	-0.02
-6	0.05	0.17	-0.04
-7	0.05	0.25	-0.07
-8	-0.02	-0.11	-0.02
-9	0.13	0.07	0.05
-0	-0.08	-0.15	-0.18
-1	0.01	-0.02	0.07
-2	-0.03	0.00	0.05
-3	0.01	-0.03	0.00
-4	-0.01	-0.05	0.00
-5	0.00	-0.04	-0.02
-6	0.04	-0.01	-0.01
-7	-0.02	0.01	0.02
-8	0.00	0.03	0.02
-9	-0.02	0.02	0.05
-0	-0.02	0.00	0.00
-1	-0.02	-0.05	0.01
-2	-0.03	-0.06	0.00
-3	0.01	-0.02	0.01
-4	0.01	0.01	0.03
-5	0.03	-0.02	-0.02
-6	0.00	-0.04	0.00
-7	-0.02	-0.03	0.04
-8	-0.01	0.00	0.04
-9	-0.01	-0.01	0.03
-0	-0.03	-0.03	0.06
-1	0.08	0.09	0.04
-2	0.00	0.07	0.07
-3	0.12	0.04	0.08
-4	0.06	0.14	-0.03
-5	0.03	0.03	0.04
-6	0.02	0.10	-0.01
-7	0.06	0.05	0.12
-8	0.04	0.03	0.05

Frequencies -- -290.5484
Red. masses -- 9.7321
Frc consts -- 0.4841
IR Inten -- 4.5206
Zero-point correction= 0.321798
(Hartree/Particle)
Thermal correction to Energy= 0.341599
Thermal correction to Enthalpy= 0.342543
Thermal correction to Gibbs Free Energy= 0.275407
Sum of electronic and zero-point Energies= -588.046125
Sum of electronic and thermal Energies= -588.026324
Sum of electronic and thermal Enthalpies= -588.025380
Sum of electronic and thermal Free Energies= -588.092516

TS-Si-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.662921	0.011493	-0.466657
6	-0.333425	-0.000112	2.275486
6	1.013804	-0.005124	1.978143
1	1.592400	-0.925897	1.986838
1	1.601912	0.909207	1.994973
1	-0.889364	-0.926765	2.404216
1	-0.879223	0.930869	2.411647
14	-0.799704	-0.002012	-2.765778
6	-0.423331	-1.374266	-1.468432
6	0.543749	-1.933499	-2.553780
6	0.411808	-1.144313	-3.677793
6	-0.247130	1.433403	-1.520029
6	-1.741729	1.824765	-1.654103
6	-2.323418	1.084986	-2.666120
6	-2.385472	2.918990	-0.834130
1	-3.432657	3.082428	-1.116657
1	-2.349351	2.686480	0.239178
1	-1.849121	3.868811	-0.975209
6	-3.722731	1.099157	-3.220462

1	-4.234192	0.138953	-3.058253
1	-4.341621	1.887024	-2.770112
1	-3.709666	1.270688	-4.306862
6	0.688855	2.620613	-1.816370
1	0.431746	3.108184	-2.770154
1	0.630328	3.387853	-1.028305
1	1.736199	2.296900	-1.876734
6	-1.424976	-2.383960	-0.893084
1	-1.919793	-2.944327	-1.706347
1	-0.948797	-3.128393	-0.235281
1	-2.213566	-1.887269	-0.311744
6	1.494725	-3.072058	-2.295361
1	2.157654	-3.273314	-3.144947
1	2.115586	-2.845299	-1.415524
1	0.941504	-3.994708	-2.066936
6	1.177142	-1.154320	-4.971017
1	1.698257	-0.197524	-5.124057
1	1.931229	-1.952516	-4.996051
1	0.510477	-1.294646	-5.833216

-1	0.11	-0.12	-0.09
-2	-0.15	0.42	0.05
-3	-0.19	0.42	0.09
-4	-0.10	0.22	0.05
-5	-0.12	0.19	0.05
-6	-0.15	0.41	0.05
-7	-0.14	0.38	0.06
-8	0.02	-0.06	0.01
-9	0.01	-0.08	0.02
-0	0.02	-0.05	0.02
-1	0.02	-0.04	-0.02
-2	0.00	-0.05	-0.01
-3	0.02	-0.05	-0.01
-4	0.01	-0.05	0.00
-5	0.02	-0.03	0.00
-6	0.02	-0.03	0.00
-7	0.03	-0.03	-0.01
-8	0.02	-0.03	0.00
-9	0.00	-0.02	0.02
-0	0.00	-0.01	0.02
-1	0.00	-0.01	0.02

-2	-0.01	-0.03	0.04
-3	-0.02	-0.02	0.00
-4	0.01	-0.02	-0.03
-5	-0.04	-0.05	0.03
-6	-0.05	0.02	-0.01
-7	-0.01	-0.02	0.00
-8	-0.01	0.00	0.04
-9	-0.02	-0.01	-0.03
-0	-0.02	-0.02	-0.01
-1	0.00	-0.03	0.02
-2	0.01	-0.02	0.02
-3	-0.02	-0.04	0.02
-4	0.00	-0.03	0.02
-5	0.02	-0.02	-0.04
-6	0.01	-0.01	-0.03
-7	0.01	0.00	-0.04
-8	0.04	-0.02	-0.05

Frequencies -- -150.9485
Red. masses -- 7.0835
Frc consts -- 0.0951
IR Inten -- 2.0007
Zero-point correction= 0.319265
(Hartree/Particle)
Thermal correction to Energy= 0.340264
Thermal correction to Enthalpy= 0.341208
Thermal correction to Gibbs Free Energy= 0.270678
Sum of electronic and zero-point Energies= -553.917304
Sum of electronic and thermal Energies= -553.896305
Sum of electronic and thermal Enthalpies= -553.895361
Sum of electronic and thermal Free Energies= -553.965891

TS-Ge-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	0.565206	-0.009929	-0.261142
6	-0.225373	-0.001033	2.227247

6	1.153766	-0.005545	1.888246
1	1.741040	-0.916229	1.996045
1	1.745256	0.903280	1.988991
1	-0.740921	-0.928498	2.469530
1	-0.735219	0.929362	2.466950
14	-0.818764	-0.003709	-2.694254
6	-0.469249	-1.426447	-1.432825
6	0.535665	-1.931278	-2.507213
6	0.403421	-1.122917	-3.616848
6	-0.301930	1.446828	-1.488687
6	-1.789315	1.859869	-1.653103
6	-2.347680	1.088750	-2.655418
6	-2.441114	2.985502	-0.887652
1	-3.482061	3.143834	-1.194971
1	-2.424636	2.788575	0.192664
1	-1.896046	3.926667	-1.052648
6	-3.726454	1.103472	-3.259169
1	-4.246370	0.146714	-3.103721
1	-4.358361	1.898379	-2.840639
1	-3.676725	1.260763	-4.346809
6	0.676589	2.591874	-1.806138
1	0.430039	3.073237	-2.766533
1	0.653642	3.374999	-1.032696
1	1.710146	2.226798	-1.869655
6	-1.493663	-2.466636	-0.961661
1	-1.940635	-2.978535	-1.832907
1	-1.050075	-3.247888	-0.326061
1	-2.312652	-2.003913	-0.396768
6	1.495371	-3.066196	-2.265804
1	2.168728	-3.239525	-3.113155
1	2.105186	-2.856032	-1.374406
1	0.949314	-3.999594	-2.066358
6	1.175531	-1.113774	-4.907367
1	1.693175	-0.153624	-5.050311
1	1.933111	-1.908637	-4.939782
1	0.513092	-1.248485	-5.773997

-1	0.09	-0.10	-0.13
-2	-0.07	0.54	0.15
-3	-0.14	0.37	0.24
-4	-0.08	0.10	0.17

-5	-0.10	0.10	0.14
-6	-0.10	0.31	0.16
-7	-0.10	0.31	0.14
-8	-0.02	-0.03	0.03
-9	-0.04	-0.06	0.06
-0	-0.02	-0.02	0.03
-1	-0.01	0.00	-0.01
-2	-0.05	-0.01	0.04
-3	-0.02	-0.05	0.01
-4	-0.02	-0.05	0.01
-5	-0.02	-0.04	0.01
-6	-0.03	-0.04	0.00
-7	-0.01	-0.04	0.01
-8	-0.02	-0.03	0.01
-9	-0.01	-0.03	0.03
-0	-0.01	-0.03	0.03
-1	-0.01	-0.02	0.03
-2	-0.03	-0.04	0.04
-3	-0.03	0.02	0.03
-4	0.05	0.00	-0.01
-5	-0.08	-0.02	0.05
-6	-0.04	0.10	0.05
-7	-0.02	-0.04	0.05
-8	0.00	-0.03	0.08
-9	-0.03	-0.02	0.03
-0	-0.02	-0.05	0.06
-1	-0.02	0.00	0.03
-2	-0.02	0.01	0.02
-3	-0.04	0.00	0.03
-4	-0.02	0.00	0.03
-5	0.00	0.02	-0.02
-6	-0.01	0.01	-0.02
-7	0.00	0.03	-0.02
-8	0.01	0.01	-0.02

Frequencies -- -211.8959
Red. masses -- 9.7164
Frc consts -- 0.2570
IR Inten -- 16.2930
Zero-point correction= 0.318429

(Hartree/Particle)

Thermal correction to Energy= 0.339525

Thermal correction to Enthalpy= 0.340469

Thermal correction to Gibbs Free Energy= 0.269676

Sum of electronic and zero-point Energies= -553.820189

Sum of electronic and thermal Energies= -553.799093

Sum of electronic and thermal Enthalpies= -553.798149

Sum of electronic and thermal Free Energies= -553.868942

TS-Sn-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	-0.393930	-0.050380	0.090523
6	0.214120	-0.015361	2.300843
6	1.523966	0.036275	1.680428
1	2.128744	-0.866657	1.633411
1	2.060725	0.981395	1.632289
1	-0.150122	-0.936314	2.754754
1	-0.224273	0.883845	2.731816
14	-0.432251	0.051052	-2.838174
6	-0.162164	-1.471137	-1.646299
6	1.112036	-1.689277	-2.495895
6	1.042035	-0.850799	-3.592252
6	-0.246160	1.491035	-1.549751
6	-1.676897	1.881343	-1.982960
6	-2.047385	1.040971	-3.013357
6	-2.478740	2.949082	-1.284973
1	-3.491241	3.057624	-1.690165
1	-2.557934	2.712763	-0.212389
1	-1.972967	3.922651	-1.357851
6	-3.364915	0.916873	-3.728405
1	-3.796517	-0.085640	-3.589296
1	-4.099463	1.647978	-3.363467
1	-3.254073	1.067316	-4.811416
6	0.808072	2.604986	-1.599399
1	0.758635	3.141950	-2.563707
1	0.671066	3.356550	-0.807264

1	1.824120	2.201693	-1.498346
6	-1.043011	-2.726592	-1.525581
1	-1.223975	-3.187047	-2.511172
1	-0.568910	-3.491418	-0.891233
1	-2.017229	-2.493217	-1.076175
6	2.182938	-2.697942	-2.163299
1	2.976434	-2.725254	-2.919683
1	2.639768	-2.467845	-1.190660
1	1.753977	-3.707495	-2.086293
6	1.969312	-0.691615	-4.766650
1	2.374058	0.329235	-4.827042
1	2.818275	-1.387425	-4.725337
1	1.437972	-0.875537	-5.712215

-1	-0.02	-0.11	0.13
-2	0.13	0.28	-0.33
-3	0.38	0.29	-0.25
-4	0.01	0.21	-0.19
-5	-0.02	0.18	-0.24
-6	-0.05	0.14	-0.20
-7	-0.05	0.15	-0.24
-8	-0.01	0.03	-0.04
-9	-0.01	0.07	-0.08
-0	-0.05	0.03	-0.02
-1	-0.05	0.01	-0.02
-2	-0.05	0.04	-0.08
-3	0.00	0.04	-0.04
-4	0.02	0.03	0.00
-5	0.00	0.04	-0.03
-6	0.01	0.04	-0.03
-7	0.00	0.05	-0.03
-8	0.01	0.03	-0.03
-9	0.03	0.02	0.00
-0	0.02	0.03	0.00
-1	0.04	0.03	0.00
-2	0.03	0.01	0.00
-3	-0.06	0.01	-0.07
-4	-0.04	-0.02	-0.07
-5	-0.04	0.02	-0.06
-6	-0.08	0.00	-0.10
-7	0.03	0.04	-0.06

-8	0.04	-0.04	-0.02
-9	-0.02	0.07	-0.06
-0	0.10	0.06	-0.09
-1	-0.06	0.03	-0.02
-2	-0.06	0.03	-0.01
-3	-0.06	0.03	-0.03
-4	-0.05	0.02	-0.02
-5	-0.04	0.00	-0.03
-6	-0.04	0.00	-0.03
-7	-0.04	0.00	-0.03
-8	-0.05	0.01	-0.03

Frequencies -- -203.1704
Red. masses -- 10.6267
Frc consts -- 0.2584
IR Inten -- 24.4337
Zero-point correction= 0.317661
(Hartree/Particle)
Thermal correction to Energy= 0.338857
Thermal correction to Enthalpy= 0.339801
Thermal correction to Gibbs Free Energy= 0.268386
Sum of electronic and zero-point Energies= -553.435708
Sum of electronic and thermal Energies= -553.414511
Sum of electronic and thermal Enthalpies= -553.413567
Sum of electronic and thermal Free Energies= -553.484982

TS-Pb-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	0.400014	-0.011288	0.039602
6	-0.133285	-0.003352	2.357553
6	1.351948	-0.002991	2.100110
1	1.929232	-0.909385	2.288613
1	1.925924	0.907607	2.278981
1	-0.555895	-0.916192	2.782666
1	-0.556395	0.908786	2.782559

14	-0.837175	0.000765	-2.706527
6	-0.542504	-1.494496	-1.514147
6	0.504965	-1.947324	-2.548409
6	0.398413	-1.107061	-3.638320
6	-0.355943	1.503387	-1.580980
6	-1.830869	1.916390	-1.744967
6	-2.383524	1.096586	-2.711142
6	-2.481998	3.041017	-0.982131
1	-3.525312	3.198327	-1.279526
1	-2.457828	2.831038	0.096317
1	-1.937576	3.983415	-1.138458
6	-3.764305	1.089257	-3.308274
1	-4.272081	0.128564	-3.138360
1	-4.400589	1.882359	-2.892723
1	-3.724770	1.235439	-4.397809
6	0.671682	2.604741	-1.874099
1	0.459304	3.099764	-2.837114
1	0.665817	3.386278	-1.099957
1	1.690681	2.199928	-1.922389
6	-1.568470	-2.543779	-1.075311
1	-2.010840	-3.038820	-1.959108
1	-1.123197	-3.334698	-0.454538
1	-2.387306	-2.093567	-0.500655
6	1.470062	-3.077646	-2.305242
1	2.153939	-3.240619	-3.145866
1	2.069999	-2.863755	-1.407501
1	0.932488	-4.016782	-2.112202
6	1.192199	-1.082087	-4.915865
1	1.710370	-0.120493	-5.045627
1	1.950539	-1.876648	-4.944295
1	0.543317	-1.212186	-5.793884

-1	-0.01	-0.06	0.08
-2	0.27	0.19	-0.21
-3	0.17	0.27	-0.35
-4	-0.01	0.18	-0.26
-5	-0.01	0.19	-0.25
-6	-0.01	0.16	-0.27
-7	-0.02	0.21	-0.23
-8	0.00	0.04	-0.05
-9	-0.05	0.04	-0.11

-0	0.01	0.04	-0.06
-1	0.03	0.04	-0.02
-2	-0.02	0.09	-0.08
-3	-0.06	0.05	-0.03
-4	-0.05	0.03	-0.02
-5	-0.06	0.05	-0.03
-6	-0.07	0.06	-0.02
-7	-0.07	0.05	-0.04
-8	-0.05	0.05	-0.03
-9	-0.05	0.01	-0.03
-0	-0.04	0.01	-0.03
-1	-0.06	0.01	-0.03
-2	-0.05	0.00	-0.03
-3	0.03	0.04	-0.07
-4	0.04	-0.02	-0.02
-5	0.00	0.07	-0.06
-6	0.10	0.05	-0.11
-7	-0.07	0.01	-0.09
-8	-0.06	-0.04	-0.09
-9	-0.05	0.02	-0.08
-0	-0.10	0.00	-0.12
-1	0.01	0.04	-0.04
-2	0.02	0.05	-0.03
-3	0.01	0.05	-0.05
-4	0.01	0.03	-0.04
-5	0.04	0.03	-0.01
-6	0.04	0.03	-0.01
-7	0.05	0.03	-0.01
-8	0.04	0.03	-0.01

Frequencies -- -186.1464
Red. masses -- 8.4256
Frc consts -- 0.1720
IR Inten -- 13.2122
Zero-point correction= 0.316684
(Hartree/Particle)
Thermal correction to Energy= 0.338024
Thermal correction to Enthalpy= 0.338969
Thermal correction to Gibbs Free Energy= 0.266793
Sum of electronic and zero-point Energies= -553.505491

Sum of electronic and thermal Energies= -553.484150

Sum of electronic and thermal Enthalpies= -553.483206

Sum of electronic and thermal Free Energies= -553.555382

TS-C-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.181500	0.081754	0.689818
1	1.979461	0.080345	1.687141
6	1.721701	0.088277	2.994533
1	0.711244	-0.191790	3.291554
1	2.462074	-0.644079	3.335364
1	1.972425	1.110358	3.293173
6	0.341507	-1.154388	0.288490
6	0.409271	1.307918	0.309041
14	-0.623127	0.014363	-0.884814
6	-1.048565	1.596892	0.784822
6	-1.972647	1.024079	-0.060639
6	-1.304960	2.378982	2.052485
1	-0.834015	1.885002	2.913692
1	-2.374973	2.490228	2.262590
1	-0.866197	3.384571	1.983973
6	-3.475103	1.003122	0.006387
1	-3.859999	-0.018170	0.139962
1	-3.855810	1.614477	0.835343
1	-3.915682	1.392200	-0.922084
6	0.960410	-1.729908	-1.036264
6	0.295049	-1.136157	-2.085354
6	2.146993	-2.655801	-1.058569
1	2.484029	-2.890477	-2.075041
1	2.981190	-2.191914	-0.514143
1	1.913483	-3.601741	-0.548452
6	0.496254	-1.259646	-3.569683
1	0.789918	-0.297869	-4.014248
1	1.276144	-1.993741	-3.813278
1	-0.427397	-1.576886	-4.073724
6	-0.167779	-2.171062	1.303265

1	-0.751169	-2.961242	0.811232
1	0.660434	-2.655982	1.844161
1	-0.813267	-1.692932	2.051772
6	1.221426	2.575818	0.054919
1	0.676328	3.286838	-0.581803
1	1.457576	3.096664	0.997631
1	2.170935	2.325942	-0.430942

-1	-0.08	-0.09	0.06
-2	0.62	0.49	-0.53
-3	-0.02	0.03	0.03
-4	-0.05	-0.05	0.05
-5	0.15	0.13	-0.09
-6	0.07	0.09	-0.08
-7	0.01	-0.01	-0.02
-8	0.03	0.02	0.00
-9	0.00	0.00	-0.01
-0	0.00	0.00	0.01
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.01	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.01	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.01	-0.01
-2	0.00	0.00	0.01
-3	0.00	0.00	-0.01

-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.01	0.00	0.01
-7	-0.01	0.01	-0.02

Frequencies -- -1066.1394
Red. masses -- 1.2589
Frc consts -- 0.8431
IR Inten -- 113.4337
Zero-point correction= 0.312906
(Hartree/Particle)
Thermal correction to Energy= 0.332762
Thermal correction to Enthalpy= 0.333706
Thermal correction to Gibbs Free Energy= 0.266285
Sum of electronic and zero-point Energies= -549.971787
Sum of electronic and thermal Energies= -549.951931
Sum of electronic and thermal Enthalpies= -549.950987
Sum of electronic and thermal Free Energies= -550.018408

TS-Si-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.414792	0.129557	0.072771
1	1.131050	0.305330	-0.030715
6	2.220811	2.024207	-0.074585
1	1.615506	1.963504	-0.972703
1	3.173197	2.557468	-0.131767
1	1.743572	1.934406	0.895673
6	-1.328367	-0.835520	1.519521
6	-1.384280	-0.945001	-1.247360
14	-2.392705	-1.789756	0.196316
6	-0.866751	-2.274511	1.903506
6	-1.640842	-3.186681	1.214503
6	0.248031	-2.544738	2.883926
1	0.399291	-3.617297	3.054618
1	1.195601	-2.114451	2.527915
1	0.030004	-2.075340	3.853731

6	-1.608242	-4.690180	1.203015
1	-1.355024	-5.078242	0.205569
1	-0.875175	-5.094038	1.914255
1	-2.590812	-5.107772	1.465292
6	-1.822172	-0.006082	2.715967
1	-2.570645	-0.560640	3.302981
1	-0.997931	0.258272	3.396800
1	-2.284242	0.934659	2.388696
6	-2.778087	-0.392954	-1.655420
6	-3.735871	-0.956018	-0.837914
6	-2.947843	0.629147	-2.750351
1	-3.991876	0.934740	-2.883639
1	-2.346057	1.524141	-2.533236
1	-2.586217	0.228802	-3.708778
6	-5.213453	-0.690667	-0.750171
1	-5.481623	-0.274583	0.232492
1	-5.548724	0.022552	-1.514959
1	-5.796642	-1.613632	-0.874830
6	-0.598480	-1.624973	-2.379556
1	-1.223967	-2.370431	-2.896576
1	-0.253266	-0.904907	-3.137485
1	0.289820	-2.148386	-2.001428

-1	-0.01	0.01	0.01
-2	-0.17	0.47	0.29
-3	0.01	-0.06	-0.03
-4	-0.21	0.19	0.34
-5	0.28	-0.17	-0.40
-6	-0.24	0.18	0.32
-7	0.01	0.01	-0.01
-8	0.02	-0.01	-0.01
-9	0.00	0.00	-0.01
-0	0.00	-0.01	0.00
-1	0.00	-0.01	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00

-9	0.00	0.00	0.00
-0	0.00	0.01	-0.01
-1	-0.01	0.00	-0.01
-2	0.01	0.00	0.00
-3	0.00	0.01	-0.01
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	-0.01
-5	0.00	0.00	-0.01
-6	0.00	0.00	0.01
-7	0.00	0.00	-0.02

Frequencies -- -599.6634
Red. masses -- 1.0864
Frc consts -- 0.2302
IR Inten -- 1.8357
Zero-point correction= 0.307250
(Hartree/Particle)
Thermal correction to Energy= 0.328100
Thermal correction to Enthalpy= 0.329044
Thermal correction to Gibbs Free Energy= 0.258349
Sum of electronic and zero-point Energies= -515.761037
Sum of electronic and thermal Energies= -515.740186
Sum of electronic and thermal Enthalpies= -515.739242
Sum of electronic and thermal Free Energies= -515.809937

TS-Ge-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z

32	-0.337670	0.195621	0.070452
1	1.307614	0.203465	-0.044905
6	2.290973	1.988350	-0.065040
1	1.698781	1.898248	-0.968639
1	3.210351	2.579660	-0.112627
1	1.821697	1.856994	0.903529
6	-1.354550	-0.833740	1.549729
6	-1.407110	-0.932737	-1.281997
14	-2.373897	-1.769315	0.190860
6	-0.872833	-2.260179	1.927419
6	-1.616431	-3.173428	1.204540
6	0.227525	-2.527968	2.924405
1	0.390777	-3.600223	3.085944
1	1.175129	-2.082202	2.587527
1	-0.011344	-2.070871	3.895128
6	-1.564196	-4.676260	1.175754
1	-1.301966	-5.050383	0.175264
1	-0.830030	-5.079303	1.886509
1	-2.543027	-5.108987	1.428594
6	-1.879577	0.000921	2.726965
1	-2.632924	-0.555520	3.306931
1	-1.072068	0.281999	3.421024
1	-2.348119	0.933044	2.383010
6	-2.801003	-0.391551	-1.669386
6	-3.741934	-0.955620	-0.830652
6	-2.999265	0.620312	-2.769891
1	-4.048917	0.910925	-2.892345
1	-2.407751	1.525931	-2.567617
1	-2.643364	0.218907	-3.729918
6	-5.220841	-0.702588	-0.725846
1	-5.484323	-0.291508	0.260129
1	-5.570730	0.008708	-1.486206
1	-5.796898	-1.630723	-0.847311
6	-0.615589	-1.608146	-2.411755
1	-1.230431	-2.368030	-2.922031
1	-0.285826	-0.888270	-3.176758
1	0.282566	-2.115548	-2.034714

-1	0.00	0.00	0.00
-2	0.00	0.60	-0.24
-3	0.00	-0.06	0.03

-4	0.18	0.19	-0.35
-5	-0.22	-0.17	0.36
-6	0.20	0.20	-0.32
-7	0.00	0.00	0.01
-8	-0.01	-0.01	0.01
-9	0.00	0.00	0.00
-0	0.00	-0.01	0.00
-1	0.00	-0.01	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.01	0.00
-1	0.01	0.00	0.01
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.01
-6	0.00	0.00	0.00
-7	0.00	0.00	0.01

Frequencies -- -721.2871
Red. masses -- 1.0635
Frc consts -- 0.3260
IR Inten -- 19.6863
Zero-point correction= 0.305733

(Hartree/Particle)

Thermal correction to Energy= 0.327034

Thermal correction to Enthalpy= 0.327978

Thermal correction to Gibbs Free Energy= 0.255959

Sum of electronic and zero-point Energies= -515.660229

Sum of electronic and thermal Energies= -515.638929

Sum of electronic and thermal Enthalpies= -515.637984

Sum of electronic and thermal Free Energies= -515.710003

TS-Sn-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	-0.265173	0.416028	0.091183
1	1.474963	-0.101457	-0.040112
6	2.870965	1.523383	-0.011160
1	2.295689	1.531718	-0.928070
1	3.902987	1.881384	-0.038638
1	2.378952	1.435785	0.948727
6	-1.484013	-0.739023	1.603654
6	-1.509950	-0.764641	-1.358347
14	-2.335261	-1.697182	0.153298
6	-0.900627	-2.114512	1.984346
6	-1.473635	-3.060758	1.153501
6	0.130127	-2.311278	3.067470
1	0.405461	-3.364189	3.199019
1	1.043484	-1.742649	2.836412
1	-0.244362	-1.933489	4.029635
6	-1.245241	-4.544437	1.063282
1	-0.880001	-4.833841	0.066654
1	-0.511758	-4.894285	1.802491
1	-2.178310	-5.101554	1.231894
6	-2.168810	0.043732	2.732178
1	-2.917769	-0.575865	3.252874
1	-1.449037	0.389474	3.489834
1	-2.687454	0.934225	2.350891
6	-2.954430	-0.357730	-1.684092
6	-3.806032	-1.030622	-0.827993

6	-3.299411	0.637094	-2.764618
1	-4.379691	0.794543	-2.862798
1	-2.824368	1.607592	-2.556161
1	-2.914464	0.300169	-3.737841
6	-5.302762	-0.958869	-0.693853
1	-5.599915	-0.621413	0.310117
1	-5.748806	-0.268531	-1.422951
1	-5.764068	-1.945285	-0.845896
6	-0.715231	-1.373372	-2.524512
1	-1.275632	-2.195490	-3.000958
1	-0.502070	-0.630402	-3.308328
1	0.248454	-1.784276	-2.195058

-1	0.00	0.00	0.00
-2	0.47	-0.40	-0.17
-3	-0.03	0.04	0.03
-4	0.03	-0.27	-0.34
-5	-0.01	0.29	0.36
-6	0.03	-0.28	-0.32
-7	0.00	-0.01	0.01
-8	0.01	0.01	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	-0.01	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00

-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.01

Frequencies -- -688.0579
Red. masses -- 1.0523
Frc consts -- 0.2935
IR Inten -- 93.2214
Zero-point correction= 0.304462
(Hartree/Particle)
Thermal correction to Energy= 0.326171
Thermal correction to Enthalpy= 0.327115
Thermal correction to Gibbs Free Energy= 0.253516
Sum of electronic and zero-point Energies= -515.275189
Sum of electronic and thermal Energies= -515.253480
Sum of electronic and thermal Enthalpies= -515.252535
Sum of electronic and thermal Free Energies= -515.326134

TS-Pb-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-0.087365	0.304445	0.038436
1	1.810097	0.353423	-0.113669
6	2.267529	2.418353	-0.084278
1	1.746554	2.167654	-0.998700
1	2.991967	3.235818	-0.120293
1	1.892325	2.120490	0.886250
6	-1.322894	-0.908050	1.616681
6	-1.408345	-1.013744	-1.367252
14	-2.310077	-1.751328	0.184986
6	-0.901215	-2.342218	1.979882

6	-1.636894	-3.210130	1.190895
6	0.141025	-2.675694	3.018916
1	0.250765	-3.756305	3.168146
1	1.120852	-2.268550	2.727194
1	-0.115420	-2.221911	3.986597
6	-1.637640	-4.713017	1.133440
1	-1.364731	-5.079295	0.132781
1	-0.938226	-5.156735	1.855132
1	-2.638032	-5.113994	1.353200
6	-1.867989	-0.052272	2.767158
1	-2.677179	-0.573099	3.306667
1	-1.088202	0.189359	3.505647
1	-2.276938	0.901628	2.405636
6	-2.782224	-0.430746	-1.715317
6	-3.699075	-0.920460	-0.802574
6	-2.997284	0.548166	-2.842740
1	-4.042636	0.863515	-2.936789
1	-2.376870	1.444811	-2.689386
1	-2.684794	0.110450	-3.801513
6	-5.161392	-0.608229	-0.640662
1	-5.369584	-0.176074	0.349443
1	-5.515983	0.105766	-1.396801
1	-5.776775	-1.515181	-0.725621
6	-0.673293	-1.774580	-2.479044
1	-1.326314	-2.549886	-2.919055
1	-0.355606	-1.116068	-3.301830
1	0.224659	-2.286330	-2.105485

-1	0.00	0.00	0.00
-2	0.68	0.11	0.25
-3	-0.03	-0.02	-0.04
-4	0.04	0.21	0.34
-5	-0.01	-0.21	-0.31
-6	0.04	0.23	0.32
-7	0.00	0.00	-0.01
-8	0.00	-0.01	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00

-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.01	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	-0.01
-6	0.00	0.00	0.00
-7	0.00	0.00	-0.01

Frequencies -- -862.4506
Red. masses -- 1.0457
Frc consts -- 0.4583
IR Inten -- 217.1051
Zero-point correction= 0.303627
(Hartree/Particle)
Thermal correction to Energy= 0.325549
Thermal correction to Enthalpy= 0.326493
Thermal correction to Gibbs Free Energy= 0.251849
Sum of electronic and zero-point Energies= -515.357032
Sum of electronic and thermal Energies= -515.335109
Sum of electronic and thermal Enthalpies= -515.334165
Sum of electronic and thermal Free Energies= -515.408810

TS-C-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.230554	-0.032877	-0.164546
1	0.066263	0.055860	1.172828
8	1.071235	0.049389	1.737889
1	1.491301	0.939603	1.696103
6	-0.035588	1.111561	-1.187246
6	-0.082511	-1.300571	-0.931641
14	-0.209933	-0.149076	-2.610312
6	-1.479373	1.575119	-1.645695
6	-1.787970	0.902107	-2.800821
6	-2.331290	2.487682	-0.806184
1	-2.444627	2.052701	0.197417
1	-1.854606	3.470321	-0.679463
1	-3.328554	2.643840	-1.233424
6	-3.032795	0.902038	-3.639710
1	-3.475667	-0.102822	-3.692153
1	-3.793448	1.584652	-3.237883
1	-2.818465	1.212092	-4.671810
6	1.243363	-1.689413	-1.657091
6	1.287360	-1.229642	-2.953719
6	2.289604	-2.447597	-0.877416
1	3.198179	-2.628322	-1.463692
1	2.547039	-1.885414	0.031431
1	1.898109	-3.420878	-0.547715
6	2.383572	-1.326215	-3.977784
1	2.797528	-0.336911	-4.221268
1	3.211174	-1.955203	-3.624396
1	2.012745	-1.760019	-4.916250
6	-0.846743	-2.505089	-0.380269
1	-0.948707	-3.298257	-1.134391
1	-0.337279	-2.932415	0.496953
1	-1.851186	-2.202916	-0.061844
6	0.950486	2.236838	-0.894550
1	0.959184	2.976757	-1.706116
1	0.691925	2.767873	0.036092
1	1.970421	1.846721	-0.783505

-1	-0.11	-0.09	0.09
-2	0.52	0.78	-0.27
-3	0.02	0.06	-0.01
-4	-0.05	0.05	0.04
-5	0.01	-0.04	-0.03
-6	0.04	0.01	0.00
-7	0.00	-0.01	-0.02
-8	-0.01	0.00	-0.01
-9	0.00	0.00	0.01
-0	0.00	0.00	0.00
-1	0.02	-0.01	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	-0.01	0.01
-9	0.00	-0.01	0.01
-0	0.00	0.00	0.00
-1	0.00	-0.01	0.00
-2	0.01	-0.01	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.01	0.00	0.00
-9	0.01	0.00	0.01
-0	0.01	0.00	0.02
-1	0.00	0.01	-0.03
-2	0.01	0.00	0.00
-3	0.00	0.02	-0.01
-4	0.00	0.00	0.02
-5	0.00	0.00	-0.02

Frequencies -- -689.4050
Red. masses -- 1.4539
Frc consts -- 0.4071
IR Inten -- 278.7943

Zero-point correction= 0.289593
(Hartree/Particle)
Thermal correction to Energy= 0.307960
Thermal correction to Enthalpy= 0.308904
Thermal correction to Gibbs Free Energy= 0.245414
Sum of electronic and zero-point Energies= -585.927326
Sum of electronic and thermal Energies= -585.908959
Sum of electronic and thermal Enthalpies= -585.908015
Sum of electronic and thermal Free Energies= -585.971506

TS-Si-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.322104	-0.206455	-0.382778
1	2.895481	0.320989	-0.002198
6	0.015481	-1.261781	0.643581
6	-0.154118	0.900925	-1.077682
14	-1.424649	-0.154090	-0.047140
6	-0.728508	-2.394035	-0.109969
6	-1.928613	-1.898552	-0.578999
6	-0.146897	-3.775508	-0.280288
1	-0.801816	-4.440744	-0.854576
1	0.827816	-3.722309	-0.788048
1	0.033853	-4.239426	0.700480
6	-2.997198	-2.560123	-1.404934
1	-3.131095	-2.048995	-2.370034
1	-2.762095	-3.612740	-1.614595
1	-3.969803	-2.532303	-0.893016
6	0.370253	-1.575229	2.103022
1	-0.526553	-1.854756	2.677785
1	1.085340	-2.409514	2.176427
1	0.834160	-0.710832	2.592791
6	-0.672184	2.065680	-0.196703
6	-1.734723	1.611533	0.558555
6	-0.059467	3.446164	-0.214796
1	-0.547733	4.131160	0.488123
1	1.013797	3.409803	0.028570

1	-0.130970	3.884103	-1.220895
6	-2.564225	2.313168	1.598585
1	-2.477652	1.819351	2.577419
1	-2.267935	3.363273	1.726990
1	-3.630056	2.299630	1.330112
6	-0.163277	1.182970	-2.588257
1	-1.145528	1.553693	-2.919959
1	0.588194	1.937641	-2.869500
1	0.060795	0.277730	-3.169206
8	2.302072	0.794742	1.026352
1	2.238743	1.762464	1.214228

-1	0.03	0.02	-0.02
-2	-0.61	-0.18	0.76
-3	-0.01	0.01	0.01
-4	-0.01	0.00	0.01
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	-0.01	0.01
-8	0.00	0.00	0.00
-9	0.00	0.00	0.01
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	-0.01	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00

-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	-0.01	0.00
-4	0.00	-0.02	-0.03
-5	-0.01	-0.08	-0.03

Frequencies -- -1408.6516
Red. masses -- 1.0714
Frc consts -- 1.2526
IR Inten -- 1577.6011
Zero-point correction= 0.285427
(Hartree/Particle)
Thermal correction to Energy= 0.305127
Thermal correction to Enthalpy= 0.306071
Thermal correction to Gibbs Free Energy= 0.239383
Sum of electronic and zero-point Energies= -551.783014
Sum of electronic and thermal Energies= -551.763315
Sum of electronic and thermal Enthalpies= -551.762370
Sum of electronic and thermal Free Energies= -551.829059

TS-Ge-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	1.413116	-0.183422	-0.374646
1	2.976637	0.377613	0.060879
6	0.021582	-1.299114	0.649153
6	-0.166236	0.918402	-1.104873
14	-1.390393	-0.156915	-0.049611
6	-0.730813	-2.412309	-0.111852
6	-1.919205	-1.892952	-0.587222
6	-0.177677	-3.805835	-0.279627
1	-0.845873	-4.457889	-0.853727
1	0.798255	-3.775472	-0.786751
1	-0.007115	-4.272004	0.701578
6	-2.995316	-2.534537	-1.419310
1	-3.121718	-2.015605	-2.381121

1	-2.774949	-3.589015	-1.635461
1	-3.967961	-2.496683	-0.908321
6	0.380404	-1.609066	2.107347
1	-0.519533	-1.851304	2.694672
1	1.065631	-2.467867	2.182804
1	0.878863	-0.755266	2.581732
6	-0.676277	2.080442	-0.222515
6	-1.710237	1.607783	0.561980
6	-0.086128	3.469911	-0.260712
1	-0.563501	4.148441	0.455941
1	0.994306	3.446642	-0.048720
1	-0.193686	3.905974	-1.264961
6	-2.528368	2.299076	1.617645
1	-2.417981	1.806439	2.594691
1	-2.242290	3.352673	1.740553
1	-3.598949	2.273062	1.369064
6	-0.191819	1.172242	-2.619246
1	-1.180019	1.530575	-2.948179
1	0.550261	1.927376	-2.922958
1	0.029788	0.257678	-3.187333
8	2.305186	0.857059	1.157803
1	2.215004	1.821489	1.350753

-1	-0.01	0.00	-0.01
-2	0.57	0.03	0.81
-3	0.01	0.01	0.00
-4	0.01	0.00	0.01
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	-0.01	0.01
-8	0.00	0.00	0.00

-9	0.00	0.00	0.01
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.01	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	-0.03	-0.02
-5	0.02	-0.09	-0.03

Frequencies -- -1365.2862
Red. masses -- 1.0466
Frc consts -- 1.1494
IR Inten -- 1510.4289
Zero-point correction= 0.283903
(Hartree/Particle)
Thermal correction to Energy= 0.304120
Thermal correction to Enthalpy= 0.305065
Thermal correction to Gibbs Free Energy= 0.236723
Sum of electronic and zero-point Energies= -551.681325
Sum of electronic and thermal Energies= -551.661107
Sum of electronic and thermal Enthalpies= -551.660163
Sum of electronic and thermal Free Energies= -551.728504

TS-Sn-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	1.561005	-0.185658	-0.495230
1	3.407379	0.114668	-0.313862

6	-0.010343	-1.283947	0.649415
6	-0.208116	1.012572	-1.156908
14	-1.382829	-0.146649	-0.126447
6	-0.763199	-2.422673	-0.062469
6	-1.907509	-1.896248	-0.632283
6	-0.254983	-3.842551	-0.105575
1	-0.916740	-4.511623	-0.667716
1	0.746559	-3.880519	-0.560243
1	-0.152003	-4.243427	0.913250
6	-2.950865	-2.553987	-1.493866
1	-3.013670	-2.075357	-2.482442
1	-2.740398	-3.620525	-1.653569
1	-3.949869	-2.477221	-1.041237
6	0.299913	-1.496793	2.138649
1	-0.614403	-1.741691	2.705191
1	1.015441	-2.318712	2.297451
1	0.739254	-0.599159	2.596115
6	-0.752851	2.118301	-0.225851
6	-1.779175	1.583508	0.529588
6	-0.197842	3.521249	-0.194381
1	-0.738984	4.169743	0.504905
1	0.863703	3.509715	0.095274
1	-0.247947	3.979855	-1.192334
6	-2.634655	2.212303	1.595527
1	-2.518015	1.697623	2.560661
1	-2.392289	3.272614	1.750713
1	-3.700656	2.151346	1.332122
6	-0.293018	1.330111	-2.659167
1	-1.307885	1.653098	-2.944029
1	0.399200	2.136308	-2.947641
1	-0.043283	0.456454	-3.278107
8	2.896274	0.697224	0.872489
1	3.165788	1.357675	1.551460

-1	-0.01	0.00	-0.01
-2	0.54	-0.01	0.82
-3	0.01	0.00	0.00
-4	0.01	0.00	0.01
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00

-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.01
-8	0.00	0.00	0.00
-9	0.00	0.00	0.01
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	-0.03	-0.02
-5	0.03	-0.16	-0.06

Frequencies -- -1336.1451
Red. masses -- 1.0348
Frc consts -- 1.0884
IR Inten -- 2090.0015
Zero-point correction= 0.282018
(Hartree/Particle)
Thermal correction to Energy= 0.302837
Thermal correction to Enthalpy= 0.303781
Thermal correction to Gibbs Free Energy= 0.233622
Sum of electronic and zero-point Energies= -551.293299
Sum of electronic and thermal Energies= -551.272480

Sum of electronic and thermal Enthalpies= -551.271536

Sum of electronic and thermal Free Energies= -551.341696

TS-Pb-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	1.688192	-0.141205	-0.415919
1	3.342155	0.526592	0.124404
6	0.030154	-1.389000	0.637283
6	-0.193365	0.983589	-1.189080
14	-1.293960	-0.163687	-0.088755
6	-0.759170	-2.468213	-0.105976
6	-1.901549	-1.879684	-0.618664
6	-0.305395	-3.902296	-0.223390
1	-1.018134	-4.523682	-0.777449
1	0.669605	-3.959070	-0.730163
1	-0.168686	-4.346716	0.772746
6	-3.006200	-2.469485	-1.451204
1	-3.091842	-1.959637	-2.422529
1	-2.849932	-3.539042	-1.648165
1	-3.980335	-2.363124	-0.952429
6	0.412695	-1.658846	2.094824
1	-0.485434	-1.791906	2.722011
1	1.017908	-2.572888	2.194064
1	0.995176	-0.828895	2.516191
6	-0.696357	2.116989	-0.283784
6	-1.644920	1.583014	0.569842
6	-0.183224	3.534381	-0.354044
1	-0.656179	4.189490	0.386770
1	0.905690	3.560572	-0.195130
1	-0.364596	3.961971	-1.351004
6	-2.425358	2.227092	1.682023
1	-2.234759	1.729380	2.644242
1	-2.176517	3.290636	1.800859
1	-3.507650	2.158376	1.499799
6	-0.277909	1.207340	-2.703974
1	-1.293120	1.513525	-3.008591

1	0.413196	1.992625	-3.047064
1	-0.033975	0.293729	-3.264657
8	2.414938	0.919764	1.367662
1	2.281847	1.845935	1.678702

-1	0.00	0.00	0.00
-2	0.33	0.41	0.84
-3	0.01	0.00	0.00
-4	0.00	0.00	0.01
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.01
-8	0.00	0.00	0.00
-9	-0.01	0.00	0.02
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-0	0.00	0.00	0.00
-1	0.00	0.00	0.00
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.02	-0.03	-0.01
-5	0.08	-0.09	-0.02

Frequencies -- -1136.8226
Red. masses -- 1.0378
Frc consts -- 0.7902
IR Inten -- 1352.8914
Zero-point correction= 0.281745
(Hartree/Particle)
Thermal correction to Energy= 0.302622
Thermal correction to Enthalpy= 0.303566
Thermal correction to Gibbs Free Energy= 0.232772
Sum of electronic and zero-point Energies= -551.371483
Sum of electronic and thermal Energies= -551.350606
Sum of electronic and thermal Enthalpies= -551.349661
Sum of electronic and thermal Free Energies= -551.420455

Pro-C-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.201250	0.138110	-0.073439
6	-0.887307	0.796986	-0.598758
6	0.839572	0.117648	0.982094
6	2.061977	-0.290530	0.101931
6	-1.996687	-1.221803	0.025293
6	1.655695	-1.271332	-0.777801
6	3.425371	0.348999	0.217555
1	4.168255	-0.133926	-0.427943
1	3.380696	1.412592	-0.054820
1	3.790104	0.298233	1.253572
6	2.420093	-2.000155	-1.847832
1	1.998514	-1.803419	-2.844214
1	3.478974	-1.708787	-1.870197
1	2.376917	-3.087595	-1.693431
6	1.044883	-0.075686	2.482384
1	1.473652	-1.063651	2.698360
1	1.728152	0.677901	2.910862
1	0.093295	0.004097	3.023596
6	-1.046582	1.575266	-1.902412
1	-1.606610	0.990627	-2.644790
1	-1.589999	2.524837	-1.756980

1	-0.069426	1.823202	-2.336368
6	-3.441108	0.921342	0.288171
1	-4.280213	0.270809	0.561137
1	-3.243646	1.592711	1.135245
1	-3.759272	1.552595	-0.553990
6	-2.916977	-2.315013	0.493083
1	-2.520351	-2.813911	1.389011
1	-3.917938	-1.935394	0.738500
1	-3.034528	-3.090409	-0.276782
6	0.057420	1.398460	0.506479
14	-0.146058	-0.959402	-0.282803
6	0.694211	2.788605	0.390196
1	0.413901	3.420607	-0.448514
1	1.724677	2.913990	0.711978
6	-0.359195	2.518425	1.467852
1	-0.027878	2.463698	2.501515
1	-1.338291	2.972787	1.341082

Zero-point correction= 0.328714
(Hartree/Particle)
Thermal correction to Energy= 0.347468
Thermal correction to Enthalpy= 0.348412
Thermal correction to Gibbs Free Energy= 0.284111
Sum of electronic and zero-point Energies= -588.160681
Sum of electronic and thermal Energies= -588.141927
Sum of electronic and thermal Enthalpies= -588.140982
Sum of electronic and thermal Free Energies= -588.205284

Pro-Si-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.002144	1.231289	-0.001149
6	2.227390	0.479457	-0.057024
6	1.072355	-0.143355	-0.886106
6	-1.082060	-0.145859	0.873100
6	-2.234678	0.487995	0.049028
6	1.763835	1.628333	0.549442

6	-1.766553	1.639711	-0.548487
6	-3.601485	-0.141456	-0.055724
1	-4.289574	0.444410	-0.676062
1	-3.523564	-1.151651	-0.484474
1	-4.052412	-0.253206	0.941168
6	-2.458979	2.604689	-1.470991
1	-1.958575	2.652619	-2.449477
1	-3.507471	2.326022	-1.644982
1	-2.449901	3.624181	-1.058810
6	-1.366834	-0.287546	2.375280
1	-1.745669	0.654405	2.800698
1	-2.119515	-1.065765	2.578479
1	-0.459789	-0.564627	2.928497
6	1.356911	-0.274400	-2.389299
1	1.738875	0.669566	-2.807372
1	2.107156	-1.053429	-2.598286
1	0.449121	-0.544352	-2.944802
6	3.591712	-0.156215	0.042913
1	4.282292	0.422525	0.667161
1	3.509929	-1.169105	0.464606
1	4.041936	-0.262740	-0.954886
6	2.460026	2.583158	1.479641
1	1.960186	2.624672	2.458706
1	3.507586	2.299341	1.650883
1	2.454391	3.606075	1.076001
14	-0.007697	-1.487958	-0.011927
6	0.438286	-3.207413	0.626972
1	1.450768	-3.592815	0.510961
1	-0.035674	-3.570948	1.539054
6	-0.462224	-3.199637	-0.665402
1	0.009912	-3.557898	-1.580514
1	-1.476674	-3.580832	-0.552680

Zero-point correction= 0.322046
(Hartree/Particle)
Thermal correction to Energy= 0.342227
Thermal correction to Enthalpy= 0.343171
Thermal correction to Gibbs Free Energy= 0.275187
Sum of electronic and zero-point Energies= -553.973773
Sum of electronic and thermal Energies= -553.953591

Sum of electronic and thermal Enthalpies= -553.952647

Sum of electronic and thermal Free Energies= -554.020632

Pro-Ge-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.002040	1.225115	-0.000765
6	2.241776	0.505917	-0.065833
6	1.094957	-0.115827	-0.902673
6	-1.104415	-0.118326	0.890662
6	-2.248576	0.514110	0.058176
6	1.758724	1.637712	0.558237
6	-1.761049	1.648903	-0.556910
6	-3.628642	-0.088592	-0.029877
1	-4.304954	0.496983	-0.663378
1	-3.574176	-1.110725	-0.433835
1	-4.080501	-0.165624	0.969942
6	-2.437785	2.611788	-1.493242
1	-1.945824	2.625405	-2.477028
1	-3.494975	2.357604	-1.651638
1	-2.397737	3.639419	-1.103739
6	-1.384225	-0.245269	2.394622
1	-1.747275	0.706659	2.813250
1	-2.148725	-1.009051	2.607390
1	-0.479572	-0.530809	2.947127
6	1.373818	-0.232388	-2.407656
1	1.740402	0.721314	-2.819094
1	2.135304	-0.997463	-2.626491
1	0.467888	-0.510237	-2.961985
6	3.619713	-0.102405	0.016911
1	4.298436	0.475949	0.654451
1	3.561912	-1.127374	0.413140
1	4.070764	-0.173464	-0.983722
6	2.439378	2.590603	1.501939
1	1.947968	2.598005	2.486061
1	3.495712	2.331353	1.657750
1	2.402831	3.621482	1.120809

32	-0.007624	-1.554834	-0.011610
6	0.435016	-3.367573	0.626170
1	1.449352	-3.750616	0.514600
1	-0.040550	-3.729143	1.538639
6	-0.460406	-3.359035	-0.666198
1	0.013182	-3.714954	-1.581917
1	-1.476887	-3.737372	-0.558148

Zero-point correction= 0.320282
(Hartree/Particle)
Thermal correction to Energy= 0.341028
Thermal correction to Enthalpy= 0.341972
Thermal correction to Gibbs Free Energy= 0.272277
Sum of electronic and zero-point Energies= -553.851736
Sum of electronic and thermal Energies= -553.830991
Sum of electronic and thermal Enthalpies= -553.830047
Sum of electronic and thermal Free Energies= -553.899742

Pro-Sn-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.002022	1.205495	-0.000898
6	2.269686	0.563080	-0.084755
6	1.141770	-0.074049	-0.930141
6	-1.150810	-0.076527	0.918594
6	-2.276140	0.571125	0.077718
6	1.745012	1.657183	0.573292
6	-1.747210	1.668230	-0.571867
6	-3.680324	0.025128	0.019137
1	-4.339518	0.624871	-0.618922
1	-3.673210	-1.006122	-0.363716
1	-4.122190	-0.013221	1.025119
6	-2.392671	2.632275	-1.528972
1	-1.901686	2.608089	-2.512870
1	-3.457638	2.410892	-1.681853
1	-2.317578	3.666060	-1.162853
6	-1.419611	-0.140405	2.430627

1	-1.747520	0.839032	2.815804
1	-2.207048	-0.867988	2.679265
1	-0.520481	-0.433355	2.988595
6	1.410029	-0.127635	-2.442677
1	1.740994	0.853583	-2.820642
1	2.195121	-0.855846	-2.696835
1	0.509852	-0.413645	-3.002562
6	3.671876	0.011460	-0.030635
1	4.333320	0.603733	0.612062
1	3.661089	-1.022750	0.344074
1	4.113500	-0.020567	-1.036949
6	2.394293	2.611361	1.537681
1	1.903495	2.581285	2.521511
1	3.458477	2.384864	1.688523
1	2.322919	3.648244	1.179684
50	-0.007728	-1.719683	-0.012041
6	0.432940	-3.723204	0.622581
1	1.446155	-4.110463	0.505574
1	-0.040394	-4.098617	1.531422
6	-0.460399	-3.714228	-0.666293
1	0.010741	-4.083854	-1.578654
1	-1.475893	-4.096589	-0.552994

Zero-point correction= 0.318731
(Hartree/Particle)
Thermal correction to Energy= 0.340075
Thermal correction to Enthalpy= 0.341020
Thermal correction to Gibbs Free Energy= 0.269028
Sum of electronic and zero-point Energies= -553.445568
Sum of electronic and thermal Energies= -553.424224
Sum of electronic and thermal Enthalpies= -553.423280
Sum of electronic and thermal Free Energies= -553.495272

Pro-Pb-C_2H_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.001028	1.209306	-0.000423

6	2.285152	0.600277	-0.092014
6	1.162762	-0.026646	-0.940458
6	-1.167108	-0.027585	0.935350
6	-2.288465	0.604732	0.089402
6	1.743816	1.677861	0.581289
6	-1.744967	1.683633	-0.580141
6	-3.697780	0.072003	0.041120
1	-4.351355	0.669201	-0.604917
1	-3.700009	-0.964000	-0.328584
1	-4.139480	0.051262	1.047668
6	-2.380111	2.642698	-1.548289
1	-1.894490	2.594666	-2.534197
1	-3.449422	2.436925	-1.692186
1	-2.285455	3.681050	-1.199668
6	-1.425504	-0.122615	2.443749
1	-1.749549	0.850853	2.849005
1	-2.214097	-0.851543	2.683135
1	-0.523501	-0.427316	2.989525
6	1.421383	-0.117004	-2.449181
1	1.746461	0.857540	-2.851179
1	2.209399	-0.845912	-2.690673
1	0.519222	-0.419208	-2.996134
6	3.693407	0.064532	-0.045336
1	4.347904	0.657739	0.603434
1	3.693549	-0.973026	0.319990
1	4.135502	0.047114	-1.051741
6	2.380797	2.632044	1.553042
1	1.894620	2.581709	2.538504
1	3.449589	2.423334	1.696722
1	2.288699	3.671794	1.208018
82	-0.004809	-1.778566	-0.006894
6	0.422774	-3.863980	0.613557
1	1.440596	-4.240344	0.498518
1	-0.051392	-4.233666	1.524495
6	-0.464029	-3.842827	-0.673188
1	0.005080	-4.201137	-1.591349
1	-1.486963	-4.207655	-0.565839

Zero-point correction= 0.317564
(Hartree/Particle)

Thermal correction to Energy= 0.338453
Thermal correction to Enthalpy= 0.339397
Thermal correction to Gibbs Free Energy= 0.268577
Sum of electronic and zero-point Energies= -553.506036
Sum of electronic and thermal Energies= -553.485147
Sum of electronic and thermal Enthalpies= -553.484203
Sum of electronic and thermal Free Energies= -553.555023

Pro-C-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.187122	0.117437	-0.080034
6	-0.884055	0.779710	-0.618514
6	0.847413	0.093814	0.962993
6	2.079915	-0.323771	0.106270
6	-1.981126	-1.242575	0.013424
6	1.673416	-1.284063	-0.797463
6	3.466250	0.250510	0.288675
1	4.199150	-0.206593	-0.387005
1	3.472565	1.335386	0.118078
1	3.811387	0.090480	1.321006
6	2.447632	-2.014910	-1.859085
1	2.039633	-1.813291	-2.860164
1	3.508609	-1.730186	-1.867591
1	2.395815	-3.102583	-1.708401
6	1.030075	-0.088229	2.468982
1	1.455056	-1.072534	2.710602
1	1.702817	0.674521	2.896942
1	0.068262	-0.001704	2.993485
6	-1.076952	1.557394	-1.920084
1	-1.623537	0.953050	-2.657160
1	-1.651425	2.486312	-1.766303
1	-0.117818	1.840061	-2.371208
6	-3.406787	0.915641	0.314473
1	-4.208805	0.288650	0.721481
1	-3.146280	1.671021	1.070740
1	-3.808182	1.461486	-0.552005

6	-2.894439	-2.335616	0.494414
1	-2.471634	-2.854385	1.366040
1	-3.882644	-1.951633	0.780201
1	-3.046574	-3.095552	-0.284152
6	0.898204	2.623576	0.098953
1	0.263558	3.475228	-0.182016
1	1.545755	2.948499	0.925164
1	1.539539	2.391657	-0.760695
6	0.048817	1.410839	0.522888
1	-0.567822	1.714621	1.385276
14	-0.132558	-0.966440	-0.313348

Zero-point correction= 0.322807
(Hartree/Particle)
Thermal correction to Energy= 0.341281
Thermal correction to Enthalpy= 0.342226
Thermal correction to Gibbs Free Energy= 0.278394
Sum of electronic and zero-point Energies= -550.105236
Sum of electronic and thermal Energies= -550.086762
Sum of electronic and thermal Enthalpies= -550.085818
Sum of electronic and thermal Free Energies= -550.149650

Pro-Si-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.012501	1.185458	-0.014518
6	2.257088	0.495346	-0.004094
6	1.127311	-0.211828	-0.795126
6	-1.026425	-0.159257	0.945585
6	-2.197671	0.390929	0.093624
6	1.760352	1.670197	0.522916
6	-1.760942	1.508257	-0.589749
6	-3.557918	-0.262139	0.052840
1	-4.263281	0.272463	-0.593976
1	-3.478803	-1.298893	-0.305214
1	-3.990695	-0.309100	1.062417
6	-2.481411	2.387696	-1.574871

1	-1.988763	2.374867	-2.558070
1	-3.524622	2.075645	-1.720333
1	-2.491668	3.434230	-1.238815
6	-1.300193	-0.206646	2.456677
1	-1.687420	0.755637	2.825737
1	-2.040857	-0.979586	2.717057
1	-0.385781	-0.435421	3.020598
6	1.432885	-0.428199	-2.285012
1	1.771104	0.504095	-2.762813
1	2.223450	-1.180014	-2.438847
1	0.546641	-0.775665	-2.832778
6	3.636459	-0.095839	0.149028
1	4.301677	0.534289	0.750653
1	3.577111	-1.086932	0.622478
1	4.104557	-0.242531	-0.835008
6	2.423066	2.700304	1.395786
1	1.901260	2.805016	2.358047
1	3.470431	2.446926	1.609420
1	2.411618	3.690614	0.918739
14	0.087132	-1.554309	0.162141
1	0.840263	-2.262628	1.243991
6	-0.744248	-2.831401	-0.973192
1	0.005933	-3.442465	-1.492867
1	-1.387581	-3.508854	-0.396293
1	-1.364345	-2.342204	-1.735426

Zero-point correction= 0.313353
(Hartree/Particle)
Thermal correction to Energy= 0.333323
Thermal correction to Enthalpy= 0.334267
Thermal correction to Gibbs Free Energy= 0.266929
Sum of electronic and zero-point Energies= -515.928437
Sum of electronic and thermal Energies= -515.908468
Sum of electronic and thermal Enthalpies= -515.907524
Sum of electronic and thermal Free Energies= -515.974862

Pro-Ge-CH_4

Atomic Coordinates (Angstroms)

Number	X	Y	Z
14	0.016783	1.167702	-0.008721
6	2.274302	0.510656	-0.006614
6	1.154357	-0.200976	-0.802887
6	-1.043127	-0.144561	0.968872
6	-2.206986	0.404447	0.110275
6	1.758158	1.670982	0.535163
6	-1.752377	1.502333	-0.593555
6	-3.577908	-0.226352	0.083166
1	-4.273685	0.304907	-0.576641
1	-3.515794	-1.272391	-0.250858
1	-4.012466	-0.243103	1.093002
6	-2.459284	2.373760	-1.595494
1	-1.970618	2.329395	-2.579883
1	-3.509086	2.079535	-1.730731
1	-2.447585	3.427633	-1.283130
6	-1.307655	-0.175393	2.481813
1	-1.675477	0.797203	2.845286
1	-2.060849	-0.932008	2.753352
1	-0.394230	-0.414857	3.042918
6	1.452612	-0.408214	-2.295331
1	1.773412	0.530867	-2.773195
1	2.253768	-1.146785	-2.457138
1	0.567851	-0.767202	-2.838266
6	3.665496	-0.055749	0.133789
1	4.322313	0.582708	0.735790
1	3.628205	-1.051119	0.600798
1	4.130310	-0.186721	-0.854051
6	2.405261	2.701605	1.419087
1	1.891118	2.777412	2.388343
1	3.460664	2.470350	1.617962
1	2.364856	3.699466	0.959517
32	0.091102	-1.628389	0.173104
1	0.866204	-2.381469	1.298717
6	-0.785067	-2.928487	-1.032408
1	-0.035921	-3.530118	-1.563020
1	-1.429155	-3.608534	-0.460601
1	-1.401285	-2.410473	-1.777700

Zero-point correction= 0.311416
(Hartree/Particle)
Thermal correction to Energy= 0.331880
Thermal correction to Enthalpy= 0.332824
Thermal correction to Gibbs Free Energy= 0.264131
Sum of electronic and zero-point Energies= -515.810828
Sum of electronic and thermal Energies= -515.790364
Sum of electronic and thermal Enthalpies= -515.789419
Sum of electronic and thermal Free Energies= -515.858112

Pro-Sn-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.024364	1.123658	0.013375
6	2.307636	0.541155	-0.016270
6	1.205034	-0.194173	-0.809419
6	-1.087724	-0.129785	1.014342
6	-2.228879	0.438416	0.142080
6	1.751889	1.665886	0.562257
6	-1.729618	1.497146	-0.591970
6	-3.625024	-0.134402	0.134492
1	-4.300330	0.409354	-0.536288
1	-3.607387	-1.190232	-0.174704
1	-4.056524	-0.109398	1.145407
6	-2.401491	2.367394	-1.619011
1	-1.907575	2.285203	-2.598390
1	-3.459335	2.104291	-1.756059
1	-2.358078	3.427383	-1.330979
6	-1.346777	-0.096136	2.530490
1	-1.670522	0.905036	2.859608
1	-2.131952	-0.806991	2.831475
1	-0.443760	-0.353725	3.100685
6	1.480712	-0.350377	-2.314957
1	1.753066	0.614220	-2.773959
1	2.308191	-1.049249	-2.513273
1	0.601209	-0.731095	-2.852389
6	3.726393	0.037548	0.080520

1	4.369181	0.698424	0.673456
1	3.747446	-0.964108	0.535259
1	4.170075	-0.060170	-0.920640
6	2.370735	2.699764	1.462936
1	1.865943	2.733981	2.439505
1	3.436355	2.504257	1.645012
1	2.287584	3.706022	1.028031
50	0.095884	-1.805446	0.207079
1	0.926723	-2.660806	1.462045
6	-0.839491	-3.190967	-1.143859
1	-0.080488	-3.769951	-1.685107
1	-1.481124	-3.890448	-0.593741
1	-1.454125	-2.653618	-1.876310

Zero-point correction= 0.309065
(Hartree/Particle)
Thermal correction to Energy= 0.330150
Thermal correction to Enthalpy= 0.331094
Thermal correction to Gibbs Free Energy= 0.260371
Sum of electronic and zero-point Energies= -515.406849
Sum of electronic and thermal Energies= -515.385763
Sum of electronic and thermal Enthalpies= -515.384819
Sum of electronic and thermal Free Energies= -515.455542

Pro-Pb-CH_4

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.026777	1.120087	0.020138
6	2.319228	0.560277	-0.020442
6	1.217989	-0.167965	-0.814438
6	-1.102298	-0.098318	1.029410
6	-2.237901	0.461295	0.151331
6	1.753197	1.673156	0.572353
6	-1.724738	1.505918	-0.594191
6	-3.638781	-0.099271	0.146463
1	-4.306820	0.442612	-0.532977
1	-3.628883	-1.158512	-0.151422

1	-4.074017	-0.059621	1.155299
6	-2.385708	2.372723	-1.630857
1	-1.890996	2.275151	-2.608551
1	-3.446319	2.120440	-1.767039
1	-2.330515	3.435207	-1.353868
6	-1.356177	-0.084023	2.544296
1	-1.670594	0.916208	2.886929
1	-2.147348	-0.790843	2.838123
1	-0.454035	-0.355938	3.108674
6	1.483490	-0.346829	-2.317019
1	1.751605	0.612040	-2.791667
1	2.311340	-1.046202	-2.510923
1	0.601003	-0.736095	-2.842808
6	3.743081	0.069312	0.064887
1	4.382264	0.731705	0.659974
1	3.775754	-0.935260	0.512333
1	4.183065	-0.016756	-0.938988
6	2.365511	2.704419	1.480111
1	1.870025	2.718079	2.462097
1	3.435820	2.523289	1.649144
1	2.262281	3.715067	1.059833
82	0.094859	-1.860325	0.218620
1	0.935586	-2.738057	1.505223
6	-0.857508	-3.285014	-1.183678
1	-0.082804	-3.811294	-1.753323
1	-1.451326	-4.012660	-0.618836
1	-1.507889	-2.735942	-1.873485

Zero-point correction= 0.307812
(Hartree/Particle)
Thermal correction to Energy= 0.329352
Thermal correction to Enthalpy= 0.330296
Thermal correction to Gibbs Free Energy= 0.257534
Sum of electronic and zero-point Energies= -515.467372
Sum of electronic and thermal Energies= -515.445832
Sum of electronic and thermal Enthalpies= -515.444888
Sum of electronic and thermal Free Energies= -515.517650

Pro-C-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.213457	0.117076	-0.053058
6	-0.891524	0.776182	-0.537756
6	0.822958	0.070199	1.041830
6	2.042327	-0.276671	0.140060
6	-2.011284	-1.243525	0.028657
6	1.658430	-1.247662	-0.761092
6	3.371198	0.423990	0.263655
1	4.112269	0.052537	-0.453901
1	3.223368	1.499633	0.106596
1	3.782390	0.298600	1.276011
6	2.437449	-1.923425	-1.854441
1	2.006987	-1.710332	-2.843906
1	3.486547	-1.598179	-1.869166
1	2.428598	-3.015819	-1.730996
6	1.050605	-0.137304	2.537449
1	1.494957	-1.120415	2.743433
1	1.725965	0.628133	2.952112
1	0.104514	-0.075070	3.093165
6	-0.999831	1.619239	-1.805120
1	-1.511472	1.064089	-2.602244
1	-1.571807	2.550249	-1.642232
1	-0.007037	1.900453	-2.176035
6	-3.445751	0.911830	0.307465
1	-4.265405	0.279146	0.667362
1	-3.216476	1.650105	1.090706
1	-3.809902	1.476959	-0.563018
6	-2.938720	-2.343501	0.463267
1	-2.539059	-2.879533	1.336474
1	-3.934765	-1.963500	0.729404
1	-3.069307	-3.088757	-0.334437
6	0.012157	1.359981	0.644611
1	-0.602855	1.686182	1.502343
14	-0.147680	-0.979860	-0.258971
8	0.901886	2.454991	0.249273
1	0.376528	3.226724	-0.051912

Zero-point correction= 0.298613
(Hartree/Particle)
Thermal correction to Energy= 0.316787
Thermal correction to Enthalpy= 0.317731
Thermal correction to Gibbs Free Energy= 0.254792
Sum of electronic and zero-point Energies= -586.034291
Sum of electronic and thermal Energies= -586.016117
Sum of electronic and thermal Enthalpies= -586.015173
Sum of electronic and thermal Free Energies= -586.078112

Pro-Si-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.407217	1.409356	0.125059
6	-2.371072	0.105674	0.156318
6	-1.029240	-0.312504	0.808924
6	0.906335	0.486031	-0.994023
6	1.923766	1.235533	-0.095793
6	-2.258807	1.408202	-0.283561
6	1.240458	2.145395	0.684743
6	3.393058	0.900694	-0.097164
1	3.971167	1.531939	0.587536
1	3.526243	-0.150748	0.193366
1	3.815775	1.013331	-1.105812
6	1.745496	3.088336	1.741652
1	1.310527	2.858592	2.725296
1	2.838292	3.042777	1.841394
1	1.475247	4.127943	1.508318
6	1.129571	0.662514	-2.503077
1	1.224835	1.725746	-2.769633
1	2.045158	0.153820	-2.842240
1	0.295051	0.248407	-3.085434
6	-1.120749	-0.741615	2.280395
1	-1.655729	0.007937	2.882857
1	-1.654992	-1.698078	2.400011
1	-0.122508	-0.868385	2.719634
6	-3.544484	-0.833979	0.030504

1	-4.404618	-0.371379	-0.466958
1	-3.258916	-1.731825	-0.537687
1	-3.869875	-1.177854	1.022873
6	-3.244975	2.277921	-1.013054
1	-2.850079	2.599996	-1.987528
1	-4.197162	1.760719	-1.192760
1	-3.465491	3.191298	-0.442619
8	1.455756	-2.071738	0.518975
1	1.324224	-2.909860	0.991334
14	0.256551	-1.197252	-0.340625
1	-0.325006	-2.055697	-1.422531

Zero-point correction= 0.289599
(Hartree/Particle)
Thermal correction to Energy= 0.309275
Thermal correction to Enthalpy= 0.310219
Thermal correction to Gibbs Free Energy= 0.243596
Sum of electronic and zero-point Energies= -551.888980
Sum of electronic and thermal Energies= -551.869304
Sum of electronic and thermal Enthalpies= -551.868360
Sum of electronic and thermal Free Energies= -551.934983

Pro-Ge-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.411413	1.396350	0.109628
6	-2.397866	0.120433	0.155829
6	-1.062295	-0.307592	0.808860
6	0.910696	0.513234	-1.028202
6	1.924398	1.245991	-0.115049
6	-2.264641	1.417306	-0.296485
6	1.232105	2.132521	0.684821
6	3.396596	0.924944	-0.122470
1	3.968860	1.552164	0.570749
1	3.540421	-0.128889	0.154818
1	3.817968	1.055595	-1.129558
6	1.729033	3.056058	1.762309

1	1.297201	2.799573	2.740656
1	2.822237	3.019022	1.860429
1	1.448276	4.097985	1.553068
6	1.125989	0.710362	-2.535635
1	1.213455	1.778225	-2.787988
1	2.043790	0.213428	-2.885335
1	0.291666	0.300204	-3.121126
6	-1.145653	-0.729974	2.282446
1	-1.666043	0.029461	2.886373
1	-1.691598	-1.678360	2.410457
1	-0.145492	-0.868378	2.713183
6	-3.590133	-0.797722	0.049920
1	-4.442696	-0.326495	-0.452412
1	-3.325169	-1.711044	-0.503455
1	-3.918526	-1.118274	1.049087
6	-3.240006	2.297959	-1.027447
1	-2.846702	2.603376	-2.007986
1	-4.203375	1.797481	-1.194761
1	-3.438760	3.220940	-0.464397
32	0.262669	-1.263232	-0.378102
1	-0.305650	-2.204909	-1.488352
8	1.543351	-2.125012	0.558757
1	1.414197	-2.983587	0.999335

Zero-point correction= 0.287499
(Hartree/Particle)
Thermal correction to Energy= 0.307727
Thermal correction to Enthalpy= 0.308671
Thermal correction to Gibbs Free Energy= 0.240498
Sum of electronic and zero-point Energies= -551.767836
Sum of electronic and thermal Energies= -551.747609
Sum of electronic and thermal Enthalpies= -551.746665
Sum of electronic and thermal Free Energies= -551.814837

Pro-Sn-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z

14	-0.406506	1.335178	0.097638
6	-2.442920	0.136648	0.170258
6	-1.125439	-0.330584	0.825705
6	0.942477	0.518823	-1.058963
6	1.938054	1.263455	-0.139190
6	-2.254976	1.415081	-0.316360
6	1.218571	2.098755	0.691796
6	3.423913	1.013386	-0.173706
1	3.977222	1.669564	0.507963
1	3.628659	-0.030288	0.105935
1	3.820217	1.161374	-1.188337
6	1.689554	3.010677	1.790857
1	1.276189	2.710269	2.764759
1	2.784180	3.013700	1.880590
1	1.366550	4.046406	1.613739
6	1.126872	0.770618	-2.564533
1	1.172241	1.849420	-2.784123
1	2.056368	0.321065	-2.945749
1	0.299089	0.351313	-3.153495
6	-1.212541	-0.706311	2.314210
1	-1.675937	0.101729	2.903215
1	-1.814796	-1.613846	2.475800
1	-0.217551	-0.899331	2.735030
6	-3.679349	-0.724934	0.100856
1	-4.516606	-0.222011	-0.396489
1	-3.468527	-1.660303	-0.439131
1	-4.005458	-1.011416	1.110917
6	-3.196674	2.317833	-1.064993
1	-2.799448	2.577143	-2.057322
1	-4.183372	1.857229	-1.210074
1	-3.348616	3.264933	-0.527913
50	0.305154	-1.459389	-0.395222
1	-0.200004	-2.599010	-1.602903
8	1.624968	-2.288892	0.758605
1	1.785332	-3.219141	0.982595

Zero-point correction= 0.285106
(Hartree/Particle)
Thermal correction to Energy= 0.306038
Thermal correction to Enthalpy= 0.306982

Thermal correction to Gibbs Free Energy= 0.236472
Sum of electronic and zero-point Energies= -551.368692
Sum of electronic and thermal Energies= -551.347760
Sum of electronic and thermal Enthalpies= -551.346815
Sum of electronic and thermal Free Energies= -551.417326

Pro-Pb-H_2O

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.413750	1.330784	0.079898
6	-2.469798	0.155347	0.173105
6	-1.154433	-0.307647	0.823052
6	0.936313	0.558700	-1.089144
6	1.935325	1.270267	-0.154263
6	-2.267144	1.426904	-0.327845
6	1.211642	2.090061	0.689073
6	3.417666	1.003090	-0.177351
1	3.972398	1.652548	0.509445
1	3.602058	-0.042666	0.109078
1	3.826594	1.143282	-1.187955
6	1.678293	2.982445	1.805120
1	1.267591	2.659130	2.772844
1	2.772837	2.990295	1.893893
1	1.348194	4.019434	1.649766
6	1.126029	0.797899	-2.593026
1	1.178882	1.876064	-2.816849
1	2.054548	0.342650	-2.968842
1	0.296951	0.381816	-3.181903
6	-1.209510	-0.719091	2.300207
1	-1.645327	0.083018	2.918733
1	-1.824106	-1.619053	2.455345
1	-0.206978	-0.938159	2.687508
6	-3.717004	-0.691616	0.122039
1	-4.551023	-0.183511	-0.375308
1	-3.521669	-1.635106	-0.409529
1	-4.039953	-0.963535	1.137090
6	-3.203746	2.336530	-1.073706
1	-2.811971	2.583561	-2.071447

1	-4.198044	1.888718	-1.206352
1	-3.337559	3.289743	-0.542540
82	0.315207	-1.513308	-0.430968
1	-0.072884	-2.812094	-1.586902
8	1.708288	-2.224398	0.864560
1	1.882973	-3.172961	1.015141

Zero-point correction= 0.283883
(Hartree/Particle)
Thermal correction to Energy= 0.305114
Thermal correction to Enthalpy= 0.306058
Thermal correction to Gibbs Free Energy= 0.234474
Sum of electronic and zero-point Energies= -551.423434
Sum of electronic and thermal Energies= -551.402203
Sum of electronic and thermal Enthalpies= -551.401259
Sum of electronic and thermal Free Energies= -551.472842

Dimer-C

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.362550	2.169830	0.392450
6	-1.672144	1.107641	-0.523845
6	-1.672894	-1.116332	0.522459
6	-2.378262	-2.168582	-0.393848
6	-3.577392	1.662269	0.806381
6	-3.594937	-1.653028	-0.791748
6	-1.815959	-3.538896	-0.685973
1	-2.522584	-4.166836	-1.241014
1	-0.885881	-3.479196	-1.263640
1	-1.571165	-4.053049	0.255162
6	-4.666368	-2.256701	-1.657453
1	-4.795410	-1.692704	-2.592730
1	-4.440450	-3.297967	-1.925674
1	-5.638286	-2.249803	-1.143948
6	-1.344865	-1.632399	1.929447
1	-2.194217	-2.189136	2.351725

1	-0.470437	-2.296229	1.947022
1	-1.121643	-0.792643	2.599943
6	-1.354259	1.610325	-1.938038
1	-2.199689	2.178549	-2.352764
1	-0.468647	2.258519	-1.971240
1	-1.154184	0.762657	-2.605908
6	-1.795557	3.541885	0.667430
1	-2.499140	4.177523	1.217693
1	-0.863583	3.487739	1.242426
1	-1.552936	4.044931	-0.280161
6	-4.637331	2.278076	1.677800
1	-4.775389	1.709711	2.609058
1	-4.392879	3.313286	1.953225
1	-5.609713	2.292121	1.165114
6	-0.686242	-0.006088	-0.003101
14	-3.169956	0.001500	0.008894
1	2.495210	4.169277	-1.239502
6	1.793903	3.535750	-0.683840
6	2.365296	2.168282	-0.395608
1	0.862781	3.471128	-1.259352
1	1.548020	4.046431	0.258927
6	1.669191	1.109333	0.519941
6	3.584318	1.661377	-0.797522
6	1.341380	1.618471	1.929751
6	0.686833	-0.005097	-0.004155
14	3.170520	0.002189	0.000113
6	4.650717	2.275538	-1.662014
1	2.183354	2.188929	2.348455
1	0.455383	2.266331	1.952460
1	1.135977	0.774328	2.600513
6	1.676886	-1.114636	-0.526091
6	3.589127	-1.653358	0.802005
1	4.796935	1.704601	-2.590395
1	4.407835	3.309736	-1.942260
1	5.618785	2.291880	-1.141321
6	2.376533	-2.169047	0.392238
6	1.355586	-1.630081	-1.934554
6	4.653673	-2.258629	1.674876
6	1.816469	-3.543418	0.670493
1	2.212076	-2.174342	-2.358704

1	0.490639	-2.306467	-1.952677
1	1.120500	-0.791766	-2.602639
1	4.771937	-1.699042	2.614341
1	4.427460	-3.301895	1.935558
1	5.630566	-2.246704	1.170922
1	2.519578	-4.171941	1.229351
1	0.879528	-3.491881	1.237722
1	1.584848	-4.052620	-0.276684

Zero-point correction= 0.544775
(Hartree/Particle)
Thermal correction to Energy= 0.579421
Thermal correction to Enthalpy= 0.580365
Thermal correction to Gibbs Free Energy= 0.480685
Sum of electronic and zero-point Energies= -1019.229245
Sum of electronic and thermal Energies= -1019.194599
Sum of electronic and thermal Enthalpies= -1019.193654
Sum of electronic and thermal Free Energies= -1019.293334

Dimer-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-1.062177	0.035046	-0.428581
14	-3.724671	0.018532	0.238863
6	-3.320004	-1.726700	-1.282672
6	-2.387204	-1.362494	-0.094605
6	-2.410423	1.417974	-0.103712
6	-2.686606	1.796400	1.376502
6	-4.485034	-0.997117	-1.163061
6	-3.752473	1.043038	1.825994
6	-1.864038	2.811646	2.128408
1	-2.192484	2.933459	3.167093
1	-0.805738	2.514093	2.132626
1	-1.919444	3.793289	1.635840
6	-4.400079	0.989820	3.182586
1	-4.285265	-0.003866	3.641435
1	-3.968632	1.727869	3.872777

1	-5.479974	1.186902	3.116980
6	-2.523261	2.586100	-1.093800
1	-3.457545	3.148297	-0.940072
1	-1.688986	3.296476	-0.983572
1	-2.511441	2.231486	-2.132991
6	-2.017855	-2.552235	0.802255
1	-2.910162	-3.142460	1.064297
1	-1.308012	-3.233663	0.306901
1	-1.547365	-2.213469	1.734089
6	-2.921488	-2.701595	-2.362099
1	-3.708302	-2.844244	-3.112150
1	-2.012660	-2.350668	-2.873786
1	-2.681268	-3.683138	-1.927573
6	-5.698793	-0.955484	-2.050033
1	-5.864762	0.054012	-2.453340
1	-5.611421	-1.645135	-2.900596
1	-6.606295	-1.228166	-1.492831
14	1.030785	0.006093	0.248313
6	2.352946	-1.400123	-0.039424
6	2.421254	1.372070	0.097996
14	3.745168	-0.040924	-0.153087
6	3.141131	-1.851091	1.221958
6	2.053550	-2.526050	-1.038764
6	2.860701	1.790182	-1.332806
6	2.455373	2.510620	1.127983
6	4.322239	-1.139968	1.275089
6	3.964931	1.040671	-1.685963
6	2.604580	-2.871649	2.193499
1	2.953190	-3.129665	-1.237328
1	1.274981	-3.209270	-0.664126
1	1.697444	-2.121637	-1.995221
6	2.129232	2.831040	-2.142248
1	3.412987	3.052441	1.087217
1	1.654492	3.246258	0.953175
1	2.328552	2.129217	2.149829
6	5.424368	-1.166859	2.298342
6	4.762634	1.026827	-2.961195
1	3.293300	-3.068753	3.023231
1	1.645967	-2.528986	2.610575
1	2.404483	-3.824270	1.682006

1	2.586076	2.995681	-3.125221
1	1.083234	2.527200	-2.293607
1	2.110222	3.792670	-1.609379
1	5.544294	-0.186810	2.782636
1	5.235683	-1.908176	3.086761
1	6.390445	-1.412764	1.835285
1	4.697004	0.049877	-3.462777
1	4.417216	1.790827	-3.671396
1	5.828648	1.212500	-2.765275

Zero-point correction= 0.536199
(Hartree/Particle)
Thermal correction to Energy= 0.572812
Thermal correction to Enthalpy= 0.573756
Thermal correction to Gibbs Free Energy= 0.468142
Sum of electronic and zero-point Energies= -950.871114
Sum of electronic and thermal Energies= -950.834501
Sum of electronic and thermal Enthalpies= -950.833557
Sum of electronic and thermal Free Energies= -950.939171

Dimer-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	1.106634	-0.035541	-0.585624
14	3.779617	-0.008877	0.344140
6	3.523246	1.765018	-1.180492
6	2.502396	1.394174	-0.077566
6	2.536620	-1.439613	-0.080015
6	2.697131	-1.800968	1.416620
6	4.659438	1.003485	-0.992926
6	3.707593	-1.019009	1.941721
6	1.844704	-2.830096	2.115491
1	2.111267	-2.948336	3.172151
1	0.783603	-2.547388	2.058069
1	1.942659	-3.810341	1.627081
6	4.246548	-0.943673	3.343921
1	4.096079	0.056046	3.777454

1	3.764364	-1.672077	4.010090
1	5.328052	-1.139525	3.365336
6	2.738246	-2.605647	-1.057518
1	3.664244	-3.158434	-0.831132
1	1.906881	-3.326842	-1.014721
1	2.807707	-2.252575	-2.095445
6	2.049609	2.565489	0.804967
1	2.911319	3.163645	1.143172
1	1.369459	3.245864	0.269054
1	1.516346	2.208164	1.695372
6	3.229019	2.776804	-2.259676
1	4.069377	2.915512	-2.949703
1	2.348473	2.468156	-2.842734
1	2.986634	3.753314	-1.816567
6	5.929545	0.945921	-1.796464
1	6.099462	-0.061408	-2.203942
1	5.915463	1.650020	-2.639844
1	6.803716	1.188537	-1.175446
32	-1.067681	0.007616	0.440106
6	-2.485425	1.425428	-0.029652
6	-2.538278	-1.401007	0.115279
14	-3.810401	0.020978	-0.251382
6	-3.390295	1.869113	1.145628
6	-2.110217	2.538127	-1.017947
6	-2.836732	-1.816804	-1.346622
6	-2.656276	-2.532023	1.146784
6	-4.544170	1.111643	1.113517
6	-3.893841	-1.054450	-1.804557
6	-2.981840	2.932200	2.135201
1	-2.998378	3.120637	-1.312453
1	-1.383749	3.244688	-0.587438
1	-1.660760	2.125274	-1.930412
6	-2.047252	-2.870236	-2.082451
1	-3.610109	-3.072058	1.036635
1	-1.847256	-3.271759	1.039759
1	-2.608941	-2.147084	2.174395
6	-5.726551	1.109801	2.043513
6	-4.565424	-1.032676	-3.150281
1	-3.743456	3.111181	2.903254
1	-2.044421	2.645845	2.635600

1	-2.786055	3.883986	1.620752
1	-2.416505	-3.035329	-3.101550
1	-0.988386	-2.578203	-2.142235
1	-2.085883	-3.829174	-1.545518
1	-5.863556	0.125236	2.514138
1	-5.619854	1.851724	2.847100
1	-6.657470	1.335787	1.503923
1	-4.460930	-0.050347	-3.634254
1	-4.148165	-1.786546	-3.831923
1	-5.643522	-1.228026	-3.058905

Zero-point correction= 0.533412
(Hartree/Particle)
Thermal correction to Energy= 0.571214
Thermal correction to Enthalpy= 0.572158
Thermal correction to Gibbs Free Energy= 0.462988
Sum of electronic and zero-point Energies= -950.663962
Sum of electronic and thermal Energies= -950.626160
Sum of electronic and thermal Enthalpies= -950.625216
Sum of electronic and thermal Free Energies= -950.734386

Dimer-Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	3.993886	0.071078	0.447186
6	3.883167	1.766039	-1.182160
6	2.760398	1.435083	-0.177160
6	2.920955	-1.492225	0.036997
6	2.974401	-1.739747	1.559214
6	4.996409	1.017096	-0.850128
6	3.844296	-0.817238	2.111014
6	2.178558	-2.814747	2.256531
1	2.373571	-2.848345	3.334904
1	1.100358	-2.651201	2.106439
1	2.412471	-3.803602	1.836199
6	4.232145	-0.587145	3.545824
1	3.945434	0.421206	3.879892

1	3.757295	-1.310249	4.223169
1	5.320036	-0.668389	3.682668
6	3.323387	-2.689180	-0.838961
1	4.287750	-3.114224	-0.513391
1	2.580367	-3.500632	-0.798506
1	3.430716	-2.402235	-1.894358
6	2.214907	2.640072	0.606212
1	3.035769	3.255285	1.012517
1	1.598024	3.298017	-0.025353
1	1.588128	2.322490	1.450423
6	3.710012	2.742854	-2.319261
1	4.623850	2.865576	-2.912235
1	2.903163	2.412804	-2.990939
1	3.416244	3.731242	-1.937491
6	6.340006	0.928410	-1.520481
1	6.553017	-0.097212	-1.855938
1	6.409385	1.587136	-2.397124
1	7.147916	1.209298	-0.829826
6	-2.732076	1.482722	-0.010512
6	-2.938482	-1.444198	0.112968
14	-4.053216	0.090187	-0.304013
6	-3.702678	1.953910	1.092573
6	-2.280337	2.570704	-0.997705
6	-3.195295	-1.833693	-1.358855
6	-3.221560	-2.551164	1.140824
6	-4.855088	1.194902	1.008644
6	-4.136670	-0.961462	-1.874329
6	-3.362228	3.047256	2.075252
1	-3.142860	3.140136	-1.383889
1	-1.595979	3.295601	-0.529761
1	-1.754512	2.139293	-1.860404
6	-2.494004	-2.975611	-2.051799
1	-4.219237	-2.994287	0.984378
1	-2.487921	-3.369628	1.077165
1	-3.190025	-2.168446	2.170468
6	-6.088436	1.208839	1.870361
6	-4.721347	-0.869740	-3.257331
1	-4.177314	3.251331	2.779453
1	-2.464412	2.777932	2.652127
1	-3.126800	3.981813	1.546185

1	-2.836418	-3.112970	-3.084393
1	-1.407090	-2.803248	-2.069521
1	-2.658635	-3.917884	-1.509299
1	-6.258477	0.229733	2.342113
1	-6.023808	1.958088	2.671682
1	-6.986492	1.433889	1.277147
1	-4.492066	0.099606	-3.724229
1	-4.340304	-1.658286	-3.920860
1	-5.817161	-0.957228	-3.232614
50	1.281199	-0.161609	-0.768467
50	-1.212719	-0.069601	0.579915

Zero-point correction= 0.531471
(Hartree/Particle)
Thermal correction to Energy= 0.570148
Thermal correction to Enthalpy= 0.571092
Thermal correction to Gibbs Free Energy= 0.458146
Sum of electronic and zero-point Energies= -949.887526
Sum of electronic and thermal Energies= -949.848849
Sum of electronic and thermal Enthalpies= -949.847905
Sum of electronic and thermal Free Energies= -949.960851

Dimer-Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	4.090351	0.137117	0.558257
6	4.048092	1.764346	-1.146539
6	2.897011	1.472357	-0.173926
6	3.077513	-1.478000	0.236507
6	3.067118	-1.608897	1.767299
6	5.142792	1.013918	-0.753563
6	3.892278	-0.623999	2.282547
6	2.256741	-2.639333	2.514971
1	2.425371	-2.600795	3.597538
1	1.182007	-2.488930	2.328417
1	2.500332	-3.653529	2.167339
6	4.205986	-0.271617	3.710748

1	3.894997	0.757246	3.946178
1	3.705712	-0.942569	4.422836
1	5.286578	-0.326489	3.906498
6	3.496878	-2.728767	-0.547591
1	4.453746	-3.133064	-0.174435
1	2.751912	-3.535844	-0.468667
1	3.630341	-2.514974	-1.617538
6	2.279976	2.690538	0.527772
1	3.060925	3.339010	0.962343
1	1.689964	3.314187	-0.161892
1	1.610556	2.391005	1.345906
6	3.923101	2.704765	-2.320994
1	4.854536	2.792769	-2.892413
1	3.128731	2.365971	-3.003339
1	3.636048	3.710422	-1.981347
6	6.501104	0.879485	-1.386239
1	6.711206	-0.163418	-1.666497
1	6.597954	1.493810	-2.292368
1	7.296725	1.185745	-0.691732
6	-2.872519	1.520967	-0.126552
6	-3.133990	-1.435704	0.136339
14	-4.181151	0.114376	-0.356640
6	-3.849860	2.065295	0.924683
6	-2.358026	2.528022	-1.165260
6	-3.370277	-1.880250	-1.315815
6	-3.423598	-2.482358	1.221029
6	-4.997877	1.292904	0.884466
6	-4.267028	-0.995448	-1.889902
6	-3.530510	3.231868	1.828330
1	-3.190015	3.092828	-1.621108
1	-1.670306	3.266038	-0.723804
1	-1.816787	2.029551	-1.981416
6	-2.692309	-3.070826	-1.948674
1	-4.429481	-2.919167	1.097293
1	-2.703933	-3.315270	1.195328
1	-3.380783	-2.048938	2.230470
6	-6.234502	1.353022	1.739390
6	-4.809957	-0.937235	-3.291346
1	-4.355845	3.479490	2.506006
1	-2.637322	3.017486	2.434885

1	-3.297948	4.127374	1.234415
1	-3.043366	-3.258610	-2.970126
1	-1.602756	-2.917757	-1.982873
1	-2.867133	-3.979267	-1.354772
1	-6.399109	0.405625	2.273904
1	-6.179022	2.153349	2.490547
1	-7.132419	1.531598	1.130335
1	-4.536469	0.006123	-3.787012
1	-4.437529	-1.761616	-3.915048
1	-5.908311	-0.988232	-3.294460
82	1.383450	-0.213735	-0.791950
82	-1.298654	-0.049953	0.599778

Zero-point correction= 0.529942
(Hartree/Particle)
Thermal correction to Energy= 0.569361
Thermal correction to Enthalpy= 0.570305
Thermal correction to Gibbs Free Energy= 0.453412
Sum of electronic and zero-point Energies= -950.067171
Sum of electronic and thermal Energies= -950.027751
Sum of electronic and thermal Enthalpies= -950.026807
Sum of electronic and thermal Free Energies= -950.143700
