

Supporting Information

Theoretical Study of the Mechanisms of [3+2] Cycloaddition Reactions of Trimetallaallenes [>M=M=M<] (M = C, Si, Ge, Sn, and Pb)

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(All geometries were calculated B3LYP/LANL2DZ)

C=C=C-Rea (singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.358841	0.000227	0.001287
6	0.000263	-0.003544	0.002654
6	1.359059	-0.001611	0.000753
6	2.337038	-0.927687	-0.915520
14	2.269202	-1.095186	-2.893775
6	2.804377	0.458115	-3.872303
1	2.828079	0.156839	-4.930286
1	2.148187	1.324539	-3.794819
1	3.821857	0.772711	-3.607217
6	3.647727	-2.303673	-3.457481
1	3.514428	-3.342157	-3.142833
1	3.644337	-2.294085	-4.557381
1	4.643224	-1.973436	-3.136073
6	0.681258	-1.734713	-3.700401
1	-0.190099	-1.129843	-3.451067
1	0.812358	-1.687162	-4.791181
1	0.464962	-2.774297	-3.437130
14	2.522636	-2.781090	-0.204420
6	2.025032	-2.963618	1.612639
1	2.855057	-2.691205	2.271251
1	1.163758	-2.349208	1.875776
1	1.775665	-4.013644	1.819205
6	1.515563	-4.095421	-1.148654
1	1.826774	-4.226821	-2.189571
1	1.665824	-5.057502	-0.637594
1	0.443392	-3.884873	-1.139713
6	4.344618	-3.360506	-0.229006
1	4.374202	-4.382834	0.176328
1	4.795842	-3.387069	-1.224976
1	4.977133	-2.738430	0.417750
6	3.737896	-0.234654	-0.723012
1	3.836363	0.639368	-1.379020
1	4.573013	-0.902726	-0.953702

6	3.737889	0.228688	0.724189
1	4.574170	0.895097	0.955547
1	3.834154	-0.645589	1.380317
6	2.338157	0.924160	0.916288
14	2.525944	2.777564	0.204842
6	1.521099	4.094007	1.148692
1	0.448661	3.883245	1.144254
1	1.836288	4.228796	2.187973
1	1.669424	5.054563	0.634182
6	4.349537	3.352786	0.230595
1	4.382253	4.375423	-0.173630
1	4.800384	3.377013	1.226878
1	4.980894	2.729626	-0.416303
6	2.027069	2.962442	-1.611708
1	2.856207	2.688659	-2.270646
1	1.163713	2.350454	-1.875172
1	1.780461	4.013375	-1.817148
14	2.272414	1.092055	2.894503
6	0.685739	1.735040	3.700785
1	-0.186845	1.132537	3.450390
1	0.815518	1.687054	4.791660
1	0.472230	2.775208	3.437408
6	2.807407	-0.461881	3.872594
1	3.826400	-0.773767	3.610493
1	2.826643	-0.162115	4.931124
1	2.154289	-1.330001	3.791870
6	3.652957	2.298158	3.458146
1	3.521869	3.336826	3.143310
1	3.648902	2.288827	4.558062
1	4.647976	1.965844	3.137440
6	-2.335708	0.928953	-0.914278
14	-2.267373	1.099509	-2.892174
6	-2.803761	-0.451824	-3.873463
1	-2.824635	-0.149429	-4.931192
1	-2.149973	-1.319862	-3.795539
1	-3.822490	-0.764530	-3.610783
6	-3.646462	2.308530	-3.454066
1	-3.513748	3.346727	-3.138140
1	-3.643276	2.300282	-4.553987
1	-4.641900	1.977439	-3.133106

6	-0.678396	1.741036	-3.696286
1	-0.463084	2.780298	-3.430814
1	0.193488	1.136461	-3.447231
1	-0.808411	1.695505	-4.787267
14	-2.520996	2.781561	-0.201138
6	-1.513499	4.096922	-1.143886
1	-1.827358	4.231996	-2.183578
1	-1.661354	5.057681	-0.629638
1	-0.441229	3.884797	-1.138227
6	-4.343373	3.360732	-0.225712
1	-4.373512	4.382997	0.179716
1	-4.794732	3.387155	-1.221775
1	-4.975835	2.738327	0.420962
6	-2.022747	2.963409	1.615645
1	-2.851197	2.686894	2.274555
1	-1.158611	2.352128	1.877324
1	-1.777492	4.014280	1.823035
6	-3.736895	0.236061	-0.724029
1	-3.834861	-0.637116	-1.381435
1	-4.571610	0.904793	-0.954418
6	-3.738542	-0.229212	0.722428
1	-4.575188	-0.895825	0.952006
1	-3.834792	0.644209	1.379724
6	-2.339689	-0.925756	0.914460
14	-2.527455	-2.777382	0.199371
6	-2.028736	-2.957782	-1.617791
1	-2.858214	-2.683348	-2.276122
1	-1.166201	-2.344322	-1.880179
1	-1.781028	-4.007924	-1.825653
6	-1.523074	-4.095436	1.141404
1	-1.671494	-5.055250	0.625577
1	-0.450894	-3.884894	1.137194
1	-1.837991	-4.231440	2.180615
6	-4.350438	-3.353586	0.222665
1	-4.801533	-3.381116	1.218760
1	-4.981817	-2.728889	-0.422756
1	-4.382144	-4.375043	-0.184648
14	-2.274635	-1.097131	2.892318
6	-3.654585	-2.305024	3.453022
1	-3.522805	-3.342898	3.135805

1	-3.650550	-2.298104	4.552951
1	-4.649694	-1.972467	3.132817
6	-0.688481	-1.740238	3.698689
1	0.182431	-1.133578	3.453204
1	-0.820897	-1.697822	4.789478
1	-0.471216	-2.778407	3.430845
6	-2.808994	0.454998	3.873272
1	-3.826880	0.769710	3.610069
1	-2.830814	0.152279	4.930891
1	-2.153500	1.321886	3.796165

Si=Si=Si-Rea (singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-2.072810	0.056458	0.051954
14	-0.044246	0.050728	-0.793548
14	2.034322	0.063994	-0.013598
6	3.411066	-0.999442	-0.876246
14	3.074031	-1.603771	-2.706021
6	2.903587	-0.193346	-3.969954
1	2.767351	-0.657614	-4.958178
1	2.031250	0.439468	-3.780142
1	3.791286	0.447708	-4.032971
6	4.587942	-2.598277	-3.317989
1	4.748758	-3.532368	-2.768170
1	4.435607	-2.859317	-4.375230
1	5.510583	-2.005311	-3.257176
6	1.507351	-2.676501	-2.895986
1	0.999651	-2.869352	-1.946373
1	0.788015	-2.167322	-3.549591
1	1.750341	-3.646819	-3.350636
14	3.881898	-2.581076	0.211655
6	3.439046	-2.458834	2.057873
1	4.060961	-1.738246	2.596001
1	2.385680	-2.198318	2.222413
1	3.607312	-3.445009	2.514779

6	3.022416	-4.189305	-0.342909
1	3.190463	-4.458297	-1.390157
1	3.417685	-5.007402	0.277081
1	1.939741	-4.145409	-0.174336
6	5.767810	-2.861168	0.145538
1	6.006630	-3.787403	0.687582
1	6.149257	-2.964502	-0.876623
1	6.318422	-2.045713	0.632877
6	4.613224	0.032111	-0.882072
1	4.532790	0.686705	-1.761141
1	5.581892	-0.476877	-0.961273
6	4.580600	0.914596	0.394264
1	5.348407	1.696932	0.332211
1	4.847866	0.285782	1.255639
6	3.139719	1.540017	0.609656
14	2.942305	3.165555	-0.490802
6	1.526896	4.284053	0.116761
1	0.577809	3.735162	0.164112
1	1.711507	4.739032	1.095840
1	1.399527	5.100595	-0.608207
6	4.579045	4.148706	-0.462387
1	4.411989	5.119639	-0.950855
1	4.959852	4.342751	0.545023
1	5.364093	3.631766	-1.030521
6	2.576246	2.899666	-2.334910
1	3.377701	2.370281	-2.859149
1	1.638736	2.358495	-2.502173
1	2.478132	3.891853	-2.800194
14	2.891506	2.022421	2.490399
6	1.072263	2.324357	2.930774
1	0.436535	1.522083	2.539590
1	0.958502	2.336267	4.024193
1	0.688243	3.273418	2.544206
6	3.498754	0.680971	3.697731
1	4.535133	0.367174	3.521098
1	3.459313	1.109213	4.710031
1	2.861173	-0.209022	3.693134
6	3.908127	3.566608	2.967447
1	3.586669	4.480493	2.455882
1	3.791014	3.735566	4.047749

1	4.979759	3.426034	2.772881
6	-3.604176	0.485764	-1.061340
14	-3.404471	0.010497	-2.952897
6	-3.111598	-1.855808	-3.191843
1	-2.904523	-2.032895	-4.257266
1	-2.247220	-2.221568	-2.625180
1	-3.989054	-2.458409	-2.928247
6	-5.022520	0.389381	-3.894358
1	-5.212148	1.463980	-4.005552
1	-4.952410	-0.037681	-4.905170
1	-5.896832	-0.062034	-3.406870
6	-1.987497	0.874452	-3.881630
1	-2.131194	1.952988	-3.994506
1	-1.018807	0.707661	-3.393275
1	-1.929017	0.438280	-4.890546
14	-4.182338	2.356521	-0.907686
6	-3.336547	3.517333	-2.157172
1	-3.667640	3.354713	-3.189284
1	-3.590376	4.552753	-1.888635
1	-2.243659	3.426350	-2.128882
6	-6.069530	2.481751	-1.166612
1	-6.345165	3.543860	-1.238529
1	-6.417619	1.985294	-2.078182
1	-6.623222	2.059816	-0.317223
6	-3.869220	3.160845	0.785690
1	-4.387071	2.644444	1.601064
1	-2.804061	3.213094	1.037653
1	-4.254385	4.190667	0.751285
6	-4.697705	-0.463349	-0.410266
1	-4.652477	-1.451449	-0.880522
1	-5.712454	-0.082886	-0.583173
6	-4.463520	-0.641763	1.117667
1	-5.138300	-1.418551	1.506589
1	-4.747066	0.291929	1.626823
6	-2.950282	-0.995460	1.435133
14	-2.661911	-2.936613	1.285175
6	-0.850551	-3.399976	0.957817
1	-0.759067	-4.495699	0.935655
1	-0.505578	-3.005995	-0.005031
1	-0.175266	-3.020721	1.733541

6	-3.197471	-3.871402	2.865330
1	-3.104221	-4.947160	2.656846
1	-2.576907	-3.652700	3.740968
1	-4.244876	-3.679247	3.129875
6	-3.716044	-3.763659	-0.067449
1	-4.787833	-3.557985	0.050993
1	-3.418411	-3.484240	-1.080565
1	-3.581910	-4.851141	0.027483
14	-2.515690	-0.421801	3.253471
6	-3.880289	-0.951025	4.478430
1	-3.886205	-2.021736	4.698827
1	-3.728724	-0.414431	5.426198
1	-4.876098	-0.675788	4.105431
6	-0.832587	-1.108031	3.818162
1	-0.040205	-0.845959	3.105293
1	-0.566403	-0.667824	4.789298
1	-0.831403	-2.197473	3.937789
6	-2.443682	1.467307	3.469751
1	-3.442850	1.917223	3.447178
1	-2.012651	1.678243	4.459455
1	-1.823915	1.975937	2.726317

Si=Ge=Si-Rea (singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-2.100181	0.056404	0.085281
32	-0.037112	0.080457	-0.958948
14	2.075321	0.068557	0.032785
6	3.522387	-0.840562	-0.898334
14	3.285175	-1.267732	-2.792452
6	3.174148	0.258473	-3.922783
1	3.082788	-0.106829	-4.956655
1	2.297825	0.879892	-3.715119
1	4.067999	0.893310	-3.881206
6	4.835704	-2.191578	-3.422926
1	4.965505	-3.185936	-2.981323

1	4.749412	-2.321709	-4.511349
1	5.750715	-1.613859	-3.234044
6	1.738568	-2.314531	-3.180168
1	1.346902	-2.860190	-2.315218
1	0.932364	-1.670615	-3.557488
1	1.975139	-3.052971	-3.963062
14	4.001393	-2.511819	0.046371
6	3.505934	-2.579045	1.883137
1	4.095127	-1.899164	2.504692
1	2.441720	-2.361908	2.043820
1	3.689033	-3.600642	2.247502
6	3.195317	-4.080032	-0.679717
1	3.367166	-4.231641	-1.749629
1	3.620365	-4.944776	-0.149150
1	2.112473	-4.090935	-0.503089
6	5.894794	-2.743628	0.013512
1	6.140141	-3.711345	0.474164
1	6.309333	-2.741925	-1.000702
1	6.410613	-1.966211	0.592475
6	4.692803	0.215792	-0.750477
1	4.621707	0.961679	-1.554273
1	5.679009	-0.255252	-0.850403
6	4.589874	0.950055	0.612034
1	5.330948	1.758648	0.663570
1	4.851593	0.239624	1.409207
6	3.122131	1.501763	0.841001
14	2.905217	3.222832	-0.103205
6	1.423431	4.225849	0.546555
1	0.491448	3.651574	0.464057
1	1.531706	4.561585	1.583315
1	1.314103	5.121508	-0.081542
6	4.503260	4.250748	0.085788
1	4.315705	5.263441	-0.299517
1	4.849098	4.345327	1.119490
1	5.321321	3.824285	-0.510259
6	2.619428	3.135973	-1.979025
1	3.456132	2.684277	-2.520472
1	1.705214	2.590948	-2.238514
1	2.509034	4.167886	-2.344589
14	2.799293	1.794774	2.748649

6	0.954540	1.959488	3.149344
1	0.391189	1.114438	2.738363
1	0.813380	1.954937	4.239352
1	0.508639	2.878345	2.757946
6	3.442663	0.379868	3.848657
1	4.496202	0.129769	3.670870
1	3.361987	0.712853	4.893770
1	2.848514	-0.534371	3.749418
6	3.717187	3.337122	3.401625
1	3.380185	4.276772	2.950430
1	3.540652	3.409319	4.484623
1	4.802435	3.257839	3.252567
6	-3.663832	0.544676	-0.974037
14	-3.478425	0.353713	-2.916737
6	-3.085522	-1.436996	-3.429936
1	-2.915295	-1.447368	-4.516322
1	-2.175372	-1.816846	-2.951133
1	-3.909838	-2.130014	-3.224015
6	-5.135892	0.768628	-3.769675
1	-5.380871	1.836957	-3.730549
1	-5.069678	0.485040	-4.829968
1	-5.973606	0.210225	-3.331531
6	-2.136891	1.422032	-3.742605
1	-2.344501	2.494564	-3.699974
1	-1.144075	1.249292	-3.308975
1	-2.084183	1.134209	-4.803167
14	-4.328484	2.348724	-0.554310
6	-3.583600	3.712361	-1.655527
1	-3.937194	3.671760	-2.692111
1	-3.884904	4.685696	-1.242658
1	-2.487058	3.682292	-1.665092
6	-6.226471	2.407296	-0.753120
1	-6.557163	3.453065	-0.673847
1	-6.572862	2.020684	-1.717188
1	-6.734976	1.845132	0.041429
6	-4.002892	2.946269	1.220260
1	-4.484573	2.315907	1.974956
1	-2.934403	3.005188	1.456066
1	-4.422400	3.958145	1.320544
6	-4.711447	-0.531932	-0.464374

1	-4.612285	-1.449026	-1.054641
1	-5.743927	-0.185021	-0.600790
6	-4.475829	-0.885562	1.030277
1	-5.114808	-1.734428	1.316350
1	-4.806022	-0.034804	1.646270
6	-2.947630	-1.203348	1.317233
14	-2.579188	-3.098315	0.929563
6	-0.739150	-3.482238	0.660492
1	-0.622081	-4.566406	0.516773
1	-0.352895	-2.975185	-0.231255
1	-0.113135	-3.185268	1.509090
6	-3.190367	-4.237533	2.339082
1	-3.062169	-5.276750	2.003252
1	-2.631222	-4.123294	3.273828
1	-4.256250	-4.092975	2.556775
6	-3.510955	-3.773693	-0.587270
1	-4.598045	-3.645389	-0.504718
1	-3.179591	-3.334974	-1.531186
1	-3.314728	-4.854824	-0.638834
14	-2.566633	-0.858513	3.206092
6	-3.963334	-1.545951	4.310718
1	-3.993282	-2.637799	4.357630
1	-3.818279	-1.169767	5.333870
1	-4.946830	-1.193886	3.971652
6	-0.903476	-1.603034	3.759829
1	-0.071200	-1.231754	3.148449
1	-0.708827	-1.305395	4.799882
1	-0.887816	-2.698081	3.722411
6	-2.511324	0.987529	3.664988
1	-3.513865	1.428301	3.699616
1	-2.081991	1.072369	4.673935
1	-1.895181	1.591508	2.993610

Ge=Si=Ge-Rea (singlet)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

32	-2.088595	0.083045	0.025715
14	-0.040714	-0.056275	-1.006296
32	2.054182	0.049753	-0.024071
6	3.578417	-1.012954	-0.840453
14	3.301461	-1.703789	-2.646646
6	3.145035	-0.347308	-3.970611
1	3.030207	-0.848096	-4.943481
1	2.264968	0.285899	-3.820797
1	4.029796	0.297685	-4.040225
6	4.839084	-2.709767	-3.177847
1	4.983042	-3.626496	-2.594484
1	4.723318	-3.003372	-4.231185
1	5.757919	-2.112410	-3.103496
6	1.753757	-2.804659	-2.830662
1	1.320998	-3.116316	-1.874215
1	0.971922	-2.263466	-3.380326
1	1.999397	-3.714872	-3.399241
14	4.075355	-2.509540	0.339719
6	3.635626	-2.281824	2.178959
1	4.228515	-1.499660	2.661664
1	2.572135	-2.061695	2.342339
1	3.853446	-3.226433	2.698839
6	3.238978	-4.160309	-0.115862
1	3.395055	-4.477758	-1.151573
1	3.656832	-4.940340	0.537321
1	2.157808	-4.125821	0.068342
6	5.966493	-2.758292	0.294112
1	6.223149	-3.643745	0.893166
1	6.351643	-2.916985	-0.719385
1	6.499622	-1.902883	0.730012
6	4.717002	0.083922	-0.851870
1	4.626202	0.701953	-1.755715
1	5.713427	-0.376272	-0.892686
6	4.631126	1.016477	0.390077
1	5.390221	1.806929	0.307448
1	4.896342	0.427470	1.279582
6	3.187016	1.636949	0.567272
14	2.949253	3.189787	-0.618303
6	1.470929	4.269354	-0.095601
1	0.543701	3.682358	-0.064442

1	1.601050	4.760527	0.874786
1	1.335000	5.058008	-0.849279
6	4.545220	4.238628	-0.600461
1	4.356744	5.175989	-1.143571
1	4.889936	4.498264	0.405198
1	5.364383	3.722842	-1.119488
6	2.640144	2.820792	-2.456210
1	3.471703	2.294874	-2.935351
1	1.724691	2.241642	-2.619708
1	2.521269	3.785462	-2.972017
14	2.892164	2.187344	2.419037
6	1.050743	2.392923	2.823666
1	0.486936	1.494480	2.546374
1	0.926978	2.541432	3.905723
1	0.590839	3.245177	2.314402
6	3.565144	0.942045	3.693628
1	4.621596	0.687531	3.541161
1	3.486101	1.411306	4.685164
1	2.986529	0.012907	3.724283
6	3.802223	3.812500	2.841523
1	3.440695	4.680048	2.278504
1	3.650286	4.025937	3.909581
1	4.884508	3.726256	2.675968
6	-3.748063	0.392446	-1.104214
14	-3.559969	-0.129469	-2.981238
6	-3.186065	-1.986304	-3.176273
1	-3.012164	-2.187437	-4.243396
1	-2.282122	-2.290011	-2.634823
1	-4.020401	-2.622855	-2.857614
6	-5.209842	0.152650	-3.902289
1	-5.446557	1.215121	-4.039187
1	-5.141495	-0.299977	-4.902080
1	-6.054565	-0.320297	-3.383753
6	-2.200307	0.776298	-3.955408
1	-2.395156	1.844427	-4.087637
1	-1.214931	0.664515	-3.485259
1	-2.139553	0.322294	-4.955844
14	-4.406303	2.233749	-0.976807
6	-3.639929	3.403818	-2.268825
1	-3.982580	3.199451	-3.289799

1	-3.937849	4.432580	-2.020781
1	-2.543313	3.365746	-2.261939
6	-6.302120	2.269397	-1.197299
1	-6.630721	3.316506	-1.267662
1	-6.641365	1.752460	-2.100996
1	-6.819407	1.824015	-0.336893
6	-4.092084	3.086790	0.694472
1	-4.596313	2.581233	1.525661
1	-3.026064	3.164139	0.938156
1	-4.494550	4.108966	0.639208
6	-4.757287	-0.594438	-0.386502
1	-4.660261	-1.596431	-0.818146
1	-5.798338	-0.286113	-0.553623
6	-4.504442	-0.701627	1.147577
1	-5.161615	-1.479589	1.565482
1	-4.818040	0.243138	1.617740
6	-2.990502	-1.004166	1.496534
14	-2.629936	-2.932340	1.405665
6	-0.791573	-3.356220	1.183301
1	-0.680766	-4.450155	1.160271
1	-0.397852	-2.952456	0.242863
1	-0.168621	-2.973245	1.999843
6	-3.226795	-3.828550	2.987400
1	-3.111774	-4.909422	2.820734
1	-2.651320	-3.572061	3.883723
1	-4.287884	-3.640775	3.196164
6	-3.580643	-3.830128	0.022283
1	-4.665536	-3.676147	0.088898
1	-3.250669	-3.549473	-0.980800
1	-3.397522	-4.908254	0.140303
14	-2.583419	-0.343745	3.289285
6	-3.972177	-0.817236	4.509392
1	-4.009197	-1.887234	4.734267
1	-3.812723	-0.280467	5.455888
1	-4.957152	-0.517340	4.126623
6	-0.920459	-1.009651	3.935159
1	-0.099841	-0.785601	3.241539
1	-0.685833	-0.525493	4.893543
1	-0.930486	-2.092090	4.106151
6	-2.490204	1.553367	3.412067

1	-3.477018	2.020504	3.322481
1	-2.095127	1.810903	4.405734
1	-1.828193	2.009378	2.669117

Ge=Ge=Ge-Rea (singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-2.138204	0.117476	-0.030800
32	-0.047469	-0.822757	-0.757384
32	2.100553	0.040688	-0.030393
6	3.649255	-1.276481	0.087465
14	3.407816	-3.015907	-0.766122
6	3.265628	-2.926499	-2.661136
1	3.171570	-3.957311	-3.033901
1	2.379640	-2.375326	-2.991761
1	4.147616	-2.486284	-3.142744
6	4.955300	-4.096771	-0.458668
1	5.093038	-4.369830	0.593990
1	4.854922	-5.030063	-1.031562
1	5.871667	-3.598112	-0.802568
6	1.867831	-3.971782	-0.163397
1	1.372395	-3.508264	0.696230
1	1.126930	-4.037328	-0.971705
1	2.141573	-4.998120	0.124607
14	4.131725	-1.565709	1.975584
6	3.668977	-0.152034	3.165126
1	4.249398	0.757381	2.986477
1	2.601785	0.104746	3.132837
1	3.889958	-0.486061	4.189646
6	3.297292	-3.092043	2.754057
1	3.471604	-4.029001	2.216037
1	3.698476	-3.213481	3.770886
1	2.212809	-2.952101	2.846285
6	6.023325	-1.762098	2.130465
1	6.272081	-2.000298	3.174563
1	6.422818	-2.564216	1.500066

1	6.549960	-0.833691	1.872555
6	4.784801	-0.466378	-0.655621
1	4.703083	-0.623847	-1.739948
1	5.783617	-0.822052	-0.367931
6	4.679917	1.058742	-0.372976
1	5.436475	1.594061	-0.964029
1	4.936291	1.230757	0.682059
6	3.230665	1.616886	-0.670686
14	2.999180	1.943372	-2.598274
6	1.508745	3.070628	-2.961381
1	0.582262	2.646145	-2.552150
1	1.619625	4.090817	-2.578229
1	1.384693	3.138689	-4.051602
6	4.589727	2.739774	-3.293627
1	4.402058	3.052744	-4.330893
1	4.923111	3.618993	-2.733955
1	5.416393	2.016976	-3.317977
6	2.713914	0.419642	-3.698024
1	3.554927	-0.280489	-3.690706
1	1.804563	-0.129311	-3.429230
1	2.593341	0.776879	-4.731790
14	2.915540	3.280678	0.305205
6	1.070753	3.695758	0.449435
1	0.513428	2.857738	0.884041
1	0.940671	4.560515	1.116014
1	0.608068	3.941688	-0.511166
6	3.577946	3.245960	2.090716
1	4.635938	2.963246	2.158923
1	3.489469	4.265125	2.494518
1	3.000226	2.584092	2.744129
6	3.818810	4.764130	-0.489621
1	3.459919	5.012102	-1.494591
1	3.657888	5.647466	0.145335
1	4.902469	4.595627	-0.547127
6	-3.835012	-0.455683	-1.008661
14	-3.686254	-2.132459	-2.005556
6	-3.290405	-3.611849	-0.873814
1	-3.147295	-4.497625	-1.509820
1	-2.365066	-3.465960	-0.303284
1	-4.103921	-3.841068	-0.174739

6	-5.358824	-2.558262	-2.824996
1	-5.604927	-1.893896	-3.662829
1	-5.310651	-3.582837	-3.221248
1	-6.188243	-2.521376	-2.106134
6	-2.365591	-2.170988	-3.375992
1	-2.556812	-1.465018	-4.188896
1	-1.357302	-1.977034	-2.988300
1	-2.357748	-3.182598	-3.808383
14	-4.518018	0.964051	-2.174320
6	-3.779730	0.919125	-3.929290
1	-4.135315	0.068674	-4.522596
1	-4.081194	1.836709	-4.454519
1	-2.682497	0.891617	-3.913841
6	-6.417174	0.838774	-2.325339
1	-6.759487	1.554071	-3.087417
1	-6.762465	-0.156494	-2.623442
1	-6.916947	1.103701	-1.383816
6	-4.196037	2.736265	-1.561051
1	-4.683801	2.943976	-0.601937
1	-3.128553	2.963004	-1.457687
1	-4.613747	3.435701	-2.300165
6	-4.812826	-0.666858	0.218042
1	-4.704906	-1.687017	0.602109
1	-5.862921	-0.562763	-0.089324
6	-4.530094	0.323418	1.386390
1	-5.166632	0.057091	2.244557
1	-4.850936	1.329115	1.073831
6	-3.005088	0.348445	1.807843
14	-2.616260	-1.099898	3.074731
6	-0.773392	-1.549964	3.190489
1	-0.653105	-2.355808	3.929619
1	-0.384816	-1.907983	2.228953
1	-0.150326	-0.706034	3.509489
6	-3.196290	-0.649453	4.842070
1	-3.073447	-1.542802	5.471422
1	-2.618198	0.158810	5.303584
1	-4.257831	-0.371443	4.872067
6	-3.557946	-2.715466	2.716549
1	-4.645474	-2.569021	2.679596
1	-3.241283	-3.203848	1.791767

1	-3.351185	-3.410060	3.544071
14	-2.576653	2.067859	2.630897
6	-3.948080	2.586613	3.852467
1	-3.986138	1.966031	4.752736
1	-3.770788	3.625194	4.167545
1	-4.937769	2.554432	3.377029
6	-0.905333	2.028536	3.544073
1	-0.094735	1.684750	2.888683
1	-0.653720	3.045101	3.877753
1	-0.917642	1.383723	4.430258
6	-2.481594	3.515465	1.398405
1	-3.468292	3.794214	1.013149
1	-2.078387	4.389618	1.930385
1	-1.824302	3.320416	0.544726

Sn=Sn=Sn-Rea (singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-2.373819	-0.005288	-0.146901
50	-0.026447	-1.551499	-0.218105
50	2.347499	-0.055053	-0.007451
6	4.225469	-1.034188	0.646780
14	4.336494	-2.961658	0.397290
6	4.374901	-3.483371	-1.433793
1	4.483677	-4.577386	-1.467285
1	3.450826	-3.229895	-1.964679
1	5.220656	-3.057468	-1.988067
6	5.975163	-3.633118	1.120818
1	6.039758	-3.545481	2.211692
1	6.066610	-4.699627	0.869457
1	6.843903	-3.118785	0.687827
6	2.894082	-3.942609	1.158114
1	2.721366	-3.729878	2.216638
1	1.955984	-3.756817	0.617450
1	3.110762	-5.016995	1.065177
14	4.587428	-0.581840	2.518399

6	3.800146	1.045916	3.127590
1	4.188656	1.929958	2.613664
1	2.704243	1.047827	3.039006
1	4.035183	1.159663	4.196308
6	3.942298	-1.874621	3.761801
1	4.390306	-2.867193	3.644605
1	4.184742	-1.519820	4.773963
1	2.851466	-1.982920	3.707649
6	6.466777	-0.388488	2.783547
1	6.667365	-0.235920	3.853627
1	7.027807	-1.273168	2.460959
1	6.867880	0.481987	2.247873
6	5.260441	-0.314268	-0.311140
1	5.284182	-0.825994	-1.283338
1	6.280550	-0.386937	0.094295
6	4.936741	1.187049	-0.566998
1	5.713900	1.605411	-1.223723
1	5.027336	1.724271	0.388176
6	3.501930	1.430722	-1.186090
14	3.493968	1.023920	-3.103951
6	2.058880	1.849588	-4.048419
1	1.081399	1.501546	-3.690134
1	2.070155	2.943929	-4.007888
1	2.140667	1.558019	-5.105335
6	5.137536	1.617540	-3.873664
1	5.085930	1.497906	-4.965327
1	5.349898	2.671558	-3.662074
1	5.989820	1.021780	-3.520710
6	3.343253	-0.814729	-3.572033
1	4.207783	-1.408068	-3.260884
1	2.439210	-1.285828	-3.165856
1	3.279201	-0.879406	-4.668473
14	2.926982	3.262628	-0.892934
6	1.055416	3.466834	-1.142914
1	0.499432	2.781757	-0.489693
1	0.753500	4.489712	-0.878615
1	0.735650	3.278599	-2.171590
6	3.280789	3.883278	0.873280
1	4.343886	3.839968	1.141944
1	2.977092	4.938910	0.925753

1	2.710839	3.342317	1.637085
6	3.853422	4.489192	-2.027176
1	3.646825	4.337904	-3.092874
1	3.546662	5.514082	-1.773228
1	4.940430	4.427086	-1.881337
6	-4.296894	-1.053448	-0.535794
14	-4.229382	-2.987227	-0.312462
6	-3.797886	-3.499569	1.471102
1	-3.758779	-4.597909	1.510237
1	-2.814735	-3.127514	1.784611
1	-4.543856	-3.173445	2.205645
6	-5.944072	-3.758220	-0.659073
1	-6.232389	-3.692508	-1.715386
1	-5.922139	-4.823505	-0.387861
1	-6.732578	-3.281737	-0.061408
6	-2.968367	-3.890279	-1.416981
1	-3.118848	-3.720112	-2.486573
1	-1.933407	-3.614846	-1.173855
1	-3.062695	-4.971053	-1.234926
14	-5.042854	-0.584522	-2.278088
6	-4.487265	-1.740919	-3.686876
1	-4.873624	-2.761775	-3.585027
1	-4.870897	-1.336789	-4.634615
1	-3.394352	-1.795483	-3.771631
6	-6.950592	-0.620714	-2.207984
1	-7.350820	-0.474397	-3.221645
1	-7.341805	-1.571022	-1.828222
1	-7.350920	0.186069	-1.579602
6	-4.595909	1.162957	-2.891457
1	-5.013774	1.948409	-2.251392
1	-3.513349	1.325034	-2.971429
1	-5.021176	1.299566	-3.896583
6	-5.175213	-0.429212	0.624380
1	-5.006953	-0.986946	1.551881
1	-6.246971	-0.534316	0.397837
6	-4.890449	1.076288	0.908204
1	-5.543360	1.400481	1.734842
1	-5.218691	1.654144	0.030365
6	-3.377411	1.411301	1.244963
14	-2.982030	1.059438	3.125322

6	-1.118825	1.015081	3.506767
1	-0.979480	0.758490	4.566942
1	-0.600721	0.252441	2.911515
1	-0.624477	1.975539	3.329039
6	-3.790141	2.384568	4.244273
1	-3.641505	2.092619	5.293871
1	-3.361116	3.384567	4.115946
1	-4.872908	2.455369	4.074396
6	-3.691304	-0.580973	3.781066
1	-4.785704	-0.625284	3.711883
1	-3.276164	-1.459578	3.278423
1	-3.428498	-0.657159	4.846511
14	-3.028627	3.285445	0.830807
6	-4.538567	4.348233	1.316247
1	-4.745518	4.320941	2.391663
1	-4.350490	5.394912	1.036591
1	-5.446596	4.026867	0.789595
6	-1.505598	4.002884	1.724122
1	-0.590937	3.440431	1.503916
1	-1.351200	5.031924	1.369461
1	-1.624799	4.044927	2.812350
6	-2.740896	3.634225	-1.021006
1	-3.643718	3.487533	-1.621700
1	-2.442875	4.687235	-1.129656
1	-1.939220	3.025126	-1.456478

Pb=Pb=Pb-Rea (singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-2.411545	0.080199	-0.147221
82	-0.023517	-1.601713	-0.162621
82	2.393586	0.019264	0.007563
6	4.376961	-0.923341	0.677928
14	4.479210	-2.847016	0.448503
6	4.544049	-3.392646	-1.375141
1	4.641254	-4.487992	-1.396239

1	3.633802	-3.133721	-1.927213
1	5.404566	-2.980648	-1.917603
6	6.090714	-3.538410	1.214132
1	6.137310	-3.429055	2.303980
1	6.169354	-4.610897	0.985046
1	6.974600	-3.044990	0.787017
6	3.004618	-3.797078	1.195060
1	2.771531	-3.516082	2.226339
1	2.097427	-3.656455	0.589225
1	3.228505	-4.873925	1.185308
14	4.715333	-0.433773	2.535097
6	3.923976	1.209060	3.098253
1	4.336030	2.082053	2.583186
1	2.831336	1.219712	2.973667
1	4.123371	1.337341	4.172427
6	4.044946	-1.699012	3.795497
1	4.467477	-2.703736	3.686781
1	4.299453	-1.340976	4.803524
1	2.950991	-1.781425	3.748016
6	6.591527	-0.241162	2.823499
1	6.780946	-0.057354	3.890635
1	7.151169	-1.138075	2.533355
1	7.003384	0.610381	2.265826
6	5.369939	-0.189833	-0.304843
1	5.390105	-0.711575	-1.271940
1	6.400363	-0.234797	0.082120
6	5.024173	1.307275	-0.576479
1	5.807822	1.723554	-1.228927
1	5.104595	1.853396	0.374480
6	3.602149	1.546355	-1.212885
14	3.580303	1.104505	-3.116349
6	2.125478	1.897478	-4.060417
1	1.155895	1.534885	-3.694207
1	2.116921	2.992240	-4.027894
1	2.205886	1.599831	-5.115760
6	5.208674	1.703711	-3.914228
1	5.158820	1.545083	-5.000982
1	5.397126	2.769262	-3.739290
1	6.074433	1.140228	-3.541248
6	3.443116	-0.744523	-3.551486

1	4.320233	-1.322113	-3.245191
1	2.551463	-1.219462	-3.121675
1	3.360178	-0.829337	-4.645314
14	2.987323	3.363126	-0.923925
6	1.107036	3.528242	-1.156588
1	0.567125	2.868909	-0.463531
1	0.794205	4.558703	-0.936934
1	0.776822	3.287386	-2.171269
6	3.343950	4.006498	0.833682
1	4.410685	3.988953	1.090843
1	3.016726	5.055338	0.881664
1	2.795548	3.458864	1.608691
6	3.871566	4.601713	-2.079818
1	3.656580	4.433878	-3.141457
1	3.546095	5.622676	-1.833489
1	4.961211	4.562935	-1.945721
6	-4.434008	-0.970971	-0.493710
14	-4.352306	-2.892956	-0.236919
6	-3.924497	-3.378382	1.555306
1	-3.874835	-4.475523	1.611664
1	-2.947077	-2.991022	1.868925
1	-4.676238	-3.047470	2.281853
6	-6.051355	-3.696213	-0.589258
1	-6.330991	-3.644810	-1.648749
1	-6.020346	-4.757877	-0.305246
1	-6.849691	-3.220008	-0.004428
6	-3.068887	-3.797012	-1.319704
1	-3.190831	-3.615364	-2.391157
1	-2.036866	-3.531374	-1.049751
1	-3.171142	-4.879124	-1.150996
14	-5.168008	-0.518358	-2.237309
6	-4.611585	-1.694861	-3.630353
1	-4.983164	-2.718858	-3.506944
1	-5.007903	-1.313679	-4.582346
1	-3.518539	-1.736444	-3.724482
6	-7.076318	-0.545159	-2.174273
1	-7.476599	-0.395514	-3.187301
1	-7.469282	-1.495606	-1.795786
1	-7.473701	0.260804	-1.542977
6	-4.706336	1.217239	-2.876688

1	-5.116476	2.015977	-2.248078
1	-3.622131	1.368395	-2.961193
1	-5.130391	1.343124	-3.883640
6	-5.271611	-0.305538	0.666600
1	-5.092101	-0.842314	1.604506
1	-6.351016	-0.401635	0.466772
6	-4.975487	1.207256	0.916247
1	-5.640923	1.549195	1.727054
1	-5.293741	1.765637	0.022008
6	-3.475253	1.555138	1.268098
14	-3.065085	1.214144	3.141807
6	-1.196931	1.137268	3.498312
1	-1.045936	0.933494	4.568523
1	-0.712676	0.327130	2.937184
1	-0.676035	2.070805	3.260964
6	-3.833709	2.570715	4.252067
1	-3.675637	2.296794	5.305123
1	-3.391038	3.561153	4.097651
1	-4.917343	2.655492	4.093949
6	-3.790898	-0.405403	3.831847
1	-4.886376	-0.435755	3.774549
1	-3.393425	-1.297554	3.338501
1	-3.517497	-0.469231	4.895442
14	-3.098676	3.409126	0.810393
6	-4.598583	4.500693	1.263070
1	-4.810787	4.492622	2.338248
1	-4.399169	5.540727	0.967296
1	-5.507178	4.177978	0.738044
6	-1.569803	4.134832	1.688279
1	-0.655412	3.573675	1.461618
1	-1.421016	5.161614	1.324409
1	-1.676951	4.184528	2.777432
6	-2.783137	3.703685	-1.046555
1	-3.656363	3.480472	-1.667461
1	-2.541257	4.767246	-1.190745
1	-1.932457	3.124938	-1.430711

C=C=C-Rea (triplet)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	-1.388487	-0.012982	0.027372
6	0	-0.063416	-0.189311	-0.162392
6	0	1.489277	-0.002799	-0.039256
6	0	2.430062	-0.967620	0.778084
14	0	2.302605	-2.951862	0.928779
6	0	2.677585	-3.938644	-0.665087
1	0	2.735691	-4.994946	-0.362252
1	0	1.926447	-3.866730	-1.451589
1	0	3.652487	-3.675695	-1.095140
6	0	3.745693	-3.554710	2.037390
1	0	3.677642	-3.248792	3.085352
1	0	3.723809	-4.654062	2.017453
1	0	4.724450	-3.243705	1.651594
6	0	0.743712	-3.716079	1.687891
1	0	-0.162263	-3.464378	1.137181
1	0	0.856160	-4.809663	1.653896
1	0	0.600422	-3.430500	2.733836
14	0	2.731917	-0.297652	2.658919
6	0	2.297905	1.532380	2.872395
1	0	3.112463	2.168719	2.514142
1	0	1.389630	1.815340	2.339386
1	0	2.154105	1.752945	3.939523
6	0	1.766448	-1.230912	4.011993
1	0	2.088263	-2.269743	4.137990
1	0	1.947167	-0.713587	4.965482
1	0	0.687646	-1.228486	3.837342
6	0	4.578689	-0.377850	3.148351
1	0	4.665591	0.000700	4.177804
1	0	5.006651	-1.384113	3.128141
1	0	5.195071	0.270960	2.512528
6	0	3.808940	-0.793083	0.029854
1	0	3.852844	-1.455581	-0.844466
1	0	4.673021	-1.031654	0.656396
6	0	3.808160	0.656198	-0.441988
1	0	4.587272	0.861244	-1.181680
1	0	3.998438	1.313240	0.416221

6	0	2.352786	0.893045	-1.000061
14	0	2.347748	0.198094	-2.898623
6	0	1.271351	1.173189	-4.134148
1	0	0.218626	1.198472	-3.842029
1	0	1.605098	2.202647	-4.297554
1	0	1.332480	0.652140	-5.100995
6	0	4.118913	0.172773	-3.620872
1	0	4.052651	-0.192282	-4.656895
1	0	4.609185	1.150514	-3.646886
1	0	4.769453	-0.522720	-3.074512
6	0	1.777645	-1.600463	-3.039211
1	0	2.586780	-2.286855	-2.775983
1	0	0.918875	-1.820981	-2.403674
1	0	1.497003	-1.810035	-4.080996
14	0	2.306382	2.874306	-1.162479
6	0	0.653144	3.636538	-1.679447
1	0	-0.184965	3.211521	-1.128582
1	0	0.668964	4.716423	-1.475876
1	0	0.459110	3.500077	-2.748172
6	0	2.966197	3.843834	0.348043
1	0	3.987772	3.540347	0.610663
1	0	3.015514	4.897486	0.034370
1	0	2.354076	3.799614	1.249283
6	0	3.584137	3.422173	-2.480506
1	0	3.365125	3.094901	-3.500507
1	0	3.586890	4.522163	-2.484631
1	0	4.601371	3.097796	-2.226868
6	0	-2.511114	-0.894034	-0.783492
14	0	-2.483897	-2.865341	-0.938724
6	0	-2.919209	-3.822912	0.656100
1	0	-3.028806	-4.877145	0.360858
1	0	-2.171231	-3.782375	1.448425
1	0	-3.882490	-3.507653	1.077536
6	0	-3.933235	-3.420224	-2.063158
1	0	-3.855532	-3.102765	-3.106984
1	0	-3.942009	-4.520170	-2.057555
1	0	-4.904399	-3.087901	-1.674710
6	0	-0.924427	-3.660799	-1.657400
1	0	-0.800342	-3.450300	-2.724194
1	0	-0.022613	-3.332699	-1.140576

1	0	-0.998643	-4.751091	-1.536493
14	0	-2.774911	-0.180337	-2.625111
6	0	-1.856730	-1.146861	-3.986903
1	0	-2.197006	-2.180746	-4.102191
1	0	-2.044860	-0.631516	-4.940138
1	0	-0.774830	-1.160595	-3.830460
6	0	-4.627121	-0.170097	-3.099344
1	0	-4.707501	0.202511	-4.131286
1	0	-5.107292	-1.152409	-3.064006
1	0	-5.202103	0.515648	-2.462985
6	0	-2.250195	1.625985	-2.854831
1	0	-3.038258	2.308086	-2.521869
1	0	-1.334455	1.870810	-2.315399
1	0	-2.081180	1.818391	-3.923575
6	0	-3.833468	-0.617068	0.010178
1	0	-3.897666	-1.251126	0.903959
1	0	-4.731077	-0.814710	-0.585113
6	0	-3.723527	0.841082	0.434111
1	0	-4.493149	1.126689	1.158269
1	0	-3.861261	1.481788	-0.446060
6	0	-2.268870	0.992919	1.015451
14	0	-2.333639	0.285465	2.879163
6	0	-1.870950	-1.542972	3.035794
1	0	-2.731761	-2.182376	2.821781
1	0	-1.058015	-1.830525	2.367793
1	0	-1.559389	-1.750055	4.068934
6	0	-1.214155	1.196189	4.124502
1	0	-1.311025	0.676329	5.088855
1	0	-0.158651	1.167446	3.843737
1	0	-1.494715	2.241239	4.288366
6	0	-4.107528	0.372780	3.588311
1	0	-4.515077	1.386391	3.648019
1	0	-4.809558	-0.244989	3.013443
1	0	-4.079252	-0.034325	4.609951
14	0	-2.114886	2.961916	1.169085
6	0	-3.373594	3.585861	2.474957
1	0	-3.161150	3.278934	3.502976
1	0	-3.339351	4.685074	2.449408
1	0	-4.401953	3.289099	2.233379
6	0	-0.441307	3.667238	1.701450

1	0	0.386509	3.265749	1.118473
1	0	-0.452812	4.755821	1.549077
1	0	-0.234921	3.481411	2.760235
6	0	-2.715864	3.960229	-0.346087
1	0	-3.767799	3.747679	-0.576520
1	0	-2.659740	5.019856	-0.054972
1	0	-2.134819	3.841551	-1.260039

Si=Si=Si-Rea (triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	2.079618	0.029135	0.026159
14	0.014552	-0.119854	-0.955281
14	-2.057993	-0.047843	0.123116
6	-3.410226	1.358928	-0.123684
14	-3.168502	2.636244	-1.579290
6	-3.194668	1.847775	-3.309480
1	-3.101141	2.663034	-4.042056
1	-2.360967	1.158110	-3.474214
1	-4.130469	1.320686	-3.530977
6	-4.629665	3.868961	-1.604347
1	-4.682184	4.509638	-0.716806
1	-4.523649	4.525848	-2.479648
1	-5.591348	3.347029	-1.702284
6	-1.536332	3.598395	-1.493407
1	-0.698204	2.914842	-1.315233
1	-1.356573	4.086475	-2.461606
1	-1.523111	4.373308	-0.721741
14	-3.710251	2.356213	1.554792
6	-3.161735	1.465696	3.143469
1	-3.763087	0.578641	3.360189
1	-2.106435	1.165740	3.111509
1	-3.283535	2.161539	3.986584
6	-2.798519	4.028888	1.647718
1	-3.106546	4.745848	0.879672
1	-3.027435	4.474472	2.626720

1	-1.709712	3.910266	1.589214
6	-5.573122	2.712645	1.763926
1	-5.715119	3.356276	2.643978
1	-6.005046	3.229807	0.899301
1	-6.150116	1.794278	1.934435
6	-4.686114	0.474382	-0.448933
1	-4.706755	0.236353	-1.521932
1	-5.615627	1.015572	-0.230739
6	-4.640333	-0.855045	0.342717
1	-5.494091	-1.489534	0.074126
1	-4.750109	-0.624738	1.412638
6	-3.262515	-1.594669	0.084103
14	-3.367774	-2.599189	-1.608813
6	-2.216454	-4.115626	-1.681681
1	-1.159774	-3.828623	-1.648676
1	-2.397851	-4.851114	-0.891807
1	-2.387480	-4.617141	-2.645439
6	-5.156234	-3.225541	-1.849267
1	-5.184248	-3.881759	-2.731091
1	-5.528879	-3.800503	-0.994098
1	-5.855405	-2.399589	-2.035760
6	-2.954125	-1.636021	-3.193084
1	-3.681416	-0.849657	-3.414303
1	-1.956685	-1.182435	-3.161355
1	-2.969996	-2.346429	-4.032966
14	-2.911262	-2.844646	1.542753
6	-1.112262	-3.451322	1.560047
1	-0.424493	-2.598751	1.635908
1	-0.949559	-4.091958	2.438676
1	-0.841109	-4.025981	0.669901
6	-3.203124	-2.100083	3.270112
1	-4.220577	-1.714120	3.410868
1	-3.056945	-2.903119	4.007494
1	-2.494193	-1.300432	3.507787
6	-4.104572	-4.336069	1.478805
1	-3.986186	-4.966829	0.591064
1	-3.927196	-4.969584	2.360034
1	-5.151395	-4.005326	1.520838
6	3.444019	-1.362963	-0.019449
14	3.347097	-2.564575	-1.556174

6	3.480719	-1.628984	-3.208898
1	3.280397	-2.342133	-4.021626
1	2.741897	-0.822487	-3.294094
1	4.480018	-1.212574	-3.381612
6	4.832146	-3.763518	-1.520724
1	4.794938	-4.470842	-0.683532
1	4.845915	-4.351517	-2.449574
1	5.784358	-3.219276	-1.462007
6	1.739167	-3.563863	-1.677528
1	1.560715	-4.222046	-0.823368
1	0.879879	-2.889624	-1.779090
1	1.778930	-4.188866	-2.581554
14	3.570841	-2.402864	1.650038
6	2.680963	-4.085396	1.618022
1	3.082757	-4.771071	0.863317
1	2.828507	-4.556807	2.600814
1	1.602173	-3.990498	1.459783
6	5.403366	-2.777605	2.033757
1	5.446027	-3.457463	2.897008
1	5.920746	-3.267396	1.200194
1	5.966396	-1.874168	2.301817
6	2.893599	-1.507213	3.185487
1	3.462661	-0.599144	3.417996
1	1.836823	-1.233089	3.081965
1	2.980587	-2.180011	4.051036
6	4.749499	-0.472727	-0.154244
1	4.935907	-0.253033	-1.209903
1	5.636457	-1.002163	0.213266
6	4.585424	0.870539	0.606765
1	5.456814	1.516392	0.423446
1	4.585653	0.664132	1.688112
6	3.236351	1.589632	0.177808
14	3.603837	2.655499	-1.430940
6	2.051586	3.157334	-2.397234
1	2.361133	3.657175	-3.326523
1	1.446294	2.284885	-2.674434
1	1.408907	3.850179	-1.846261
6	4.580290	4.234217	-0.967084
1	4.848108	4.755180	-1.897790
1	4.024263	4.941073	-0.343323

1	5.518069	3.989452	-0.450284
6	4.763183	1.819073	-2.690609
1	5.729351	1.533576	-2.255905
1	4.322353	0.942854	-3.172298
1	4.968882	2.558962	-3.478452
14	2.612170	2.778059	1.612259
6	4.104310	3.555611	2.509309
1	4.703340	4.197926	1.854978
1	3.740438	4.173364	3.342968
1	4.768264	2.792042	2.934916
6	1.480554	4.180221	0.998219
1	0.592815	3.790624	0.488153
1	1.134555	4.751614	1.871787
1	1.975806	4.883871	0.321080
6	1.590519	1.889979	2.951515
1	2.167988	1.143714	3.504991
1	1.245119	2.643139	3.675204
1	0.703558	1.393638	2.537154

Si=Ge=Si-Rea (triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	2.117912	0.052751	0.039503
32	0.013753	-0.328051	-1.074444
14	-2.097994	-0.042451	0.156343
6	-3.477257	1.339791	-0.097788
14	-3.236822	2.597767	-1.568505
6	-3.267173	1.789888	-3.290362
1	-3.173484	2.597051	-4.031897
1	-2.436033	1.096049	-3.451320
1	-4.204383	1.262208	-3.504162
6	-4.690505	3.838356	-1.614166
1	-4.747509	4.485966	-0.732120
1	-4.575581	4.487629	-2.493988
1	-5.653316	3.318786	-1.714979
6	-1.595962	3.547618	-1.494566

1	-0.760056	2.858389	-1.324897
1	-1.420419	4.038690	-2.462098
1	-1.570973	4.319297	-0.719754
14	-3.783302	2.355186	1.566724
6	-3.246451	1.482247	3.169030
1	-3.845469	0.594012	3.387751
1	-2.189356	1.187802	3.150577
1	-3.380619	2.185140	4.004417
6	-2.866898	4.026402	1.643993
1	-3.170325	4.736260	0.867425
1	-3.096409	4.483585	2.617451
1	-1.778329	3.903056	1.589463
6	-5.646758	2.716779	1.762233
1	-5.792448	3.377104	2.629261
1	-6.075648	3.216647	0.886089
1	-6.223756	1.801389	1.948266
6	-4.743444	0.436276	-0.408567
1	-4.765600	0.187075	-1.478851
1	-5.678966	0.968373	-0.192360
6	-4.678609	-0.884746	0.396933
1	-5.524772	-1.532840	0.135403
1	-4.791255	-0.645119	1.464470
6	-3.289710	-1.605232	0.145316
14	-3.387471	-2.645671	-1.525808
6	-2.165266	-4.106471	-1.596171
1	-1.122701	-3.770223	-1.555737
1	-2.317388	-4.849429	-0.806902
1	-2.306521	-4.615502	-2.560687
6	-5.151068	-3.354286	-1.719263
1	-5.164552	-4.035986	-2.581952
1	-5.488569	-3.918553	-0.843028
1	-5.885530	-2.562697	-1.919139
6	-3.060816	-1.702304	-3.143326
1	-3.809055	-0.931032	-3.347324
1	-2.069564	-1.235171	-3.166548
1	-3.102525	-2.429221	-3.968196
14	-2.899734	-2.828083	1.619593
6	-1.086926	-3.397623	1.639531
1	-0.412763	-2.533575	1.703143
1	-0.912113	-4.025096	2.525464

1	-0.806612	-3.978327	0.756093
6	-3.203633	-2.065558	3.336993
1	-4.230085	-1.703254	3.475502
1	-3.034423	-2.853131	4.085981
1	-2.514708	-1.244477	3.559350
6	-4.049279	-4.354752	1.586273
1	-3.907818	-5.001672	0.713541
1	-3.855153	-4.962406	2.482093
1	-5.105899	-4.055936	1.617770
6	3.532330	-1.291033	0.030395
14	3.520256	-2.522598	-1.487910
6	3.652489	-1.606323	-3.152246
1	3.516734	-2.341810	-3.958486
1	2.873231	-0.843379	-3.274210
1	4.631678	-1.136299	-3.302009
6	5.053957	-3.654988	-1.394169
1	5.021019	-4.347117	-0.544116
1	5.114215	-4.260076	-2.310152
1	5.982666	-3.073176	-1.321966
6	1.971425	-3.611479	-1.639404
1	1.812229	-4.277042	-0.787142
1	1.072975	-2.994554	-1.764974
1	2.072449	-4.236220	-2.539098
14	3.635333	-2.304531	1.719586
6	2.764300	-3.996877	1.695579
1	3.199605	-4.695133	0.971496
1	2.882021	-4.443980	2.693671
1	1.690156	-3.917159	1.497663
6	5.463615	-2.644249	2.153241
1	5.495201	-3.311063	3.027041
1	6.011057	-3.135989	1.340486
1	6.003702	-1.727260	2.422698
6	2.912331	-1.396491	3.227031
1	3.451221	-0.467540	3.448366
1	1.849107	-1.157009	3.105311
1	3.007963	-2.049456	4.106761
6	4.815644	-0.366848	-0.074894
1	5.023139	-0.144854	-1.126417
1	5.708224	-0.869557	0.316624
6	4.594156	0.971756	0.679873

1	5.446145	1.646495	0.507737
1	4.586334	0.768255	1.761444
6	3.227562	1.643861	0.231185
14	3.585340	2.718644	-1.374230
6	2.030151	3.184497	-2.354817
1	2.336189	3.704426	-3.274165
1	1.460930	2.294226	-2.652486
1	1.354796	3.847900	-1.807550
6	4.531402	4.311561	-0.897644
1	4.800746	4.840385	-1.823439
1	3.959520	5.007262	-0.275816
1	5.467481	4.077972	-0.372422
6	4.761668	1.902451	-2.630488
1	5.735143	1.641219	-2.197106
1	4.338379	1.013101	-3.104007
1	4.948009	2.640987	-3.424374
14	2.535500	2.817085	1.648471
6	3.987904	3.616315	2.590637
1	4.607303	4.251532	1.947527
1	3.589975	4.245675	3.399727
1	4.640688	2.864176	3.052899
6	1.401688	4.206325	1.007420
1	0.524665	3.804817	0.487855
1	1.037785	4.776843	1.874284
1	1.897976	4.913187	0.334617
6	1.473937	1.915405	2.947580
1	2.042490	1.197317	3.545509
1	1.066659	2.668959	3.638015
1	0.625695	1.385715	2.493855

Ge=Si=Ge-Rea (triplet)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
32	0	2.071908	0.023871	0.007097
14	0	0.011585	-0.111905	-1.143197
32	0	-2.044945	-0.041576	0.141945

6	0	-3.482501	1.393159	-0.131921
14	0	-3.214366	2.657191	-1.589353
6	0	-3.228149	1.860524	-3.316462
1	0	-3.126010	2.671136	-4.053044
1	0	-2.394851	1.167654	-3.471263
1	0	-4.163241	1.334086	-3.542842
6	0	-4.664142	3.902928	-1.632259
1	0	-4.721084	4.540451	-0.742493
1	0	-4.545317	4.561609	-2.504439
1	0	-5.627831	3.386336	-1.740180
6	0	-1.573227	3.607718	-1.491801
1	0	-0.737642	2.918327	-1.320477
1	0	-1.390281	4.104190	-2.455323
1	0	-1.555711	4.375413	-0.712774
14	0	-3.776210	2.374443	1.546274
6	0	-3.228725	1.469894	3.129933
1	0	-3.822217	0.574467	3.335041
1	0	-2.169886	1.180656	3.101378
1	0	-3.359915	2.155272	3.980201
6	0	-2.847564	4.037506	1.648192
1	0	-3.148953	4.761024	0.883469
1	0	-3.068160	4.481592	2.629622
1	0	-1.759980	3.907053	1.585556
6	0	-5.636493	2.737156	1.756811
1	0	-5.781044	3.376304	2.639448
1	0	-6.063027	3.258796	0.892007
1	0	-6.215343	1.818406	1.919253
6	0	-4.728641	0.474038	-0.460145
1	0	-4.738616	0.235459	-1.533198
1	0	-5.672233	0.995862	-0.249495
6	0	-4.683948	-0.861360	0.331032
1	0	-5.549216	-1.480898	0.060033
1	0	-4.794738	-0.630660	1.401045
6	0	-3.325781	-1.632443	0.079394
14	0	-3.409682	-2.620251	-1.615740
6	0	-2.231574	-4.116493	-1.690865
1	0	-1.179937	-3.810180	-1.648236
1	0	-2.405531	-4.859552	-0.906213
1	0	-2.385826	-4.615694	-2.658524
6	0	-5.190094	-3.266615	-1.860576

1	0	-5.213135	-3.921494	-2.743295
1	0	-5.556610	-3.844907	-1.004863
1	0	-5.895942	-2.445721	-2.044727
6	0	-3.005740	-1.648426	-3.198112
1	0	-3.730635	-0.857673	-3.411489
1	0	-2.005958	-1.199327	-3.170303
1	0	-3.028055	-2.354253	-4.041788
14	0	-2.960697	-2.869121	1.540151
6	0	-1.152009	-3.455993	1.556054
1	0	-0.470950	-2.597375	1.629739
1	0	-0.981120	-4.093612	2.435273
1	0	-0.875451	-4.029094	0.666416
6	0	-3.250672	-2.111766	3.263014
1	0	-4.269221	-1.728435	3.403160
1	0	-3.097785	-2.906158	4.008169
1	0	-2.544933	-1.306016	3.491370
6	0	-4.132657	-4.376722	1.486677
1	0	-4.003316	-5.008244	0.600690
1	0	-3.949566	-5.004876	2.370363
1	0	-5.183606	-4.058549	1.523442
6	0	3.519201	-1.392827	-0.015106
14	0	3.413397	-2.584850	-1.556202
6	0	3.546895	-1.640644	-3.204260
1	0	3.358397	-2.352149	-4.021232
1	0	2.797887	-0.843371	-3.290762
1	0	4.541261	-1.210066	-3.370553
6	0	4.889806	-3.793265	-1.523681
1	0	4.846253	-4.498517	-0.684982
1	0	4.900919	-4.382357	-2.451633
1	0	5.844759	-3.254100	-1.463394
6	0	1.796761	-3.572914	-1.679787
1	0	1.604854	-4.220789	-0.820672
1	0	0.941451	-2.895461	-1.797878
1	0	1.839881	-4.208120	-2.576559
14	0	3.616924	-2.417893	1.657022
6	0	2.701446	-4.086750	1.624157
1	0	3.092524	-4.779402	0.870184
1	0	2.837750	-4.560712	2.607203
1	0	1.624020	-3.973636	1.463018
6	0	5.442588	-2.801761	2.056801

1	0	5.479358	-3.476827	2.923755
1	0	5.961080	-3.297048	1.227089
1	0	6.007500	-1.898475	2.321287
6	0	2.928699	-1.509434	3.181945
1	0	3.497153	-0.601532	3.416102
1	0	1.872228	-1.235263	3.071053
1	0	3.006014	-2.178049	4.051600
6	0	4.798931	-0.469279	-0.139504
1	0	4.987859	-0.245907	-1.194336
1	0	5.695493	-0.980763	0.232692
6	0	4.625391	0.878421	0.621456
1	0	5.509006	1.511056	0.448296
1	0	4.614087	0.669643	1.702540
6	0	3.297703	1.626377	0.187203
14	0	3.651108	2.685327	-1.423302
6	0	2.090150	3.179459	-2.381578
1	0	2.391230	3.691189	-3.307179
1	0	1.494941	2.302307	-2.666073
1	0	1.438234	3.858598	-1.824175
6	0	4.621589	4.267326	-0.961437
1	0	4.890738	4.790919	-1.890063
1	0	4.058305	4.970032	-0.339015
1	0	5.557434	4.025887	-0.439659
6	0	4.797689	1.837260	-2.685332
1	0	5.764419	1.547041	-2.255200
1	0	4.345741	0.959996	-3.155511
1	0	5.002761	2.568214	-3.481417
14	0	2.646378	2.795112	1.620174
6	0	4.121776	3.582116	2.534203
1	0	4.719538	4.230726	1.884655
1	0	3.748493	4.194133	3.367690
1	0	4.789241	2.821715	2.960030
6	0	1.500173	4.185853	1.005872
1	0	0.617268	3.789757	0.491328
1	0	1.145068	4.750261	1.880311
1	0	1.989996	4.897485	0.333113
6	0	1.619035	1.888218	2.945246
1	0	2.193404	1.137496	3.495858
1	0	1.268922	2.633877	3.674443
1	0	0.730983	1.397061	2.525426

Ge=Ge=Ge-Rea (triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	2.112175	0.035796	0.034495
32	0.005886	-0.220008	-1.241845
32	-2.083690	-0.030634	0.186736
6	-3.537721	1.396194	-0.087414
14	-3.259958	2.650103	-1.551043
6	-3.270432	1.841429	-3.273239
1	-3.160761	2.645809	-4.015558
1	-2.440239	1.142792	-3.420177
1	-4.206995	1.317714	-3.499741
6	-4.701113	3.905164	-1.612656
1	-4.763229	4.546314	-0.725860
1	-4.570886	4.559856	-2.486286
1	-5.666497	3.393098	-1.727455
6	-1.611235	3.590431	-1.455255
1	-0.777790	2.896877	-1.286737
1	-1.428147	4.088555	-2.418049
1	-1.587704	4.356367	-0.674525
14	-3.831107	2.387365	1.583442
6	-3.285875	1.490804	3.172398
1	-3.876772	0.594058	3.379028
1	-2.225829	1.205324	3.147451
1	-3.421479	2.178611	4.020012
6	-2.898697	4.049222	1.677116
1	-3.197397	4.769388	0.908100
1	-3.119066	4.499392	2.655827
1	-1.811321	3.915519	1.616286
6	-5.690869	2.756283	1.789854
1	-5.835511	3.400501	2.668823
1	-6.114339	3.274435	0.921342
1	-6.272487	1.839950	1.955919
6	-4.780461	0.470923	-0.409989
1	-4.790195	0.227084	-1.481924

1	-5.726699	0.989441	-0.201666
6	-4.730781	-0.861199	0.387439
1	-5.595032	-1.483995	0.119149
1	-4.842757	-0.626101	1.456415
6	-3.369484	-1.627622	0.140318
14	-3.452203	-2.633564	-1.544041
6	-2.239484	-4.102829	-1.618405
1	-1.194899	-3.772052	-1.570207
1	-2.399967	-4.850410	-0.834929
1	-2.377824	-4.604837	-2.587067
6	-5.221125	-3.318846	-1.767342
1	-5.236856	-3.987303	-2.640110
1	-5.572496	-3.890332	-0.901012
1	-5.942760	-2.513683	-1.960256
6	-3.093765	-1.675375	-3.147487
1	-3.822376	-0.884594	-3.348191
1	-2.092049	-1.229698	-3.158065
1	-3.143168	-2.390774	-3.982048
14	-2.987004	-2.853661	1.607679
6	-1.171912	-3.424357	1.625284
1	-0.496115	-2.560568	1.683595
1	-0.994077	-4.048268	2.513059
1	-0.893632	-4.008469	0.743260
6	-3.281989	-2.088617	3.326520
1	-4.303708	-1.713146	3.465246
1	-3.121388	-2.876985	4.076428
1	-2.583048	-1.275314	3.549065
6	-4.137124	-4.379180	1.569947
1	-3.997091	-5.018434	0.690997
1	-3.944076	-4.994902	2.460372
1	-5.193102	-4.077796	1.603130
6	3.582712	-1.364979	0.043793
14	3.503863	-2.580190	-1.482917
6	3.636798	-1.652489	-3.141241
1	3.471866	-2.376701	-3.952232
1	2.872752	-0.871469	-3.246328
1	4.623629	-1.202476	-3.301372
6	4.992079	-3.772906	-1.425700
1	4.945317	-4.469119	-0.579496
1	5.014368	-4.372693	-2.346703

1	5.942847	-3.226962	-1.363341
6	1.907038	-3.601930	-1.613528
1	1.715800	-4.241139	-0.747973
1	1.036729	-2.948254	-1.754594
1	1.978611	-4.249502	-2.499824
14	3.663051	-2.373721	1.727907
6	2.739432	-4.038568	1.708256
1	3.135733	-4.744764	0.969759
1	2.861705	-4.498214	2.700004
1	1.664145	-3.922535	1.532801
6	5.484154	-2.759306	2.147403
1	5.511303	-3.425508	3.021605
1	6.008621	-3.264327	1.327489
1	6.049304	-1.854957	2.407669
6	2.966285	-1.449454	3.239565
1	3.530626	-0.537271	3.466371
1	1.909070	-1.181140	3.122206
1	3.042515	-2.108745	4.116451
6	4.856828	-0.433318	-0.070937
1	5.057360	-0.215047	-1.124996
1	5.753910	-0.934102	0.315300
6	4.663159	0.917337	0.680812
1	5.541549	1.558094	0.509046
1	4.648311	0.714807	1.762926
6	3.329629	1.648862	0.237510
14	3.675237	2.707343	-1.375657
6	2.108902	3.187999	-2.333828
1	2.405176	3.709348	-3.255641
1	1.526446	2.304652	-2.626141
1	1.445531	3.854215	-1.774444
6	4.636175	4.297013	-0.920820
1	4.904457	4.817422	-1.851536
1	4.067229	4.999628	-0.303349
1	5.572094	4.063909	-0.395448
6	4.820316	1.857957	-2.637850
1	5.790946	1.576421	-2.210866
1	4.370368	0.973817	-3.097255
1	5.016611	2.582719	-3.441744
14	2.652967	2.818174	1.659112
6	4.112525	3.623079	2.583319

1	4.708282	4.275478	1.935468
1	3.726489	4.234765	3.411263
1	4.785107	2.871806	3.017105
6	1.500922	4.198528	1.030623
1	0.621087	3.794388	0.516632
1	1.140308	4.765589	1.901153
1	1.988226	4.909704	0.355605
6	1.614760	1.909751	2.974390
1	2.188574	1.174068	3.545104
1	1.238971	2.658025	3.687892
1	0.742183	1.401818	2.541559

Sn=Sn=Sn-Rea (triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	2.363934	0.003973	-0.092944
50	0.025032	-0.719747	-1.600230
50	-2.246063	-0.042629	0.226828
6	-3.885446	1.437230	-0.178343
14	-3.598122	2.547324	-1.744212
6	-3.724194	1.589040	-3.384882
1	-3.544177	2.299302	-4.205231
1	-2.978441	0.791589	-3.471967
1	-4.716005	1.149051	-3.547800
6	-4.933312	3.909638	-1.889513
1	-4.912505	4.630613	-1.064074
1	-4.778048	4.469759	-2.823043
1	-5.941117	3.474184	-1.931383
6	-1.884151	3.375807	-1.776367
1	-1.086435	2.624152	-1.851509
1	-1.810576	4.019361	-2.664953
1	-1.685922	3.997354	-0.898033
14	-4.207598	2.553649	1.391456
6	-3.830633	1.747448	3.077752
1	-4.445543	0.864299	3.277295
1	-2.775790	1.459322	3.179960

1	-4.046472	2.483991	3.866077
6	-3.161246	4.148616	1.413036
1	-3.367566	4.824864	0.575989
1	-3.387052	4.693502	2.341162
1	-2.085807	3.929351	1.415935
6	-6.049657	3.051912	1.473117
1	-6.190604	3.785417	2.280089
1	-6.407631	3.505484	0.541988
1	-6.691990	2.190192	1.699065
6	-5.094050	0.440573	-0.406309
1	-5.104037	0.101713	-1.451037
1	-6.054135	0.955447	-0.246151
6	-5.054769	-0.823768	0.507020
1	-5.960250	-1.419490	0.314635
1	-5.131531	-0.492447	1.552667
6	-3.751276	-1.699951	0.311121
14	-3.924132	-2.817360	-1.277012
6	-2.686787	-4.268631	-1.322792
1	-1.644806	-3.922732	-1.321709
1	-2.814008	-4.975823	-0.495870
1	-2.844204	-4.824082	-2.258602
6	-5.687652	-3.553208	-1.352752
1	-5.742317	-4.271256	-2.183749
1	-5.968295	-4.080980	-0.434749
1	-6.441731	-2.777628	-1.542560
6	-3.696368	-1.963916	-2.965788
1	-4.433686	-1.176734	-3.152016
1	-2.696469	-1.532192	-3.097585
1	-3.825647	-2.727660	-3.747140
14	-3.393616	-2.806683	1.869524
6	-1.596538	-3.442411	1.921541
1	-0.879068	-2.610996	1.956135
1	-1.449783	-4.043388	2.830855
1	-1.339339	-4.069868	1.062336
6	-3.654415	-1.871004	3.509788
1	-4.688573	-1.528212	3.643405
1	-3.431348	-2.560988	4.336739
1	-2.991770	-1.004745	3.616656
6	-4.563775	-4.313037	1.991219
1	-4.428294	-5.032065	1.175332

1	-4.372316	-4.842436	2.935836
1	-5.616893	-4.000984	1.996056
6	4.188272	-1.210817	0.144828
14	4.583377	-2.284157	-1.431724
6	4.918531	-1.189357	-2.956633
1	5.041680	-1.844497	-3.831011
1	4.086261	-0.508221	-3.180425
1	5.835662	-0.595458	-2.863148
6	6.167325	-3.318214	-1.173865
1	6.036212	-4.111357	-0.427250
1	6.445712	-3.799788	-2.122113
1	7.013709	-2.693004	-0.859317
6	3.185720	-3.462145	-1.960208
1	2.922023	-4.202551	-1.199500
1	2.270365	-2.917622	-2.228067
1	3.512791	-4.008773	-2.856934
14	4.120988	-2.318865	1.750741
6	3.288056	-4.008858	1.476706
1	3.855035	-4.664259	0.805542
1	3.214872	-4.517069	2.448784
1	2.268854	-3.910826	1.080531
6	5.887910	-2.625500	2.404253
1	5.846615	-3.363407	3.218404
1	6.564380	-3.013697	1.635001
1	6.333501	-1.710615	2.817004
6	3.175320	-1.544357	3.212614
1	3.635758	-0.613684	3.564448
1	2.120091	-1.343526	2.987247
1	3.196384	-2.255083	4.051804
6	5.265682	-0.061880	0.312900
1	5.604151	0.268747	-0.674984
1	6.160117	-0.442001	0.828501
6	4.756972	1.195576	1.087683
1	5.573071	1.935860	1.113666
1	4.586398	0.908867	2.137203
6	3.445952	1.841149	0.478734
14	3.858578	3.027383	-1.016441
6	2.390808	3.230081	-2.209519
1	2.664427	3.938443	-3.004641
1	2.126761	2.280040	-2.693941

1	1.489419	3.613755	-1.719258
6	4.396437	4.761365	-0.415946
1	4.674172	5.360238	-1.295345
1	3.614272	5.307888	0.121064
1	5.280015	4.706194	0.233983
6	5.342589	2.454264	-2.064675
1	6.247524	2.303773	-1.462025
1	5.146570	1.538627	-2.629997
1	5.564851	3.247986	-2.792954
14	2.447836	2.807731	1.844328
6	3.626222	3.839409	2.931709
1	4.133766	4.633278	2.373799
1	3.053757	4.311992	3.742725
1	4.395021	3.209817	3.398959
6	1.107864	3.939611	1.105244
1	0.389400	3.369606	0.502161
1	0.548891	4.405787	1.929026
1	1.505051	4.746441	0.480406
6	1.498952	1.675312	3.051052
1	2.152105	1.028331	3.645124
1	0.949275	2.316968	3.755770
1	0.753670	1.042536	2.548387

Pb=Pb=Pb-Rea (triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	2.403662	0.041423	-0.073449
82	0.022549	-0.856122	-1.644724
82	-2.264120	0.029485	0.332995
6	-3.994619	1.512708	-0.173361
14	-3.663882	2.555294	-1.770576
6	-3.772946	1.536988	-3.376900
1	-3.572101	2.212268	-4.221509
1	-3.034493	0.728865	-3.420115
1	-4.766487	1.100071	-3.538306
6	-4.973620	3.932657	-1.997390

1	-4.958530	4.682047	-1.197539
1	-4.792056	4.456559	-2.947072
1	-5.986502	3.509451	-2.042701
6	-1.935560	3.357678	-1.802306
1	-1.150391	2.591168	-1.865383
1	-1.844809	3.992870	-2.695348
1	-1.732195	3.982808	-0.927379
14	-4.318599	2.669262	1.355516
6	-3.955202	1.906114	3.066582
1	-4.582654	1.037384	3.289462
1	-2.904043	1.606487	3.181232
1	-4.160791	2.666944	3.834170
6	-3.254450	4.253479	1.340751
1	-3.437302	4.901342	0.476279
1	-3.488257	4.834831	2.244405
1	-2.181582	4.021797	1.369781
6	-6.156266	3.187246	1.411972
1	-6.305763	3.921742	2.216438
1	-6.491299	3.644046	0.473478
1	-6.810649	2.330886	1.623778
6	-5.173109	0.485701	-0.380958
1	-5.155134	0.103619	-1.410683
1	-6.147380	0.988990	-0.264536
6	-5.152214	-0.743436	0.583299
1	-6.068249	-1.329496	0.402312
1	-5.240357	-0.368475	1.613374
6	-3.869914	-1.653023	0.447135
14	-4.004588	-2.815413	-1.101672
6	-2.758677	-4.261262	-1.073250
1	-1.717926	-3.910357	-1.058161
1	-2.900203	-4.939868	-0.224756
1	-2.890899	-4.850174	-1.992339
6	-5.761933	-3.564362	-1.197868
1	-5.800861	-4.299716	-2.014415
1	-6.052866	-4.073722	-0.272391
1	-6.516588	-2.796024	-1.413491
6	-3.740915	-2.020541	-2.816390
1	-4.478045	-1.245067	-3.047492
1	-2.741976	-1.581912	-2.940501
1	-3.843867	-2.811094	-3.574587

14	-3.538878	-2.691883	2.050643
6	-1.740231	-3.318030	2.170187
1	-1.035223	-2.480600	2.270522
1	-1.632353	-3.946547	3.066550
1	-1.431802	-3.914822	1.305479
6	-3.826457	-1.692137	3.648781
1	-4.862177	-1.343884	3.752571
1	-3.615515	-2.347963	4.506105
1	-3.165389	-0.821570	3.731921
6	-4.701335	-4.201624	2.213539
1	-4.543108	-4.951347	1.429598
1	-4.526240	-4.691585	3.182288
1	-5.756301	-3.897346	2.182351
6	4.303550	-1.151015	0.344183
14	4.752753	-2.261358	-1.186195
6	5.119354	-1.204712	-2.731485
1	5.277105	-1.880352	-3.584400
1	4.284939	-0.541368	-2.998757
1	6.023931	-0.593683	-2.627487
6	6.330085	-3.285668	-0.858447
1	6.179040	-4.049836	-0.085780
1	6.630755	-3.802654	-1.780857
1	7.168924	-2.649613	-0.545828
6	3.376325	-3.462870	-1.725837
1	3.095678	-4.186259	-0.954681
1	2.463692	-2.934026	-2.033950
1	3.731905	-4.029666	-2.598899
14	4.167048	-2.198477	1.978334
6	3.362274	-3.904769	1.719888
1	3.969687	-4.577547	1.103132
1	3.238274	-4.380626	2.703128
1	2.366288	-3.828023	1.264254
6	5.905209	-2.467727	2.720415
1	5.836640	-3.176991	3.557730
1	6.614915	-2.876965	1.992451
1	6.327669	-1.535094	3.117376
6	3.143211	-1.389455	3.367821
1	3.576315	-0.442931	3.711251
1	2.097333	-1.208681	3.086548
1	3.129978	-2.072988	4.229339

6	5.334107	0.033767	0.511302
1	5.702381	0.343352	-0.473094
1	6.220148	-0.302149	1.072190
6	4.775331	1.305971	1.230861
1	5.590610	2.047245	1.279296
1	4.559822	1.039398	2.277334
6	3.498255	1.942685	0.558018
14	3.941814	3.083007	-0.958891
6	2.500036	3.233474	-2.193688
1	2.782218	3.925257	-3.000282
1	2.258400	2.268973	-2.661809
1	1.582273	3.616990	-1.734496
6	4.442690	4.841953	-0.400781
1	4.740015	5.417783	-1.289116
1	3.636703	5.393319	0.095000
1	5.305632	4.817644	0.278127
6	5.454028	2.487258	-1.952886
1	6.345006	2.362418	-1.324225
1	5.276775	1.551116	-2.490577
1	5.689193	3.256359	-2.703072
14	2.426947	2.916169	1.856154
6	3.543497	3.995428	2.963417
1	4.063382	4.778994	2.401892
1	2.933606	4.484799	3.736360
1	4.301013	3.390205	3.478997
6	1.099630	4.010539	1.040156
1	0.418539	3.421562	0.411909
1	0.495388	4.477959	1.830807
1	1.511475	4.816854	0.423632
6	1.452152	1.794930	3.053498
1	2.094536	1.182124	3.693577
1	0.858003	2.442867	3.715135
1	0.742458	1.129136	2.541085

C=C=C (TS)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

6	0.858584	0.266600	-1.735170
6	-0.237746	-0.573017	-2.185387
6	-1.399655	0.193836	0.089164
6	-0.117840	-0.158475	0.433984
6	1.265503	-0.128945	-0.186473
6	2.511015	0.850589	0.466205
14	2.422979	1.844743	2.198039
6	1.824084	0.852761	3.708239
1	1.772468	1.557519	4.551366
1	0.841139	0.393374	3.591903
1	2.535925	0.068544	3.987559
6	4.217562	2.294914	2.712324
1	4.717105	2.980014	2.018707
1	4.149769	2.812110	3.681414
1	4.862971	1.420557	2.856547
6	1.546676	3.530656	2.285916
1	0.666671	3.616065	1.654987
1	1.223991	3.690521	3.323159
1	2.232968	4.342311	2.025348
14	3.449751	2.106700	-0.837877
6	3.236463	1.938100	-2.734839
1	3.479619	0.940651	-3.117368
1	2.247767	2.219264	-3.105690
1	3.965378	2.635053	-3.173458
6	3.154822	3.969911	-0.524036
1	3.754447	4.339486	0.316050
1	3.482526	4.507712	-1.424832
1	2.114090	4.245680	-0.337476
6	5.352000	1.910294	-0.691025
1	5.802467	2.670105	-1.346579
1	5.750187	2.068726	0.316108
1	5.698189	0.930500	-1.044758
6	3.637627	-0.194531	0.796995
1	3.433642	-0.704181	1.748148
1	4.625662	0.255593	0.895261
6	3.563933	-1.198121	-0.339101
1	4.259797	-2.029386	-0.210290
1	3.837320	-0.702676	-1.282801
6	2.070654	-1.662465	-0.339238

14	1.997683	-2.971766	1.193256
6	1.143368	-4.632529	0.770370
1	1.024933	-5.189911	1.710714
1	0.156905	-4.554403	0.310199
1	1.770562	-5.241367	0.108648
6	3.759524	-3.572390	1.672266
1	3.630777	-4.289865	2.497091
1	4.289614	-4.095029	0.867980
1	4.408547	-2.769330	2.042165
6	1.316275	-2.371744	2.862050
1	2.113293	-1.903763	3.448210
1	0.498396	-1.658734	2.760111
1	0.959574	-3.239514	3.432124
14	1.984523	-2.770125	-2.008634
6	0.440248	-3.863989	-2.312292
1	-0.425322	-3.605819	-1.698294
1	0.137700	-3.773437	-3.364905
1	0.670494	-4.917983	-2.121275
6	2.287729	-1.855221	-3.663511
1	3.135566	-1.159752	-3.636530
1	2.526253	-2.625775	-4.410374
1	1.404935	-1.311179	-4.015244
6	3.465313	-3.973295	-1.980034
1	3.526828	-4.601719	-1.087761
1	3.354211	-4.639800	-2.847419
1	4.418689	-3.442761	-2.093913
6	-2.661072	-0.779991	0.425511
14	-2.699678	-1.751165	2.150757
6	-2.218841	-0.687841	3.648684
1	-2.225451	-1.342094	4.532251
1	-1.224876	-0.243984	3.565866
1	-2.941723	0.114480	3.832039
6	-4.520433	-2.225154	2.496654
1	-4.915472	-2.954393	1.780038
1	-4.558356	-2.694602	3.490372
1	-5.195026	-1.361005	2.514757
6	-1.782357	-3.405017	2.344581
1	-2.418097	-4.246454	2.051561
1	-0.853636	-3.470948	1.784923
1	-1.534953	-3.530618	3.407201

14	-3.335876	-2.090888	-0.987568
6	-2.992886	-3.937077	-0.618209
1	-3.214807	-4.497633	-1.537909
1	-1.965404	-4.171325	-0.330300
1	-3.655050	-4.322400	0.166078
6	-5.252302	-1.999865	-1.037375
1	-5.594780	-2.812527	-1.694841
1	-5.738345	-2.136739	-0.066492
1	-5.612135	-1.058414	-1.472514
6	-2.959566	-1.949564	-2.860723
1	-3.161868	-0.960812	-3.283981
1	-1.951778	-2.251735	-3.149984
1	-3.657828	-2.653365	-3.338348
6	-3.829829	0.254392	0.541246
1	-3.764221	0.803679	1.489890
1	-4.819168	-0.199690	0.505908
6	-3.570715	1.205981	-0.618737
1	-4.252062	2.057744	-0.628387
1	-3.714333	0.670811	-1.568836
6	-2.068884	1.639267	-0.438499
14	-2.159773	3.059398	0.989158
6	-1.290860	4.707356	0.550462
1	-0.271119	4.621974	0.171964
1	-1.870137	5.275867	-0.185763
1	-1.250014	5.307698	1.470485
6	-3.962604	3.632872	1.284765
1	-3.931992	4.379953	2.091421
1	-4.415850	4.114437	0.410828
1	-4.627192	2.825738	1.612304
6	-1.568613	2.512964	2.705287
1	-2.389276	2.036225	3.249181
1	-0.734531	1.810120	2.679162
1	-1.259445	3.395209	3.279613
14	-1.730359	2.631375	-2.159318
6	-3.204872	3.835208	-2.371886
1	-3.404425	4.486236	-1.516350
1	-2.974589	4.483313	-3.230372
1	-4.129499	3.295443	-2.612299
6	-0.164319	3.717623	-2.339572
1	0.644631	3.489768	-1.643765

1	0.231826	3.594161	-3.357096
1	-0.417676	4.776738	-2.213290
6	-1.820732	1.696846	-3.828075
1	-2.633943	0.966536	-3.901867
1	-2.018244	2.472665	-4.583069
1	-0.884773	1.203289	-4.107287
1	-0.146477	-1.643376	-2.225669
1	-1.136724	-0.172215	-2.627335
1	1.761806	0.117610	-2.323318
1	0.597942	1.325783	-1.784094

1

A

Frequencies -- -194.0258

Red. masses -- 3.3374

Frc consts -- 0.0740

IR Inten -- 39.3136

Atom	AN	X	Y	Z
1	6	0.00	0.01	0.15
2	6	-0.12	-0.02	0.33
3	6	0.03	-0.02	-0.11
4	6	0.01	-0.06	0.12
5	6	0.02	0.04	-0.05
6	6	0.01	0.01	-0.02
7	14	0.00	0.00	-0.01
8	6	0.00	0.00	-0.01
9	1	-0.01	0.00	-0.01
10	1	0.01	-0.01	-0.02
11	1	0.00	0.00	0.00
12	6	0.00	0.00	0.00
13	1	0.00	0.00	0.00
14	1	0.00	0.00	0.00
15	1	0.00	0.00	0.00
16	6	0.00	0.00	0.00
17	1	0.00	0.00	0.00
18	1	0.01	0.00	0.00
19	1	0.00	0.00	0.00
20	14	0.01	0.01	0.00
21	6	-0.01	-0.01	0.00
22	1	-0.03	-0.01	0.01

23	1	-0.01	0.00	0.01
24	1	-0.01	-0.02	-0.01
25	6	0.01	0.01	-0.01
26	1	0.00	0.01	0.00
27	1	0.01	0.01	0.00
28	1	0.01	0.00	0.00
29	6	0.01	0.01	-0.01
30	1	0.01	0.00	-0.01
31	1	0.01	0.01	-0.01
32	1	0.00	0.00	0.00
33	6	0.00	0.00	-0.01
34	1	-0.01	0.01	-0.01
35	1	0.00	0.00	0.00
36	6	0.01	0.00	0.00
37	1	0.01	0.00	0.00
38	1	0.01	-0.01	-0.01
39	6	0.00	0.00	0.00
40	14	0.00	0.01	0.00
41	6	0.01	0.00	0.00
42	1	0.02	0.00	0.00
43	1	0.00	-0.01	0.01
44	1	0.00	0.01	-0.01
45	6	0.00	0.00	-0.01
46	1	0.00	0.00	-0.01
47	1	0.00	0.00	-0.01
48	1	0.00	0.00	-0.01
49	6	0.01	-0.01	0.01
50	1	0.01	-0.01	0.01
51	1	0.02	0.00	0.00
52	1	0.01	-0.01	0.01
53	14	-0.01	0.01	0.00
54	6	0.00	-0.01	0.00
55	1	0.01	-0.07	0.04
56	1	-0.04	0.04	0.02
57	1	0.03	-0.01	-0.06
58	6	-0.08	0.03	0.00
59	1	-0.11	0.07	-0.02
60	1	-0.08	0.04	-0.02
61	1	-0.12	-0.01	0.04
62	6	0.00	0.01	-0.02

63	1	0.00	0.01	-0.02
64	1	0.00	0.01	-0.02
65	1	0.00	0.02	-0.02
66	6	0.01	-0.01	-0.06
67	14	0.02	0.01	-0.03
68	6	0.00	0.00	-0.02
69	1	-0.01	0.00	-0.03
70	1	0.00	0.00	-0.01
71	1	0.00	0.00	-0.02
72	6	0.02	0.01	-0.02
73	1	0.01	0.01	-0.02
74	1	0.02	0.02	-0.02
75	1	0.01	0.01	-0.02
76	6	0.00	0.00	-0.01
77	1	0.00	0.00	-0.01
78	1	0.01	0.00	0.01
79	1	-0.01	0.01	0.00
80	14	-0.02	-0.01	-0.01
81	6	-0.01	-0.01	-0.01
82	1	0.00	-0.01	0.00
83	1	-0.01	0.00	0.00
84	1	-0.01	0.00	-0.01
85	6	-0.01	0.00	-0.02
86	1	-0.02	0.00	-0.01
87	1	-0.01	0.00	-0.01
88	1	-0.01	0.00	-0.01
89	6	0.00	-0.01	-0.01
90	1	-0.01	-0.01	-0.01
91	1	0.01	0.01	-0.01
92	1	0.02	-0.01	-0.02
93	6	0.01	0.00	-0.03
94	1	0.03	-0.01	-0.02
95	1	0.01	0.01	-0.02
96	6	0.01	0.01	-0.02
97	1	0.01	0.01	-0.01
98	1	0.00	0.02	-0.02
99	6	0.01	0.00	-0.02
100	14	0.01	-0.01	0.00
101	6	0.00	0.00	0.00
102	1	0.00	0.00	0.00

103	1	0.00	0.00	0.00
104	1	0.00	-0.01	0.00
105	6	0.01	-0.01	0.00
106	1	0.01	-0.01	0.00
107	1	0.01	0.00	0.00
108	1	0.00	-0.01	-0.01
109	6	0.01	-0.01	-0.01
110	1	0.00	0.00	0.00
111	1	0.00	-0.02	0.00
112	1	0.02	-0.01	-0.01
113	14	0.01	0.01	0.00
114	6	0.00	0.00	-0.01
115	1	0.00	0.00	-0.01
116	1	0.00	0.00	-0.01
117	1	0.00	0.00	-0.01
118	6	0.00	0.01	-0.01
119	1	0.00	0.02	-0.01
120	1	0.00	0.01	-0.01
121	1	0.00	0.01	-0.01
122	6	0.02	-0.01	0.01
123	1	0.04	-0.03	0.02
124	1	0.00	-0.03	0.00
125	1	0.04	0.02	0.00
126	1	-0.21	-0.05	0.75
127	1	0.12	-0.07	-0.21
128	1	-0.14	0.03	-0.07
129	1	-0.04	0.01	0.07

Si=Si=Si (TS)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	1.276190	-1.045307	1.932152
6	0	0.093316	-0.572800	2.552121
14	0	-1.994989	-0.069636	0.004484
14	0	-0.023477	0.205120	-1.153887
14	0	1.947725	-0.037833	0.151375

6	0	3.513425	-0.986934	-0.621796
14	0	3.268221	-1.696182	-2.442065
6	0	3.101701	-0.347295	-3.772436
1	0	3.030011	-0.858809	-4.743763
1	0	2.200359	0.260294	-3.652232
1	0	3.969572	0.321577	-3.822745
6	0	4.777819	-2.710315	-3.034926
1	0	4.952478	-3.628688	-2.463565
1	0	4.589873	-3.002389	-4.078466
1	0	5.702996	-2.119492	-3.024824
6	0	1.748380	-2.813399	-2.664559
1	0	1.702551	-3.638405	-1.948888
1	0	0.811944	-2.245792	-2.592555
1	0	1.789236	-3.247199	-3.674707
14	0	4.277874	-2.434412	0.486768
6	0	4.300157	-2.250412	2.392473
1	0	4.591058	-1.254497	2.744046
1	0	3.353846	-2.525129	2.871466
1	0	5.062562	-2.955989	2.756941
6	0	3.409334	-4.106867	0.195883
1	0	3.588950	-4.517841	-0.803914
1	0	3.794501	-4.832637	0.926366
1	0	2.322978	-4.040804	0.340858
6	0	6.142047	-2.624427	0.111405
1	0	6.485666	-3.573345	0.549493
1	0	6.395550	-2.637489	-0.951039
1	0	6.718406	-1.821171	0.590732
6	0	4.580058	0.183174	-0.685966
1	0	4.416944	0.793736	-1.583870
1	0	5.605095	-0.203547	-0.760261
6	0	4.438665	1.092851	0.556206
1	0	5.142865	1.933004	0.494388
1	0	4.727412	0.515188	1.444561
6	0	2.947108	1.608765	0.690976
14	0	2.718612	3.136224	-0.551171
6	0	1.259063	4.244351	-0.030587
1	0	1.093764	4.993831	-0.817093
1	0	0.332419	3.665823	0.070733
1	0	1.429469	4.781445	0.909001
6	0	4.317094	4.187141	-0.596202

1	0	4.100757	5.109004	-1.156056
1	0	4.709048	4.476691	0.381796
1	0	5.113448	3.661773	-1.140962
6	0	2.435754	2.780159	-2.396622
1	0	3.313752	2.338667	-2.878767
1	0	1.572515	2.137523	-2.590242
1	0	2.248705	3.749548	-2.882783
14	0	2.716238	2.308523	2.508720
6	0	0.919672	2.774529	2.964119
1	0	0.182251	2.385509	2.254200
1	0	0.671088	2.389306	3.963205
1	0	0.806435	3.865306	2.998756
6	0	3.391077	1.154096	3.877106
1	0	4.445604	0.893256	3.716853
1	0	3.343935	1.720188	4.819222
1	0	2.828475	0.227684	4.034535
6	0	3.760381	3.885874	2.789279
1	0	3.427267	4.739526	2.189324
1	0	3.661752	4.169009	3.847514
1	0	4.828204	3.724619	2.591926
6	0	-3.421576	1.086524	-0.708919
14	0	-3.134021	1.987959	-2.430774
6	0	-2.826901	0.777218	-3.867166
1	0	-2.769469	1.367560	-4.793679
1	0	-1.875027	0.247248	-3.753218
1	0	-3.627444	0.039840	-3.998520
6	0	-4.746271	2.905105	-2.899988
1	0	-4.974888	3.745919	-2.234607
1	0	-4.639267	3.310654	-3.916415
1	0	-5.612862	2.230743	-2.905957
6	0	-1.713838	3.248889	-2.528186
1	0	-1.785728	4.065069	-1.804996
1	0	-0.742923	2.757664	-2.399828
1	0	-1.727863	3.693482	-3.534911
14	0	-4.036729	2.418428	0.606741
6	0	-3.329780	4.170835	0.353601
1	0	-3.724483	4.804351	1.161199
1	0	-2.235411	4.186701	0.431217
1	0	-3.613458	4.634008	-0.597168
6	0	-5.939715	2.564216	0.546617

1	0	-6.255062	3.354011	1.243612
1	0	-6.313978	2.829797	-0.448742
1	0	-6.435051	1.635546	0.859140
6	0	-3.605361	2.033758	2.417091
1	0	-4.151083	1.169456	2.802404
1	0	-2.533121	1.855326	2.566217
1	0	-3.886093	2.902118	3.030809
6	0	-4.561519	0.018778	-0.963415
1	0	-4.383714	-0.487486	-1.919278
1	0	-5.548474	0.493146	-1.042481
6	0	-4.586544	-1.042017	0.157441
1	0	-5.292669	-1.844191	-0.104421
1	0	-4.988307	-0.569070	1.067355
6	0	-3.145299	-1.643216	0.453687
14	0	-2.720004	-3.110240	-0.785448
6	0	-0.944266	-3.734231	-0.520139
1	0	-0.240437	-2.907235	-0.364780
1	0	-0.870403	-4.416224	0.332487
1	0	-0.614195	-4.278258	-1.414314
6	0	-3.884269	-4.609649	-0.562431
1	0	-3.679596	-5.316468	-1.379603
1	0	-3.728247	-5.144745	0.381024
1	0	-4.944276	-4.332418	-0.628700
6	0	-2.905718	-2.661231	-2.622854
1	0	-3.948559	-2.457235	-2.897917
1	0	-2.295209	-1.804951	-2.920904
1	0	-2.576272	-3.526954	-3.216172
14	0	-3.289000	-2.401744	2.265777
6	0	-4.988517	-3.256770	2.449499
1	0	-5.142776	-4.085623	1.752578
1	0	-5.062415	-3.660477	3.470129
1	0	-5.816137	-2.547686	2.319773
6	0	-1.985567	-3.723675	2.708103
1	0	-0.949885	-3.402282	2.552192
1	0	-2.099454	-3.958608	3.776167
1	0	-2.138629	-4.656300	2.152425
6	0	-3.295339	-1.164042	3.719289
1	0	-4.263772	-0.656195	3.801248
1	0	-3.162363	-1.749217	4.641490
1	0	-2.515129	-0.399460	3.694286

1	0	0.089489	0.305093	3.188781
1	0	-0.837388	-1.112209	2.463214
1	0	2.191273	-0.809685	2.477004
1	0	1.246154	-2.082988	1.590271

1

A

Frequencies -- -134.4541

Red. masses -- 5.8682

Frc consts -- 0.0625

IR Inten -- 13.5427

Atom	AN	X	Y	Z
1	6	0.05	-0.19	0.26
2	6	0.23	-0.11	0.34
3	14	-0.07	0.05	-0.08
4	14	-0.02	0.00	0.16
5	14	0.02	0.04	-0.06
6	6	0.02	0.02	-0.02
7	14	0.00	0.00	-0.02
8	6	0.00	0.00	-0.01
9	1	-0.01	0.01	-0.01
10	1	0.00	0.00	0.00
11	1	-0.01	0.01	-0.01
12	6	0.01	0.01	-0.01
13	1	0.01	0.01	-0.01
14	1	0.01	0.01	-0.01
15	1	0.01	0.01	-0.01
16	6	0.02	-0.01	-0.01
17	1	0.03	-0.02	-0.02
18	1	0.01	-0.02	0.01
19	1	0.02	0.00	-0.01
20	14	0.01	0.00	-0.01
21	6	0.05	-0.02	-0.01
22	1	-0.01	-0.01	0.01
23	1	0.09	-0.11	0.02
24	1	0.12	0.03	-0.05
25	6	0.00	0.01	-0.01
26	1	0.01	0.00	-0.01
27	1	0.00	0.01	0.00
28	1	0.00	0.01	-0.02

29	6	0.00	0.01	-0.03
30	1	0.00	-0.01	-0.05
31	1	0.00	0.03	-0.03
32	1	0.01	-0.01	-0.01
33	6	0.03	0.01	0.00
34	1	0.04	0.01	0.00
35	1	0.02	0.00	0.01
36	6	0.02	0.00	0.00
37	1	0.02	0.01	0.00
38	1	0.03	0.00	0.00
39	6	0.02	-0.01	0.01
40	14	0.00	0.00	0.00
41	6	0.00	-0.01	0.00
42	1	-0.01	-0.02	-0.01
43	1	0.01	-0.02	0.02
44	1	0.01	0.01	-0.01
45	6	0.01	-0.01	0.00
46	1	0.00	0.00	0.01
47	1	0.01	-0.01	0.00
48	1	0.00	0.00	0.00
49	6	0.00	0.00	0.00
50	1	0.00	-0.01	0.00
51	1	0.00	0.01	0.00
52	1	0.01	0.00	0.00
53	14	0.00	0.00	0.00
54	6	-0.01	-0.01	-0.02
55	1	0.00	-0.08	0.00
56	1	0.00	0.04	0.00
57	1	-0.03	-0.01	-0.09
58	6	-0.01	-0.01	0.00
59	1	-0.01	-0.02	0.00
60	1	0.00	0.00	0.00
61	1	-0.02	0.00	0.01
62	6	0.00	0.00	0.00
63	1	0.00	-0.01	0.00
64	1	-0.01	0.00	0.00
65	1	0.00	0.00	0.01
66	6	-0.06	-0.01	-0.06
67	14	-0.03	0.00	-0.04
68	6	-0.01	-0.01	-0.02

69	1	0.02	-0.02	-0.03
70	1	-0.01	-0.01	0.01
71	1	-0.01	-0.01	-0.03
72	6	-0.02	0.02	-0.04
73	1	-0.02	0.01	-0.04
74	1	-0.02	0.02	-0.04
75	1	-0.02	0.02	-0.05
76	6	-0.01	-0.02	-0.01
77	1	-0.03	-0.01	-0.02
78	1	-0.02	-0.03	0.04
79	1	0.03	-0.04	-0.02
80	14	-0.02	-0.01	-0.03
81	6	-0.01	-0.01	-0.02
82	1	0.00	-0.02	-0.01
83	1	-0.01	-0.02	-0.03
84	1	-0.01	0.00	-0.01
85	6	-0.02	0.01	-0.01
86	1	0.00	0.01	0.00
87	1	-0.02	0.01	0.00
88	1	-0.02	0.01	0.00
89	6	-0.01	-0.02	-0.03
90	1	0.00	-0.02	-0.03
91	1	0.00	-0.01	-0.03
92	1	0.00	-0.02	-0.03
93	6	-0.07	0.00	-0.03
94	1	-0.08	-0.01	-0.03
95	1	-0.07	-0.02	-0.01
96	6	-0.03	0.00	-0.01
97	1	-0.02	-0.01	0.00
98	1	-0.03	0.01	-0.02
99	6	-0.01	0.03	-0.01
100	14	0.00	0.01	0.00
101	6	0.00	0.02	-0.01
102	1	-0.01	0.03	-0.07
103	1	0.02	0.05	0.02
104	1	-0.02	-0.02	0.00
105	6	0.00	0.01	0.01
106	1	0.00	0.01	0.01
107	1	0.01	0.01	0.01
108	1	0.00	0.01	0.01

109	6	-0.01	0.00	-0.01
110	1	-0.01	-0.01	0.00
111	1	-0.01	0.00	-0.01
112	1	-0.01	-0.01	0.00
113	14	0.00	0.02	-0.01
114	6	0.01	0.01	0.00
115	1	0.01	0.01	0.00
116	1	0.02	0.01	0.00
117	1	0.00	0.01	0.01
118	6	0.01	0.03	-0.01
119	1	0.01	0.05	0.03
120	1	-0.01	0.01	-0.01
121	1	0.04	0.04	-0.03
122	6	0.00	0.01	0.00
123	1	0.00	0.01	0.01
124	1	0.01	0.01	-0.01
125	1	0.00	0.02	0.00
126	1	0.38	-0.17	0.42
127	1	0.04	0.26	0.02
128	1	0.21	-0.17	-0.05
129	1	-0.04	-0.09	-0.03

Si=Ge=Si (TS)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.263299	-1.124796	2.098088
6	0.075609	-0.663932	2.665085
14	-2.060994	-0.057220	0.074810
32	-0.030974	0.184048	-1.180094
14	2.019961	-0.038529	0.174058
6	3.587677	-0.990626	-0.591622
14	3.333424	-1.695332	-2.411822
6	3.189958	-0.339814	-3.739127
1	3.116894	-0.846175	-4.712985
1	2.296984	0.280959	-3.623512
1	4.067079	0.317526	-3.781722

6	4.824062	-2.733546	-3.009611
1	4.984402	-3.655913	-2.440551
1	4.629882	-3.020161	-4.053544
1	5.758921	-2.158214	-2.999330
6	1.791863	-2.784977	-2.628718
1	1.727169	-3.602517	-1.905916
1	0.865134	-2.200153	-2.562175
1	1.823705	-3.228196	-3.635100
14	4.323429	-2.452393	0.517428
6	4.342741	-2.268462	2.421659
1	4.655210	-1.279311	2.773227
1	3.388464	-2.520191	2.896929
1	5.086579	-2.992022	2.789960
6	3.425823	-4.107895	0.220376
1	3.601265	-4.520454	-0.779476
1	3.795057	-4.841761	0.950857
1	2.340468	-4.022011	0.361925
6	6.184730	-2.671757	0.143648
1	6.513413	-3.625590	0.582393
1	6.439084	-2.689048	-0.918567
1	6.772974	-1.877363	0.623110
6	4.664562	0.169408	-0.641387
1	4.513082	0.785742	-1.537613
1	5.687011	-0.225699	-0.709737
6	4.523002	1.073633	0.605422
1	5.226024	1.915056	0.545123
1	4.813858	0.493152	1.490913
6	3.031639	1.586016	0.748249
14	2.791763	3.126600	-0.478430
6	1.317452	4.210221	0.050668
1	1.140222	4.963943	-0.729230
1	0.399427	3.617044	0.148038
1	1.480048	4.741549	0.994845
6	4.382234	4.189027	-0.512547
1	4.158834	5.117929	-1.057729
1	4.774340	4.465916	0.468915
1	5.180325	3.676573	-1.066894
6	2.512447	2.785657	-2.327980
1	3.386547	2.338174	-2.811554
1	1.642341	2.154373	-2.530177

1	2.336462	3.760422	-2.807578
14	2.793006	2.265912	2.573028
6	0.987563	2.689149	3.030065
1	0.258933	2.284840	2.319457
1	0.747609	2.295461	4.028016
1	0.849159	3.777065	3.067606
6	3.497752	1.114693	3.927516
1	4.557296	0.879689	3.761896
1	3.439634	1.670767	4.875075
1	2.957279	0.174514	4.077363
6	3.806052	3.861269	2.865188
1	3.460539	4.712314	2.268749
1	3.698237	4.136744	3.924540
1	4.877336	3.719779	2.671810
6	-3.485687	1.095595	-0.654596
14	-3.190279	2.015391	-2.361696
6	-2.908510	0.822542	-3.819469
1	-2.846687	1.426772	-4.736662
1	-1.966260	0.271668	-3.724764
1	-3.722180	0.100838	-3.957131
6	-4.780543	2.973429	-2.821011
1	-4.991611	3.810883	-2.145726
1	-4.665360	3.387900	-3.832906
1	-5.660652	2.316859	-2.833507
6	-1.741475	3.247632	-2.441985
1	-1.785170	4.040825	-1.691588
1	-0.775921	2.737314	-2.344457
1	-1.759735	3.724948	-3.433439
14	-4.088647	2.419925	0.675790
6	-3.349785	4.163131	0.447674
1	-3.737108	4.794338	1.260608
1	-2.255671	4.156602	0.532358
1	-3.619045	4.642788	-0.499124
6	-5.988950	2.593570	0.609399
1	-6.296371	3.382215	1.311230
1	-6.356671	2.870414	-0.385237
1	-6.496415	1.668758	0.913960
6	-3.673156	2.009677	2.484424
1	-4.219502	1.138631	2.853494
1	-2.601707	1.831594	2.639580

1	-3.961214	2.869151	3.107370
6	-4.629294	0.035290	-0.916498
1	-4.453229	-0.464459	-1.876111
1	-5.615932	0.512119	-0.990982
6	-4.656338	-1.034810	0.196590
1	-5.363222	-1.834115	-0.072619
1	-5.059303	-0.568641	1.109622
6	-3.216315	-1.638261	0.491587
14	-2.784848	-3.090084	-0.763622
6	-1.003527	-3.710049	-0.518479
1	-0.302456	-2.882374	-0.353530
1	-0.921865	-4.405456	0.322772
1	-0.675599	-4.238131	-1.423358
6	-3.941073	-4.597889	-0.549874
1	-3.731076	-5.300245	-1.369574
1	-3.786117	-5.136296	0.391727
1	-5.002066	-4.324515	-0.618038
6	-2.986218	-2.633142	-2.598361
1	-4.031742	-2.430673	-2.864334
1	-2.379813	-1.774839	-2.898623
1	-2.659438	-3.496382	-3.196891
14	-3.358741	-2.419849	2.293431
6	-5.063259	-3.266440	2.473134
1	-5.223319	-4.085863	1.766077
1	-5.136981	-3.682531	3.488814
1	-5.887302	-2.551309	2.353886
6	-2.064804	-3.759521	2.712083
1	-1.027001	-3.442880	2.562843
1	-2.180891	-4.011906	3.775896
1	-2.224145	-4.681182	2.140289
6	-3.343880	-1.199479	3.761216
1	-4.308168	-0.686419	3.859452
1	-3.202945	-1.793836	4.676353
1	-2.558778	-0.439827	3.732207
1	0.039599	0.215713	3.299415
1	-0.857161	-1.185089	2.504722
1	2.190836	-0.821271	2.577211
1	1.272390	-2.135549	1.687881

A

Frequencies	--	-175.6979		
Red. masses	--	9.2733		
Frc consts	--	0.1687		
IR Inten	--	13.9773		
Atom	AN	X	Y	Z
1	6	-0.15	-0.32	0.52
2	6	0.00	-0.11	0.34
3	14	-0.04	0.06	-0.06
4	32	-0.01	-0.01	0.08
5	14	0.07	0.08	-0.19
6	6	0.05	0.04	-0.06
7	14	0.02	0.00	-0.04
8	6	0.01	0.00	-0.03
9	1	-0.01	0.02	-0.03
10	1	0.01	0.01	-0.01
11	1	0.01	0.00	-0.03
12	6	0.02	0.00	-0.02
13	1	0.02	0.00	-0.01
14	1	0.03	-0.01	-0.02
15	1	0.02	0.00	-0.02
16	6	0.03	-0.01	-0.01
17	1	0.04	-0.01	-0.01
18	1	0.03	-0.02	0.01
19	1	0.02	-0.01	-0.01
20	14	0.00	0.02	-0.02
21	6	0.01	0.01	-0.02
22	1	-0.04	0.02	0.00
23	1	0.03	-0.06	-0.01
24	1	0.05	0.04	-0.04
25	6	-0.01	0.02	-0.01
26	1	0.00	0.01	-0.01
27	1	-0.02	0.03	0.00
28	1	-0.01	0.03	-0.03
29	6	0.00	0.01	-0.01
30	1	-0.02	0.00	-0.02
31	1	0.00	0.02	-0.01
32	1	0.00	-0.01	0.00
33	6	0.07	0.02	-0.02
34	1	0.10	0.02	-0.02

35	1	0.07	0.01	0.01
36	6	0.04	0.01	-0.01
37	1	0.03	0.02	0.00
38	1	0.04	0.01	-0.01
39	6	0.04	-0.01	-0.02
40	14	0.01	0.01	-0.02
41	6	0.01	0.00	0.00
42	1	0.00	-0.01	0.00
43	1	0.01	-0.02	-0.01
44	1	0.00	0.00	0.00
45	6	0.01	0.01	0.00
46	1	0.02	0.01	0.01
47	1	0.01	0.00	0.00
48	1	0.01	0.01	0.00
49	6	0.02	0.02	-0.02
50	1	0.02	0.01	-0.01
51	1	0.01	0.05	-0.03
52	1	0.05	0.03	-0.01
53	14	0.00	-0.01	-0.01
54	6	0.00	-0.03	-0.03
55	1	0.01	-0.06	-0.03
56	1	0.00	0.00	-0.02
57	1	-0.02	-0.03	-0.06
58	6	0.00	-0.01	-0.01
59	1	0.00	0.00	-0.01
60	1	0.00	0.00	-0.01
61	1	0.01	-0.01	-0.01
62	6	-0.01	-0.01	-0.01
63	1	-0.01	-0.01	-0.01
64	1	-0.02	-0.01	-0.01
65	1	0.00	0.00	0.00
66	6	-0.04	-0.01	-0.05
67	14	-0.02	0.00	-0.02
68	6	0.00	0.00	-0.01
69	1	0.01	-0.01	-0.02
70	1	-0.01	-0.01	0.00
71	1	0.00	0.00	-0.02
72	6	-0.01	0.01	-0.03
73	1	-0.01	0.01	-0.02
74	1	-0.02	0.02	-0.03

75	1	-0.01	0.01	-0.03
76	6	-0.01	-0.01	-0.01
77	1	-0.01	-0.01	-0.01
78	1	-0.01	-0.01	0.01
79	1	0.00	-0.01	-0.01
80	14	0.00	-0.01	-0.02
81	6	0.00	-0.01	-0.01
82	1	0.00	-0.01	0.00
83	1	0.00	-0.01	-0.02
84	1	0.00	0.00	-0.01
85	6	0.00	0.00	0.00
86	1	0.00	0.00	0.00
87	1	-0.01	0.00	0.00
88	1	-0.01	0.00	0.00
89	6	0.00	-0.01	-0.02
90	1	0.01	-0.02	-0.02
91	1	0.00	0.00	-0.02
92	1	-0.01	-0.01	-0.02
93	6	-0.04	0.00	-0.02
94	1	-0.06	-0.01	-0.02
95	1	-0.05	-0.02	0.00
96	6	-0.01	0.00	-0.01
97	1	0.00	-0.01	0.01
98	1	-0.01	0.01	-0.01
99	6	0.00	0.03	-0.01
100	14	0.01	0.01	0.00
101	6	0.00	0.00	0.00
102	1	0.00	0.01	-0.03
103	1	0.01	0.02	0.01
104	1	-0.01	-0.02	0.00
105	6	0.00	0.01	0.01
106	1	0.00	0.01	0.01
107	1	0.00	0.01	0.01
108	1	0.00	0.01	0.01
109	6	-0.01	0.00	0.00
110	1	-0.01	-0.01	0.00
111	1	-0.01	-0.01	-0.01
112	1	-0.01	-0.01	0.00
113	14	0.00	0.01	0.00
114	6	0.00	0.00	-0.01

115	1	0.00	0.00	-0.01
116	1	0.00	0.01	-0.01
117	1	0.00	0.00	-0.01
118	6	0.00	0.02	0.00
119	1	0.00	0.02	0.02
120	1	-0.01	0.01	0.00
121	1	0.01	0.02	-0.01
122	6	-0.03	0.00	0.01
123	1	-0.05	-0.03	0.01
124	1	-0.02	-0.01	0.00
125	1	-0.06	0.03	0.03
126	1	0.10	-0.08	0.31
127	1	-0.13	0.20	0.09
128	1	0.01	-0.15	0.05
129	1	-0.21	-0.15	0.11

Ge=Si=Ge (TS)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.004876	-0.963225	-2.185686
6	0.279836	-0.531507	-2.524903
32	1.982186	-0.018683	-0.075132
14	-0.000319	0.084726	1.298306
32	-1.981846	-0.055447	-0.120765
6	-3.620432	-1.077851	0.633472
14	-3.376726	-1.801564	2.440735
6	-3.283516	-0.455850	3.782167
1	-3.202763	-0.964005	4.754416
1	-2.406648	0.189273	3.674111
1	-4.179184	0.176697	3.821092
6	-4.857554	-2.882674	2.985817
1	-4.975688	-3.801598	2.400209
1	-4.692505	-3.177742	4.032374
1	-5.805585	-2.330051	2.948702
6	-1.813073	-2.860641	2.662818
1	-1.708473	-3.652030	1.915578

1	-0.900711	-2.248778	2.641519
1	-1.856738	-3.337802	3.653128
14	-4.270333	-2.510027	-0.542418
6	-4.197339	-2.234302	-2.430622
1	-4.650772	-1.290894	-2.750654
1	-3.188878	-2.292914	-2.851784
1	-4.784214	-3.045520	-2.887501
6	-3.334442	-4.147254	-0.266144
1	-3.527430	-4.591749	0.716859
1	-3.658843	-4.871601	-1.026642
1	-2.248415	-4.023888	-0.371217
6	-6.136913	-2.798972	-0.250562
1	-6.432564	-3.725005	-0.765074
1	-6.416309	-2.898893	0.801592
1	-6.732238	-1.984402	-0.685161
6	-4.694323	0.080869	0.682316
1	-4.558620	0.681407	1.591713
1	-5.716034	-0.322703	0.731843
6	-4.568963	1.019363	-0.544541
1	-5.306707	1.830410	-0.461952
1	-4.840604	0.450435	-1.443224
6	-3.110351	1.609125	-0.690709
14	-2.887871	3.121854	0.557118
6	-1.417833	4.214423	0.036387
1	-1.265830	4.992327	0.797804
1	-0.490820	3.629511	-0.022582
1	-1.563179	4.715183	-0.927126
6	-4.487707	4.168144	0.599102
1	-4.287180	5.083071	1.175563
1	-4.861738	4.468491	-0.382807
1	-5.291031	3.630003	1.120597
6	-2.600234	2.732569	2.394925
1	-3.472898	2.270138	2.867982
1	-1.731178	2.091721	2.573233
1	-2.420227	3.690722	2.905202
14	-2.890973	2.291564	-2.512227
6	-1.078377	2.674248	-2.973917
1	-0.368192	2.340380	-2.210622
1	-0.811756	2.190737	-3.923494
1	-0.938639	3.754697	-3.106037

6	-3.630533	1.154215	-3.859143
1	-4.708636	1.003514	-3.718251
1	-3.502349	1.673579	-4.820359
1	-3.164514	0.169933	-3.962530
6	-3.877570	3.904780	-2.794387
1	-3.521430	4.747763	-2.192669
1	-3.766535	4.184595	-3.852375
1	-4.950492	3.775304	-2.601920
6	3.452282	1.196391	0.731999
14	3.092592	2.081234	2.442894
6	2.822310	0.868956	3.886681
1	2.723676	1.464852	4.806182
1	1.900549	0.288647	3.770412
1	3.656962	0.173927	4.036693
6	4.641115	3.085255	2.950272
1	4.848120	3.932491	2.286142
1	4.488052	3.488786	3.961630
1	5.538140	2.452240	2.982402
6	1.597779	3.257345	2.489520
1	1.631338	4.053583	1.741342
1	0.655242	2.709072	2.367379
1	1.568501	3.732770	3.481618
14	4.066680	2.529703	-0.570753
6	3.292163	4.258079	-0.345757
1	3.692736	4.908792	-1.136457
1	2.201240	4.234546	-0.464179
1	3.522321	4.728040	0.616143
6	5.962058	2.730336	-0.457003
1	6.279188	3.526664	-1.145571
1	6.297830	3.006390	0.549341
1	6.490245	1.813622	-0.750871
6	3.695768	2.124953	-2.392408
1	4.245216	1.251603	-2.751514
1	2.627010	1.956646	-2.578742
1	4.004969	2.984175	-3.005532
6	4.581043	0.129132	1.016072
1	4.376894	-0.376862	1.966460
1	5.563986	0.609153	1.128149
6	4.672453	-0.944664	-0.092155
1	5.409670	-1.705854	0.207412

1	5.082250	-0.466674	-0.996385
6	3.284734	-1.630707	-0.430566
14	2.839827	-3.073400	0.819991
6	1.078303	-3.727147	0.519977
1	0.359521	-2.913988	0.358640
1	1.030883	-4.402901	-0.340033
1	0.743200	-4.285519	1.404104
6	4.026074	-4.563707	0.649708
1	3.810940	-5.262267	1.471176
1	3.899902	-5.112907	-0.290290
1	5.080467	-4.270637	0.736593
6	2.973833	-2.592312	2.653611
1	4.006437	-2.367013	2.950334
1	2.342393	-1.740282	2.919124
1	2.642224	-3.451912	3.254549
14	3.527646	-2.397885	-2.223623
6	5.245550	-3.229971	-2.326310
1	5.369293	-4.074499	-1.641510
1	5.383461	-3.607434	-3.350447
1	6.055426	-2.514610	-2.131787
6	2.258857	-3.738594	-2.708841
1	1.213610	-3.431889	-2.591518
1	2.411736	-3.982156	-3.769872
1	2.404174	-4.663798	-2.138233
6	3.594373	-1.156215	-3.672660
1	4.546298	-0.611389	-3.681414
1	3.552833	-1.741870	-4.602931
1	2.784021	-0.424440	-3.706931
1	0.452130	0.403592	-3.045239
1	1.115078	-1.209958	-2.454522
1	-1.846060	-0.497425	-2.691600
1	-1.140711	-2.013846	-1.932599

1

A

Frequencies -- -215.7562

Red. masses -- 11.4088

Frc consts -- 0.3129

IR Inten -- 4.9064

Atom AN X Y Z

1	6	-0.09	0.28	0.56
2	6	0.10	0.15	0.47
3	32	-0.06	-0.05	-0.08
4	14	-0.01	0.00	0.19
5	32	0.05	-0.03	-0.11
6	6	0.04	-0.03	-0.04
7	14	0.01	0.00	-0.02
8	6	0.00	0.00	-0.01
9	1	0.00	-0.01	-0.01
10	1	0.01	-0.01	0.00
11	1	0.00	0.00	-0.01
12	6	0.01	0.00	-0.01
13	1	0.01	0.00	-0.01
14	1	0.02	0.01	-0.01
15	1	0.02	0.00	-0.01
16	6	0.02	0.01	-0.01
17	1	0.04	0.02	-0.02
18	1	0.02	0.02	0.03
19	1	0.02	0.00	-0.01
20	14	0.00	-0.01	-0.01
21	6	0.01	0.00	-0.01
22	1	-0.03	-0.01	0.00
23	1	0.02	0.06	0.01
24	1	0.05	-0.02	-0.03
25	6	0.00	-0.01	-0.01
26	1	0.01	0.00	0.00
27	1	0.00	-0.02	0.00
28	1	0.00	-0.01	-0.02
29	6	0.00	0.00	0.00
30	1	-0.01	0.00	-0.01
31	1	0.00	-0.01	0.00
32	1	0.00	0.00	0.00
33	6	0.05	-0.01	-0.01
34	1	0.07	-0.02	-0.01
35	1	0.05	-0.01	0.02
36	6	0.03	0.00	0.00
37	1	0.01	-0.01	0.01
38	1	0.03	0.00	0.00
39	6	0.02	0.02	0.01
40	14	0.00	0.00	0.00

41	6	0.00	0.01	0.00
42	1	0.00	0.01	0.00
43	1	0.01	0.02	-0.01
44	1	0.00	0.01	0.00
45	6	0.00	0.01	0.01
46	1	0.00	0.01	0.01
47	1	0.01	0.01	0.01
48	1	0.00	0.00	0.00
49	6	0.01	-0.01	-0.01
50	1	0.01	0.01	0.00
51	1	-0.01	-0.04	-0.02
52	1	0.05	-0.02	0.00
53	14	0.00	0.00	0.00
54	6	0.00	0.00	0.00
55	1	0.00	0.01	0.01
56	1	0.01	-0.02	0.01
57	1	0.01	0.00	-0.01
58	6	0.01	0.00	0.01
59	1	0.00	0.00	0.00
60	1	0.02	-0.02	0.00
61	1	0.00	-0.01	0.03
62	6	0.00	0.00	0.00
63	1	0.00	0.00	0.00
64	1	0.00	0.00	0.00
65	1	0.00	0.00	0.00
66	6	-0.04	0.02	-0.05
67	14	-0.02	0.00	-0.02
68	6	0.01	0.01	-0.01
69	1	0.02	0.02	-0.01
70	1	0.00	0.01	0.01
71	1	0.01	0.01	-0.01
72	6	-0.01	0.00	-0.02
73	1	-0.01	0.00	-0.02
74	1	-0.01	-0.01	-0.02
75	1	-0.01	-0.01	-0.02
76	6	-0.01	0.00	-0.01
77	1	-0.02	0.00	-0.01
78	1	-0.02	0.00	0.02
79	1	-0.01	0.00	-0.01
80	14	0.00	0.01	-0.02

81	6	0.00	0.01	-0.01
82	1	0.00	0.02	0.00
83	1	0.00	0.02	-0.02
84	1	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	1	0.01	0.00	0.00
87	1	-0.01	0.00	0.00
88	1	-0.01	0.00	0.01
89	6	0.01	0.01	-0.01
90	1	0.01	0.01	-0.01
91	1	0.01	0.00	-0.01
92	1	0.00	0.01	-0.02
93	6	-0.06	0.01	-0.02
94	1	-0.08	0.01	-0.02
95	1	-0.07	0.02	0.01
96	6	-0.02	0.00	0.00
97	1	0.00	0.02	0.02
98	1	-0.02	0.00	0.00
99	6	0.00	-0.02	0.01
100	14	0.01	-0.01	0.00
101	6	0.00	0.01	0.00
102	1	0.00	0.00	-0.04
103	1	0.00	-0.01	0.01
104	1	-0.02	0.03	0.01
105	6	0.00	-0.01	0.01
106	1	0.00	-0.02	0.01
107	1	0.00	-0.01	0.01
108	1	0.00	-0.01	0.01
109	6	-0.01	0.00	0.00
110	1	-0.01	0.00	0.01
111	1	0.00	0.01	0.00
112	1	-0.01	0.01	0.01
113	14	-0.01	0.00	0.00
114	6	0.00	0.00	0.00
115	1	0.00	0.00	0.00
116	1	0.00	0.00	0.00
117	1	0.00	0.00	0.00
118	6	0.00	-0.01	0.00
119	1	0.00	-0.01	0.01
120	1	-0.01	0.00	0.00

121	1	0.00	-0.01	0.00
122	6	-0.02	0.00	0.01
123	1	-0.03	0.02	0.01
124	1	-0.01	0.01	0.01
125	1	-0.04	-0.01	0.02
126	1	0.12	0.04	0.29
127	1	-0.10	-0.15	-0.03
128	1	0.12	0.11	0.02
129	1	-0.08	0.15	0.11

Ge=Ge=Ge (TS)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.907917	-0.953284	2.324744
6	-0.372745	-0.492359	2.604746
32	-2.021451	-0.009557	0.142134
32	0.001758	0.053813	-1.329688
32	2.024429	-0.057983	0.170944
6	3.657052	-1.086992	-0.585735
14	3.415400	-1.797612	-2.396334
6	3.337615	-0.446079	-3.734214
1	3.269084	-0.950238	-4.709532
1	2.459509	0.199414	-3.635234
1	4.233192	0.187521	-3.759036
6	4.891323	-2.887292	-2.935652
1	4.993824	-3.811156	-2.354785
1	4.737189	-3.173292	-3.986311
1	5.843369	-2.342984	-2.881465
6	1.845910	-2.847622	-2.641417
1	1.716277	-3.630024	-1.888380
1	0.934475	-2.232739	-2.652804
1	1.910141	-3.336153	-3.625469
14	4.261897	-2.533807	0.592976
6	4.141489	-2.262047	2.478039
1	4.609683	-1.331753	2.815012
1	3.118616	-2.293377	2.866327

1	4.690705	-3.090022	2.951002
6	3.309589	-4.157196	0.290240
1	3.506959	-4.596263	-0.694386
1	3.617298	-4.891799	1.047926
1	2.224196	-4.020761	0.386909
6	6.129057	-2.847445	0.335727
1	6.405663	-3.775158	0.857493
1	6.422554	-2.953806	-0.712347
1	6.726861	-2.037773	0.776222
6	4.742941	0.060158	-0.617775
1	4.621425	0.666477	-1.525869
1	5.761295	-0.353304	-0.659055
6	4.615992	0.995276	0.612023
1	5.361424	1.800317	0.538128
1	4.875689	0.419814	1.510326
6	3.161257	1.594521	0.753798
14	2.943733	3.113441	-0.485536
6	1.481359	4.216942	0.037219
1	1.354649	5.013237	-0.709800
1	0.543513	3.646928	0.068600
1	1.617466	4.694920	1.013239
6	4.549824	4.148582	-0.529418
1	4.358405	5.062105	-1.111094
1	4.921036	4.450190	0.453331
1	5.351392	3.601449	-1.044357
6	2.641563	2.736494	-2.324422
1	3.507495	2.271087	-2.806895
1	1.767789	2.100808	-2.500429
1	2.461415	3.698152	-2.828085
14	2.932028	2.266940	2.577463
6	1.119169	2.662299	3.030373
1	0.410674	2.351538	2.255377
1	0.839230	2.161847	3.967152
1	0.990833	3.741588	3.184530
6	3.645504	1.113377	3.923774
1	4.722534	0.945901	3.791515
1	3.516121	1.629707	4.886770
1	3.161780	0.136105	4.016178
6	3.933101	3.869156	2.871697
1	3.585139	4.718946	2.274522

1	3.824881	4.144319	3.931218
1	5.004817	3.730088	2.677978
6	-3.484071	1.203879	-0.690075
14	-3.098745	2.087249	-2.393954
6	-2.826880	0.879829	-3.843683
1	-2.728766	1.480347	-4.760275
1	-1.906079	0.296125	-3.735501
1	-3.661375	0.185369	-3.996549
6	-4.623181	3.115036	-2.922284
1	-4.833286	3.958330	-2.254464
1	-4.447921	3.524944	-3.927351
1	-5.525728	2.491476	-2.975115
6	-1.583639	3.241346	-2.419622
1	-1.630116	4.053180	-1.688622
1	-0.646371	2.691593	-2.259138
1	-1.517596	3.695975	-3.419817
14	-4.097023	2.542081	0.606533
6	-3.301957	4.262507	0.385840
1	-3.697542	4.917181	1.175777
1	-2.211820	4.225594	0.509377
1	-3.522143	4.737027	-0.576160
6	-5.989143	2.757689	0.479511
1	-6.306920	3.555705	1.165680
1	-6.314892	3.035599	-0.529640
1	-6.524830	1.843912	0.768671
6	-3.736167	2.136880	2.430000
1	-4.293440	1.268809	2.789274
1	-2.669291	1.959872	2.618567
1	-4.038898	2.999771	3.041250
6	-4.611763	0.138211	-0.986932
1	-4.399619	-0.364029	-1.937716
1	-5.594269	0.618183	-1.105219
6	-4.712913	-0.942709	0.114943
1	-5.443446	-1.704653	-0.198848
1	-5.136415	-0.470401	1.015814
6	-3.326350	-1.622720	0.470691
14	-2.852316	-3.063513	-0.770130
6	-1.084575	-3.697624	-0.453368
1	-0.377127	-2.880298	-0.262123
1	-1.043869	-4.387865	0.396017

1	-0.727487	-4.237420	-1.340692
6	-4.017394	-4.571013	-0.609078
1	-3.790122	-5.264518	-1.431545
1	-3.886300	-5.120619	0.329976
1	-5.075292	-4.292068	-0.697873
6	-2.979770	-2.592767	-2.607779
1	-4.013045	-2.378758	-2.910178
1	-2.355752	-1.736553	-2.876015
1	-2.637197	-3.452541	-3.202418
14	-3.582576	-2.392309	2.260522
6	-5.286692	-3.253560	2.343297
1	-5.376197	-4.119289	1.679917
1	-5.444684	-3.604520	3.374035
1	-6.103980	-2.559392	2.107174
6	-2.293300	-3.707105	2.764555
1	-1.253345	-3.381676	2.650594
1	-2.446720	-3.945932	3.826642
1	-2.418093	-4.639064	2.200013
6	-3.693570	-1.148339	3.704926
1	-4.647946	-0.608066	3.687904
1	-3.673743	-1.733113	4.636469
1	-2.887501	-0.413442	3.760238
1	-0.544635	0.461731	3.090266
1	-1.214123	-1.163451	2.540616
1	1.758489	-0.463549	2.788234
1	1.046403	-2.002894	2.070131

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A

Frequencies -- -193.7942

Red. masses -- 11.2136

Frc consts -- 0.2481

IR Inten -- 1.2889

Atom	AN	X	Y	Z
1	6	-0.13	-0.26	0.56
2	6	0.05	-0.11	0.47
3	32	-0.06	0.04	-0.08
4	32	0.00	0.00	0.10
5	32	0.06	0.01	-0.11
6	6	0.05	0.03	-0.05

7	14	0.02	0.00	-0.03
8	6	0.01	0.00	-0.02
9	1	0.00	0.01	-0.02
10	1	0.01	0.01	-0.01
11	1	0.01	0.00	-0.02
12	6	0.02	0.00	-0.02
13	1	0.01	0.00	-0.01
14	1	0.02	-0.01	-0.02
15	1	0.02	-0.01	-0.02
16	6	0.02	-0.01	-0.01
17	1	0.04	-0.01	-0.01
18	1	0.02	-0.02	0.02
19	1	0.02	0.00	-0.01
20	14	0.00	0.01	-0.02
21	6	0.00	0.01	-0.01
22	1	-0.02	0.01	-0.01
23	1	0.01	-0.03	0.00
24	1	0.03	0.02	-0.03
25	6	0.00	0.01	-0.01
26	1	0.01	0.00	0.00
27	1	0.00	0.02	0.00
28	1	0.00	0.02	-0.02
29	6	0.00	0.00	-0.01
30	1	-0.01	0.00	-0.01
31	1	0.01	0.00	0.00
32	1	0.01	0.00	0.00
33	6	0.06	0.01	-0.01
34	1	0.08	0.02	-0.01
35	1	0.06	0.02	0.02
36	6	0.03	0.00	0.00
37	1	0.02	0.01	0.01
38	1	0.03	0.00	-0.01
39	6	0.02	-0.01	0.00
40	14	0.00	0.00	-0.01
41	6	0.00	-0.01	0.00
42	1	0.00	-0.01	0.00
43	1	0.01	-0.02	-0.01
44	1	0.00	-0.01	0.00
45	6	0.01	0.00	0.01
46	1	0.00	0.00	0.01

47	1	0.01	-0.01	0.01
48	1	0.00	0.00	0.00
49	6	0.02	0.02	-0.01
50	1	0.01	-0.01	-0.01
51	1	-0.01	0.05	-0.02
52	1	0.06	0.03	0.00
53	14	0.00	-0.01	0.00
54	6	0.01	0.00	0.00
55	1	-0.01	0.00	0.02
56	1	0.02	0.02	0.01
57	1	0.01	0.00	-0.01
58	6	0.01	0.00	0.00
59	1	0.01	0.00	0.00
60	1	0.01	0.01	0.00
61	1	0.01	0.00	0.02
62	6	0.00	0.00	0.00
63	1	0.00	-0.01	-0.01
64	1	0.00	0.00	-0.01
65	1	0.00	0.00	0.00
66	6	-0.04	-0.02	-0.05
67	14	-0.02	0.00	-0.02
68	6	0.01	-0.01	-0.01
69	1	0.02	-0.02	-0.02
70	1	0.01	-0.01	0.01
71	1	0.01	-0.01	-0.01
72	6	-0.01	0.00	-0.03
73	1	-0.01	0.00	-0.02
74	1	-0.02	0.01	-0.02
75	1	-0.02	0.00	-0.02
76	6	-0.02	0.01	-0.01
77	1	-0.03	0.01	-0.02
78	1	-0.02	0.01	0.01
79	1	-0.02	0.00	-0.01
80	14	0.00	-0.01	-0.02
81	6	0.00	-0.01	-0.01
82	1	0.00	-0.02	0.00
83	1	0.00	-0.02	-0.02
84	1	-0.01	0.00	0.00
85	6	0.00	0.00	0.00
86	1	0.01	0.00	0.00

87	1	-0.01	0.00	0.00
88	1	-0.01	0.00	0.00
89	6	0.00	-0.01	-0.02
90	1	0.01	-0.02	-0.01
91	1	0.01	0.00	-0.01
92	1	-0.01	-0.01	-0.02
93	6	-0.06	-0.01	-0.02
94	1	-0.08	-0.01	-0.02
95	1	-0.07	-0.02	0.01
96	6	-0.02	0.00	0.00
97	1	-0.01	-0.02	0.01
98	1	-0.02	0.00	-0.01
99	6	-0.01	0.02	0.01
100	14	0.00	0.01	0.00
101	6	0.00	-0.01	0.00
102	1	0.00	-0.01	-0.04
103	1	0.00	0.00	0.01
104	1	-0.02	-0.03	0.00
105	6	-0.01	0.01	0.01
106	1	-0.01	0.02	0.01
107	1	0.00	0.01	0.01
108	1	-0.01	0.01	0.01
109	6	-0.01	0.00	0.00
110	1	-0.01	0.00	0.00
111	1	0.00	-0.01	0.00
112	1	-0.01	-0.01	0.01
113	14	-0.01	0.00	0.00
114	6	0.00	0.00	0.00
115	1	0.00	0.00	0.00
116	1	0.00	0.00	0.00
117	1	-0.01	0.00	0.00
118	6	0.00	0.01	0.00
119	1	0.00	0.02	0.00
120	1	0.00	0.01	0.00
121	1	0.00	0.01	0.00
122	6	-0.03	0.00	0.01
123	1	-0.05	-0.03	0.01
124	1	-0.02	-0.01	0.00
125	1	-0.05	0.02	0.02
126	1	0.09	0.00	0.26

127	1	-0.13	0.14	0.05
128	1	0.07	-0.13	0.05
129	1	-0.14	-0.17	0.20

Sn=Sn=Sn (TS)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	0.848802	-0.788928	2.665506
6	0	-0.484889	-0.461551	2.805385
50	0	-2.239780	-0.005643	0.222893
50	0	-0.007377	0.004968	-1.651335
50	0	2.252553	-0.080648	0.180189
6	0	4.099663	-1.243404	-0.353581
14	0	3.920813	-2.174682	-2.051208
6	0	3.982096	-1.006027	-3.552746
1	0	3.859543	-1.613044	-4.461762
1	0	3.181844	-0.258472	-3.546677
1	0	4.941197	-0.479194	-3.640687
6	0	5.324262	-3.431766	-2.378560
1	0	5.332691	-4.269331	-1.671674
1	0	5.188941	-3.849931	-3.386596
1	0	6.312178	-2.953518	-2.351511
6	0	2.270366	-3.122886	-2.190679
1	0	1.974126	-3.626551	-1.264866
1	0	1.451031	-2.450005	-2.488291
1	0	2.347397	-3.888414	-2.976537
14	0	4.604753	-2.511311	1.038960
6	0	4.383262	-1.945143	2.847553
1	0	4.984038	-1.063517	3.095214
1	0	3.343121	-1.741899	3.123224
1	0	4.731617	-2.765602	3.492848
6	0	3.607354	-4.134595	0.936442
1	0	3.759302	-4.689001	0.003381
1	0	3.916251	-4.789410	1.763773
1	0	2.528883	-3.955924	1.048222
6	0	6.468047	-2.915156	0.922254

1	0	6.706921	-3.718978	1.633564
1	0	6.779043	-3.245280	-0.073457
1	0	7.080237	-2.045834	1.198156
6	0	5.153434	-0.068899	-0.442207
1	0	5.095183	0.412885	-1.427514
1	0	6.180873	-0.457904	-0.358241
6	0	4.955116	1.027154	0.647663
1	0	5.753627	1.777181	0.535887
1	0	5.115064	0.562203	1.629004
6	0	3.536385	1.726722	0.608617
14	0	3.486102	3.066334	-0.818265
6	0	2.021801	4.269575	-0.618622
1	0	1.990759	4.932571	-1.494863
1	0	1.060036	3.742101	-0.576757
1	0	2.099713	4.903627	0.271229
6	0	5.116198	4.064720	-0.809940
1	0	5.020125	4.909356	-1.507449
1	0	5.376241	4.469793	0.172567
1	0	5.957397	3.450566	-1.158895
6	0	3.352551	2.447025	-2.614078
1	0	4.203681	1.829361	-2.919373
1	0	2.431294	1.885036	-2.808007
1	0	3.340803	3.333451	-3.266259
14	0	3.145217	2.580820	2.313425
6	0	1.284787	2.919157	2.551651
1	0	0.661239	2.068108	2.256245
1	0	1.080647	3.133405	3.610504
1	0	0.956797	3.788291	1.970517
6	0	3.764045	1.563205	3.805007
1	0	4.859673	1.488923	3.810945
1	0	3.471634	2.097083	4.720892
1	0	3.363320	0.548313	3.877463
6	0	4.046540	4.250152	2.558450
1	0	3.747384	5.024717	1.843641
1	0	3.810163	4.623188	3.565866
1	0	5.137148	4.136216	2.500062
6	0	-3.904707	1.354607	-0.446264
14	0	-3.510468	2.367723	-2.055396
6	0	-3.447596	1.298172	-3.632935
1	0	-3.226792	1.960790	-4.482778

1	0	-2.660679	0.535225	-3.604336
1	0	-4.400315	0.798174	-3.847357
6	0	-4.861208	3.667534	-2.437234
1	0	-4.924328	4.461843	-1.684746
1	0	-4.636413	4.142031	-3.403391
1	0	-5.852069	3.201613	-2.522467
6	0	-1.834188	3.279440	-1.979605
1	0	-1.606259	3.692842	-0.992671
1	0	-1.003061	2.617072	-2.272007
1	0	-1.832478	4.111571	-2.698378
14	0	-4.442254	2.569519	0.977268
6	0	-3.432491	4.189295	1.003218
1	0	-3.813146	4.818851	1.820404
1	0	-2.371205	3.996199	1.210886
1	0	-3.496463	4.775341	0.079860
6	0	-6.292664	3.011564	0.811678
1	0	-6.557024	3.758320	1.574106
1	0	-6.542309	3.431388	-0.168811
1	0	-6.933697	2.135390	0.977954
6	0	-4.246394	1.899201	2.748875
1	0	-4.867617	1.019563	2.942644
1	0	-3.206703	1.640981	2.988879
1	0	-4.558457	2.684971	3.452580
6	0	-5.029658	0.290819	-0.758145
1	0	-4.879881	-0.113870	-1.765284
1	0	-6.025254	0.763156	-0.766780
6	0	-5.080729	-0.908819	0.232519
1	0	-5.883938	-1.587757	-0.099918
1	0	-5.402918	-0.526024	1.213770
6	0	-3.724470	-1.712760	0.392006
14	0	-3.461408	-3.003480	-1.046950
6	0	-1.670016	-3.649642	-1.142564
1	0	-1.037804	-2.974449	-1.734114
1	0	-1.202793	-3.779263	-0.159508
1	0	-1.662240	-4.626640	-1.649131
6	0	-4.576994	-4.547669	-0.856228
1	0	-4.531710	-5.114300	-1.797860
1	0	-4.245856	-5.217411	-0.053313
1	0	-5.628474	-4.290614	-0.675144
6	0	-3.895487	-2.350317	-2.781479

1	0	-4.961255	-2.106189	-2.881435
1	0	-3.311461	-1.471001	-3.068166
1	0	-3.672941	-3.145555	-3.508462
14	0	-3.793911	-2.638282	2.105108
6	0	-5.430718	-3.606991	2.301171
1	0	-5.472904	-4.526494	1.709640
1	0	-5.545991	-3.884825	3.359164
1	0	-6.298237	-2.989904	2.030432
6	0	-2.363120	-3.874844	2.353279
1	0	-1.372216	-3.416224	2.240142
1	0	-2.420232	-4.286308	3.371265
1	0	-2.421636	-4.718890	1.655164
6	0	-3.833227	-1.494738	3.635053
1	0	-4.829670	-1.054671	3.766324
1	0	-3.637473	-2.116241	4.521249
1	0	-3.107117	-0.679309	3.637670
1	0	-0.795195	0.506541	3.188978
1	0	-1.241721	-1.233290	2.754447
1	0	1.615623	-0.114714	3.032894
1	0	1.140674	-1.824531	2.506488

1

A

Frequencies -- -113.1558

Red. masses -- 9.1673

Frc consts -- 0.0692

IR Inten -- 0.0877

Atom	AN	X	Y	Z
1	6	-0.09	-0.16	0.50
2	6	-0.01	-0.09	0.44
3	50	-0.06	0.03	-0.05
4	50	0.01	0.00	0.07
5	50	0.06	-0.01	-0.05
6	6	0.05	0.02	-0.04
7	14	0.04	0.00	-0.03
8	6	0.02	0.01	-0.03
9	1	0.01	0.01	-0.03
10	1	0.01	0.00	-0.02
11	1	0.01	0.01	-0.03
12	6	0.03	0.00	-0.03

13	1	0.03	0.00	-0.02
14	1	0.03	-0.01	-0.03
15	1	0.03	-0.01	-0.03
16	6	0.04	0.00	-0.02
17	1	0.04	0.00	-0.01
18	1	0.03	-0.01	-0.01
19	1	0.04	0.00	-0.01
20	14	0.02	0.01	-0.03
21	6	0.02	0.00	-0.02
22	1	0.01	0.01	-0.02
23	1	0.02	-0.01	-0.02
24	1	0.03	0.00	-0.03
25	6	0.01	0.01	-0.02
26	1	0.02	0.00	-0.02
27	1	0.00	0.02	-0.01
28	1	0.01	0.02	-0.04
29	6	0.02	0.00	-0.02
30	1	0.01	-0.01	-0.02
31	1	0.02	0.00	-0.02
32	1	0.02	-0.01	-0.01
33	6	0.06	0.01	-0.02
34	1	0.08	0.02	-0.02
35	1	0.06	0.01	0.00
36	6	0.03	0.01	-0.01
37	1	0.03	0.01	0.00
38	1	0.03	0.00	-0.01
39	6	0.03	0.00	-0.01
40	14	0.01	0.00	-0.01
41	6	0.01	0.00	0.00
42	1	0.02	0.01	0.01
43	1	0.01	-0.01	-0.02
44	1	0.00	-0.01	0.01
45	6	0.01	0.00	0.00
46	1	0.01	0.01	0.00
47	1	0.01	0.00	0.00
48	1	0.01	0.01	-0.01
49	6	0.01	0.01	-0.01
50	1	0.00	-0.01	-0.01
51	1	0.00	0.03	-0.01
52	1	0.03	0.01	-0.01

53	14	0.02	-0.01	-0.01
54	6	0.02	-0.03	0.01
55	1	0.03	-0.08	0.12
56	1	0.05	0.07	0.00
57	1	-0.03	-0.10	-0.06
58	6	0.04	0.01	-0.01
59	1	0.04	0.04	0.00
60	1	0.01	-0.01	-0.01
61	1	0.08	-0.01	-0.02
62	6	0.00	0.00	-0.01
63	1	-0.01	0.00	-0.01
64	1	0.00	0.00	-0.01
65	1	0.00	0.01	-0.01
66	6	-0.04	-0.01	-0.04
67	14	-0.03	0.00	-0.03
68	6	-0.01	0.00	-0.02
69	1	0.00	-0.01	-0.03
70	1	0.00	0.00	-0.01
71	1	0.00	-0.02	-0.03
72	6	-0.04	0.00	-0.03
73	1	-0.03	0.00	-0.03
74	1	-0.04	0.00	-0.03
75	1	-0.04	0.00	-0.03
76	6	-0.04	0.02	-0.02
77	1	-0.04	0.01	-0.01
78	1	-0.03	0.04	-0.02
79	1	-0.06	0.03	0.00
80	14	-0.01	-0.01	-0.02
81	6	-0.01	-0.01	-0.02
82	1	0.00	-0.02	-0.01
83	1	-0.01	-0.01	-0.03
84	1	-0.02	0.00	-0.01
85	6	-0.01	0.00	0.00
86	1	0.00	0.00	0.00
87	1	-0.02	0.00	0.00
88	1	-0.02	0.00	0.01
89	6	0.00	-0.01	-0.02
90	1	0.03	-0.02	-0.02
91	1	0.01	0.03	-0.02
92	1	-0.02	-0.01	-0.03

93	6	-0.05	0.00	-0.02
94	1	-0.07	-0.01	-0.02
95	1	-0.06	-0.01	0.00
96	6	-0.03	0.00	-0.01
97	1	-0.02	-0.01	-0.01
98	1	-0.04	0.00	-0.02
99	6	-0.02	0.01	0.00
100	14	-0.01	0.00	0.00
101	6	-0.02	-0.03	0.01
102	1	0.00	-0.04	0.04
103	1	-0.03	-0.06	0.02
104	1	-0.04	-0.03	0.00
105	6	-0.02	0.01	0.00
106	1	-0.03	0.01	0.00
107	1	-0.02	0.00	0.00
108	1	-0.02	0.01	0.01
109	6	0.00	0.00	0.00
110	1	0.00	-0.01	-0.01
111	1	0.00	0.00	0.00
112	1	0.01	0.00	0.00
113	14	-0.02	0.01	0.00
114	6	-0.01	-0.01	-0.01
115	1	0.00	-0.02	0.00
116	1	-0.01	0.00	0.00
117	1	-0.02	-0.02	-0.01
118	6	-0.01	0.02	0.01
119	1	-0.01	0.03	-0.01
120	1	0.00	0.04	0.01
121	1	-0.01	0.01	0.02
122	6	-0.06	0.00	0.01
123	1	-0.09	-0.06	0.02
124	1	-0.02	0.01	0.00
125	1	-0.11	0.04	0.01
126	1	0.00	-0.02	0.27
127	1	-0.10	0.02	0.17
128	1	0.01	-0.12	0.22
129	1	-0.09	-0.13	0.26

Pb=Pb=Pb (TS)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.882878	-0.622617	2.730696
6	-0.469902	-0.375288	2.891641
82	-2.232167	-0.007926	0.376826
82	-0.026055	0.007427	-1.731869
82	2.243126	-0.067986	0.257214
6	4.059958	-1.483924	-0.134383
14	3.787336	-2.502972	-1.766965
6	4.183073	-1.502249	-3.336795
1	4.000924	-2.146287	-4.209245
1	3.555189	-0.612879	-3.444572
1	5.233624	-1.185930	-3.378775
6	4.888167	-4.059626	-1.936189
1	4.681230	-4.835328	-1.190317
1	4.707395	-4.497998	-2.928400
1	5.954854	-3.806986	-1.878979
6	1.980337	-3.100220	-1.983335
1	1.487542	-3.386338	-1.047755
1	1.375291	-2.322090	-2.479790
1	1.955264	-3.974664	-2.649260
14	4.362236	-2.672448	1.367981
6	4.334130	-1.901659	3.113758
1	5.088828	-1.118408	3.247986
1	3.362037	-1.491915	3.405379
1	4.570382	-2.704898	3.827339
6	3.046198	-4.054265	1.420509
1	3.052199	-4.688781	0.527022
1	3.234789	-4.704260	2.286596
1	2.031399	-3.647584	1.535153
6	6.100006	-3.460592	1.270521
1	6.239256	-4.136488	2.126505
1	6.256701	-4.041088	0.357473
1	6.887582	-2.696310	1.326783
6	5.202305	-0.408847	-0.285184
1	5.208687	-0.010766	-1.308185

1	6.191402	-0.876752	-0.138986
6	5.104255	0.804422	0.695551
1	5.989248	1.439848	0.525554
1	5.203726	0.428116	1.721154
6	3.784807	1.660033	0.561615
14	3.875982	2.858556	-0.969564
6	2.479496	4.156056	-0.950045
1	2.526293	4.737282	-1.881734
1	1.486219	3.690661	-0.906847
1	2.559214	4.863301	-0.117388
6	5.560748	3.762585	-0.969461
1	5.555447	4.540146	-1.746850
1	5.791441	4.245442	-0.014656
1	6.380596	3.071029	-1.206659
6	3.781765	2.073801	-2.703589
1	4.616475	1.394978	-2.908856
1	2.844560	1.531565	-2.878480
1	3.833960	2.888450	-3.441259
14	3.393954	2.658798	2.181010
6	1.539405	3.077901	2.338827
1	0.897096	2.195201	2.230736
1	1.342203	3.518980	3.326258
1	1.227032	3.809308	1.584380
6	3.923140	1.725803	3.759719
1	5.015219	1.623762	3.813279
1	3.610349	2.322327	4.629000
1	3.492660	0.727010	3.876952
6	4.340303	4.314692	2.346380
1	4.109816	5.041310	1.559596
1	4.062312	4.771573	3.307485
1	5.427488	4.160389	2.360052
6	-3.868070	1.559798	-0.291418
14	-3.284005	2.616862	-1.799778
6	-3.363959	1.686713	-3.462593
1	-2.985077	2.353272	-4.251168
1	-2.751828	0.777287	-3.478160
1	-4.388883	1.405216	-3.735802
6	-4.349901	4.176048	-2.115995
1	-4.295539	4.913575	-1.307388
1	-3.998091	4.664930	-3.036172

1	-5.405839	3.914344	-2.265588
6	-1.469717	3.209675	-1.610341
1	-1.137083	3.247056	-0.567536
1	-0.774680	2.568185	-2.184143
1	-1.346096	4.217480	-2.031678
14	-4.325721	2.723949	1.186579
6	-3.048218	4.127700	1.400732
1	-3.361483	4.768955	2.237002
1	-2.057963	3.724420	1.655669
1	-2.933246	4.769624	0.520148
6	-6.062325	3.485575	0.949937
1	-6.277541	4.174536	1.779502
1	-6.157610	4.047211	0.014657
1	-6.840852	2.710484	0.959437
6	-4.385237	1.912440	2.908197
1	-5.175828	1.160229	2.998622
1	-3.435248	1.438403	3.183711
1	-4.588453	2.695396	3.653554
6	-5.030963	0.582371	-0.696647
1	-4.867207	0.222964	-1.718408
1	-5.998543	1.114275	-0.715960
6	-5.209492	-0.668066	0.218459
1	-6.078385	-1.233397	-0.163692
1	-5.507088	-0.314864	1.217843
6	-3.955701	-1.621305	0.338880
14	-3.779588	-2.826869	-1.170796
6	-2.064717	-3.648216	-1.290264
1	-1.288903	-2.920233	-1.559111
1	-1.757754	-4.142925	-0.363403
1	-2.086387	-4.407160	-2.085479
6	-5.047299	-4.261087	-1.110171
1	-5.051607	-4.763100	-2.088270
1	-4.796659	-5.014537	-0.353440
1	-6.067568	-3.907790	-0.913538
6	-4.076554	-2.014362	-2.868068
1	-5.093988	-1.616394	-2.973900
1	-3.368843	-1.204700	-3.073708
1	-3.939100	-2.780334	-3.645360
14	-4.081823	-2.607175	2.004508
6	-5.778066	-3.473771	2.175531

1	-5.900517	-4.327619	1.501625
1	-5.891116	-3.840675	3.206026
1	-6.602957	-2.773620	1.985252
6	-2.725878	-3.935540	2.198273
1	-1.717531	-3.541681	2.012473
1	-2.746624	-4.323301	3.226480
1	-2.879268	-4.788666	1.525369
6	-4.009246	-1.529629	3.578648
1	-4.938225	-0.964694	3.719301
1	-3.906653	-2.203536	4.441829
1	-3.180716	-0.817213	3.617308
1	-0.827684	0.586728	3.249887
1	-1.170970	-1.201912	2.917930
1	1.606143	0.116745	3.062523
1	1.229946	-1.650018	2.647968

1

A

Frequencies -- -76.9166

Red. masses -- 8.7738

Frc consts -- 0.0306

IR Inten -- 2.5071

Atom	AN	X	Y	Z
1	6	-0.03	-0.16	0.43
2	6	0.04	-0.09	0.43
3	82	-0.06	0.02	0.00
4	82	0.01	0.00	0.04
5	82	0.06	-0.01	-0.02
6	6	0.05	0.01	-0.04
7	14	0.04	0.01	-0.03
8	6	0.03	0.00	-0.03
9	1	0.02	0.00	-0.03
10	1	0.04	0.01	-0.03
11	1	0.04	-0.01	-0.04
12	6	0.02	-0.01	-0.03
13	1	0.01	0.00	-0.03
14	1	0.00	-0.01	-0.03
15	1	0.02	-0.02	-0.04
16	6	0.03	0.02	-0.01
17	1	0.02	0.07	0.00

18	1	0.04	0.01	-0.04
19	1	0.01	0.00	0.03
20	14	0.04	0.01	-0.03
21	6	0.06	0.00	-0.03
22	1	0.04	0.01	-0.03
23	1	0.06	-0.03	0.01
24	1	0.09	-0.01	-0.04
25	6	0.02	0.02	-0.03
26	1	0.01	0.02	-0.02
27	1	0.01	0.02	-0.02
28	1	0.02	0.03	-0.03
29	6	0.03	-0.01	-0.03
30	1	0.01	-0.02	-0.04
31	1	0.02	-0.01	-0.04
32	1	0.03	-0.02	-0.02
33	6	0.06	0.01	-0.03
34	1	0.07	0.01	-0.03
35	1	0.06	0.01	-0.01
36	6	0.05	0.01	-0.02
37	1	0.04	0.01	-0.02
38	1	0.05	0.01	-0.02
39	6	0.04	0.00	-0.02
40	14	0.02	0.01	-0.02
41	6	0.00	-0.02	-0.01
42	1	0.00	0.00	0.00
43	1	0.01	-0.04	-0.03
44	1	-0.02	-0.03	0.00
45	6	0.01	0.02	-0.01
46	1	0.01	0.03	-0.01
47	1	0.00	0.02	-0.01
48	1	0.02	0.03	-0.01
49	6	0.03	0.01	-0.02
50	1	0.03	0.01	-0.01
51	1	0.03	0.01	-0.02
52	1	0.04	0.01	-0.02
53	14	0.02	-0.01	-0.01
54	6	0.01	-0.06	0.00
55	1	0.04	-0.10	0.08
56	1	0.02	-0.01	-0.02
57	1	-0.03	-0.13	-0.04

58	6	0.06	0.01	-0.02
59	1	0.07	0.05	-0.02
60	1	0.03	-0.01	-0.02
61	1	0.11	-0.01	-0.02
62	6	-0.01	0.01	-0.02
63	1	-0.03	0.01	-0.02
64	1	-0.02	0.00	-0.02
65	1	-0.01	0.03	-0.02
66	6	-0.05	-0.01	-0.05
67	14	-0.04	0.00	-0.04
68	6	-0.01	-0.01	-0.04
69	1	0.00	-0.01	-0.04
70	1	-0.01	-0.01	-0.02
71	1	-0.01	-0.01	-0.05
72	6	-0.03	0.00	-0.05
73	1	-0.03	0.00	-0.04
74	1	-0.03	0.00	-0.04
75	1	-0.03	0.00	-0.05
76	6	-0.04	0.00	-0.02
77	1	-0.05	-0.01	-0.02
78	1	-0.03	0.00	-0.01
79	1	-0.04	0.00	-0.02
80	14	-0.03	-0.01	-0.04
81	6	-0.03	-0.01	-0.04
82	1	-0.02	-0.01	-0.04
83	1	-0.02	-0.01	-0.05
84	1	-0.03	0.00	-0.04
85	6	-0.03	0.00	-0.02
86	1	-0.01	0.01	-0.03
87	1	-0.04	-0.01	-0.03
88	1	-0.03	0.00	-0.01
89	6	-0.01	0.00	-0.04
90	1	0.02	-0.03	-0.03
91	1	0.01	0.04	-0.02
92	1	-0.04	0.00	-0.05
93	6	-0.06	0.00	-0.04
94	1	-0.07	-0.01	-0.04
95	1	-0.06	-0.01	-0.03
96	6	-0.05	0.00	-0.03
97	1	-0.04	-0.01	-0.03

98	1	-0.05	0.00	-0.04
99	6	-0.04	0.00	-0.02
100	14	-0.02	0.00	-0.02
101	6	-0.02	0.00	0.00
102	1	-0.02	0.01	0.01
103	1	-0.02	0.00	0.00
104	1	-0.01	0.00	0.00
105	6	-0.01	-0.01	-0.02
106	1	-0.01	-0.01	-0.02
107	1	-0.01	-0.01	-0.02
108	1	-0.02	-0.01	-0.02
109	6	-0.01	-0.01	-0.02
110	1	-0.01	-0.02	-0.03
111	1	-0.02	0.00	-0.01
112	1	0.01	-0.01	-0.02
113	14	-0.03	0.01	-0.02
114	6	-0.02	-0.02	-0.02
115	1	-0.01	-0.03	-0.01
116	1	-0.02	-0.01	-0.02
117	1	-0.03	-0.03	-0.03
118	6	-0.01	0.03	0.00
119	1	-0.02	0.04	0.00
120	1	-0.02	0.03	0.00
121	1	0.00	0.02	0.00
122	6	-0.07	0.01	-0.02
123	1	-0.10	-0.04	-0.01
124	1	-0.02	0.01	-0.02
125	1	-0.11	0.06	-0.02
126	1	0.05	-0.03	0.30
127	1	-0.07	0.00	0.21
128	1	0.06	-0.14	0.19
129	1	-0.05	-0.14	0.19

C=C=C (pro)

Atomic Atomic Coordinates (Angstroms)
Number Type X Y Z

6	0	0.719524	0.287825	-1.516815
6	0	-0.697125	-0.292521	-1.524162
6	0	-1.274116	0.178658	-0.154112
6	0	-0.005416	0.004175	0.785579
6	0	1.276504	-0.176752	-0.136447
6	0	2.610426	0.680037	0.417846
14	0	2.634133	1.652224	2.158918
6	0	2.026051	0.678048	3.672917
1	0	2.045678	1.364748	4.531936
1	0	1.011098	0.297605	3.554321
1	0	2.686441	-0.162276	3.914703
6	0	4.471498	1.986273	2.596578
1	0	4.982621	2.646027	1.886399
1	0	4.478311	2.494289	3.572576
1	0	5.064923	1.070418	2.704259
6	0	1.862673	3.386434	2.274810
1	0	0.973300	3.527142	1.666911
1	0	1.574496	3.559045	3.319999
1	0	2.588735	4.157904	1.999438
14	0	3.550527	1.875860	-0.928409
6	0	3.211735	1.716844	-2.805945
1	0	3.358292	0.702536	-3.190343
1	0	2.224518	2.065022	-3.119034
1	0	3.959500	2.358811	-3.295097
6	0	3.390099	3.751625	-0.594061
1	0	4.044407	4.072601	0.225125
1	0	3.716080	4.278432	-1.502168
1	0	2.377597	4.091383	-0.362178
6	0	5.440675	1.559358	-0.873827
1	0	5.912574	2.299293	-1.537055
1	0	5.887500	1.677408	0.118759
1	0	5.709080	0.564969	-1.253643
6	0	3.662855	-0.452761	0.690484
1	0	3.461764	-0.953873	1.646677
1	0	4.686674	-0.081479	0.742784
6	0	3.447547	-1.433073	-0.446471
1	0	4.082663	-2.317644	-0.367353
1	0	3.699046	-0.946825	-1.400584
6	0	1.920196	-1.787263	-0.366085
14	0	1.839158	-3.141622	1.117216

6	0	0.861614	-4.725704	0.666849
1	0	0.723393	-5.301163	1.593208
1	0	-0.126627	-4.568123	0.230841
1	0	1.431452	-5.355506	-0.026387
6	0	3.575833	-3.860375	1.500378
1	0	3.440089	-4.584424	2.317837
1	0	4.030177	-4.399330	0.661068
1	0	4.291443	-3.107111	1.850790
6	0	1.247539	-2.520013	2.808457
1	0	2.094037	-2.115149	3.372512
1	0	0.491209	-1.737267	2.734440
1	0	0.840075	-3.361546	3.382774
14	0	1.656674	-2.800780	-2.081624
6	0	0.043878	-3.785845	-2.366702
1	0	-0.799915	-3.476794	-1.748641
1	0	-0.258022	-3.668757	-3.416768
1	0	0.208080	-4.854505	-2.187207
6	0	1.922581	-1.857667	-3.725321
1	0	2.807900	-1.212162	-3.733734
1	0	2.082562	-2.629722	-4.493041
1	0	1.056100	-1.264175	-4.037728
6	0	3.063518	-4.095967	-2.171164
1	0	3.140460	-4.747852	-1.296221
1	0	2.865837	-4.738516	-3.041703
1	0	4.041013	-3.623284	-2.329779
6	0	-2.616421	-0.678575	0.382334
14	0	-2.683780	-1.615670	2.143680
6	0	-2.130368	-0.604549	3.654051
1	0	-2.169084	-1.273714	4.526118
1	0	-1.115979	-0.216542	3.558008
1	0	-2.806114	0.233263	3.859216
6	0	-4.529905	-1.958431	2.535621
1	0	-5.011094	-2.645837	1.831036
1	0	-4.560294	-2.437365	3.525783
1	0	-5.137324	-1.047661	2.598020
6	0	-1.903198	-3.339630	2.325542
1	0	-2.612658	-4.123647	2.042452
1	0	-0.991606	-3.486057	1.753728
1	0	-1.651769	-3.485390	3.384378
14	0	-3.506626	-1.907839	-0.966240

6	0	-3.292180	-3.775746	-0.616984
1	0	-3.583316	-4.319379	-1.526951
1	0	-2.274070	-4.081277	-0.362610
1	0	-3.951243	-4.112040	0.192262
6	0	-5.405830	-1.648968	-0.934588
1	0	-5.847187	-2.409927	-1.595170
1	0	-5.860067	-1.770738	0.053957
1	0	-5.700332	-0.667299	-1.328079
6	0	-3.156361	-1.743796	-2.841734
1	0	-3.333026	-0.735334	-3.230056
1	0	-2.156160	-2.060210	-3.146478
1	0	-3.879039	-2.410900	-3.335096
6	0	-3.686207	0.449605	0.602717
1	0	-3.523465	0.962918	1.559570
1	0	-4.708548	0.071006	0.622749
6	0	-3.438101	1.419952	-0.536200
1	0	-4.081623	2.300649	-0.487454
1	0	-3.653088	0.922570	-1.493661
6	0	-1.916774	1.785250	-0.405398
14	0	-1.895022	3.148299	1.074895
6	0	-0.950650	4.756099	0.638429
1	0	0.051452	4.623575	0.226921
1	0	-1.520592	5.368177	-0.070329
1	0	-0.849972	5.338161	1.565612
6	0	-3.655722	3.825245	1.423501
1	0	-3.553222	4.554968	2.240776
1	0	-4.107307	4.350253	0.573777
1	0	-4.359270	3.056012	1.763004
6	0	-1.313844	2.554054	2.778696
1	0	-2.157876	2.134586	3.334694
1	0	-0.538535	1.788961	2.721719
1	0	-0.933769	3.409965	3.350727
14	0	-1.597245	2.795117	-2.112682
6	0	-3.016080	4.072020	-2.261169
1	0	-3.140979	4.719850	-1.388556
1	0	-2.790040	4.719769	-3.120806
1	0	-3.978627	3.585708	-2.463647
6	0	0.017317	3.794695	-2.332642
1	0	0.832204	3.504655	-1.667540
1	0	0.373804	3.666696	-3.364020

1	0	-0.168085	4.863762	-2.177312
6	0	-1.782407	1.845072	-3.763482
1	0	-2.657893	1.187618	-3.807790
1	0	-1.919187	2.613217	-4.539603
1	0	-0.895604	1.262360	-4.036567
1	0	-0.637868	-1.384176	-1.529974
1	0	-1.294493	0.000687	-2.379003
1	0	1.328039	-0.011990	-2.361538
1	0	0.662718	1.379905	-1.530406

Si=Si=Si (pro)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.687095	-0.371200	1.615298
6	-0.683817	0.374653	1.614131
14	-1.814170	0.072440	0.069129
14	0.001231	-0.013551	-1.669822
14	1.819010	-0.071967	0.070045
6	3.068713	-1.583829	-0.309334
14	2.618683	-2.608268	-1.902911
6	2.851116	-1.656539	-3.534561
1	2.632678	-2.353898	-4.357068
1	2.175449	-0.803386	-3.637597
1	3.882934	-1.308144	-3.673240
6	3.706934	-4.157350	-2.169048
1	3.663421	-4.891064	-1.357896
1	3.365942	-4.658547	-3.086872
1	4.759509	-3.883660	-2.322881
6	0.804863	-3.190957	-1.815416
1	0.169243	-2.522028	-1.207982
1	0.362696	-3.250605	-2.817504
1	0.727167	-4.181398	-1.350642
14	3.371437	-2.842915	1.171015
6	3.324716	-2.178010	2.957584
1	4.013471	-1.345758	3.130810
1	2.325905	-1.869301	3.280892

1	3.641190	-3.004035	3.611937
6	2.131542	-4.292591	1.185116
1	2.235905	-4.959000	0.322202
1	2.315835	-4.893394	2.087385
1	1.090194	-3.954731	1.228946
6	5.129753	-3.579487	1.028664
1	5.210688	-4.432452	1.718199
1	5.380308	-3.938095	0.025392
1	5.892732	-2.848081	1.327834
6	4.411901	-0.791679	-0.570065
1	4.426515	-0.389417	-1.592581
1	5.289959	-1.445701	-0.484836
6	4.514432	0.385581	0.420372
1	5.439546	0.951459	0.255292
1	4.581532	-0.024697	1.436711
6	3.236403	1.322793	0.292563
14	3.540839	2.525968	-1.242061
6	2.707514	4.234625	-1.072481
1	2.986097	4.828033	-1.955558
1	1.615304	4.167285	-1.060014
1	3.026132	4.794618	-0.187286
6	5.411774	2.856681	-1.452506
1	5.541291	3.612317	-2.240853
1	5.893234	3.237278	-0.545326
1	5.951626	1.956105	-1.773708
6	2.990468	1.896157	-2.951045
1	3.591097	1.048322	-3.295687
1	1.937064	1.596775	-2.999423
1	3.135928	2.715087	-3.671358
14	3.190788	2.401561	1.921843
6	1.609579	3.430555	2.158308
1	0.787106	2.811554	2.534140
1	1.798360	4.210932	2.909361
1	1.276966	3.928476	1.242840
6	3.421159	1.418642	3.540944
1	4.401235	0.928008	3.594146
1	3.379051	2.143368	4.367657
1	2.653273	0.663512	3.729980
6	4.687237	3.593184	1.971984
1	4.681329	4.362747	1.193068

1	4.684824	4.107221	2.944182
1	5.635517	3.044051	1.897339
6	-3.062978	1.586638	-0.306988
14	-2.629160	2.618921	-1.901258
6	-2.852391	1.661257	-3.530507
1	-2.638722	2.356461	-4.355954
1	-2.170549	0.812263	-3.629860
1	-3.881103	1.303869	-3.668771
6	-3.742553	4.152061	-2.154937
1	-3.694381	4.888638	-1.346490
1	-3.423872	4.654710	-3.079825
1	-4.793900	3.863958	-2.289384
6	-0.830547	3.242214	-1.844672
1	-0.707225	4.060933	-1.128118
1	-0.106652	2.458054	-1.559203
1	-0.520693	3.602734	-2.834516
14	-3.377367	2.836986	1.180679
6	-2.150410	4.297307	1.215825
1	-2.353278	4.890392	2.119229
1	-1.106504	3.969083	1.273498
1	-2.250779	4.968636	0.356151
6	-5.139343	3.564831	1.036078
1	-5.229970	4.406441	1.738194
1	-5.384097	3.937815	0.036730
1	-5.900515	2.824807	1.317969
6	-3.333957	2.163815	2.964020
1	-4.021299	1.329760	3.132350
1	-2.335254	1.856129	3.289001
1	-3.654272	2.986852	3.620288
6	-4.404803	0.790522	-0.571243
1	-4.414283	0.386312	-1.592859
1	-5.283968	1.443400	-0.490705
6	-4.509048	-0.385989	0.420392
1	-5.434027	-0.951847	0.254060
1	-4.577479	0.024195	1.436652
6	-3.231292	-1.322682	0.293145
14	-3.537424	-2.527418	-1.240392
6	-2.693085	-4.230984	-1.074094
1	-1.601423	-4.157627	-1.082772
1	-2.991836	-4.785957	-0.178988

1	-2.985229	-4.832274	-1.947322
6	-5.407437	-2.870120	-1.440822
1	-5.535400	-3.625706	-2.229498
1	-5.882094	-3.255096	-0.532071
1	-5.955014	-1.973061	-1.758724
6	-3.004242	-1.892986	-2.953461
1	-3.621063	-1.055841	-3.296761
1	-1.956424	-1.575607	-3.006744
1	-3.139779	-2.715519	-3.671598
14	-3.175882	-2.402248	1.921786
6	-4.657965	-3.611384	1.973434
1	-4.641555	-4.383231	1.196962
1	-4.650231	-4.122416	2.947249
1	-5.612756	-3.074045	1.896118
6	-1.581745	-3.412180	2.154283
1	-0.773733	-2.787967	2.552508
1	-1.765380	-4.211994	2.885912
1	-1.230684	-3.884642	1.232244
6	-3.414579	-1.424624	3.542619
1	-4.399802	-0.944663	3.598372
1	-3.363626	-2.150744	4.367693
1	-2.654214	-0.661975	3.731974
1	-0.502220	1.458814	1.646844
1	-1.216529	0.133894	2.542172
1	1.218620	-0.129533	2.543499
1	0.503138	-1.454851	1.650269

Si=Ge=Si (pro)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.691061	-0.372925	1.651224
6	-0.681046	0.374083	1.650157
14	-1.836113	0.063657	0.121578
32	0.001149	-0.024884	-1.708218
14	1.845274	-0.065364	0.121462
6	3.096885	-1.581191	-0.247225

14	2.646205	-2.596688	-1.845902
6	2.902631	-1.643866	-3.474997
1	2.678852	-2.335915	-4.300550
1	2.244119	-0.778210	-3.585195
1	3.940961	-1.312064	-3.605009
6	3.712763	-4.159563	-2.116860
1	3.654370	-4.897746	-1.310638
1	3.370498	-4.650186	-3.039942
1	4.769850	-3.899370	-2.262618
6	0.821545	-3.157298	-1.776801
1	0.191193	-2.505096	-1.145229
1	0.379397	-3.189244	-2.780623
1	0.734449	-4.159935	-1.339582
14	3.384869	-2.848278	1.226051
6	3.343466	-2.190124	3.014546
1	4.045460	-1.369904	3.191755
1	2.348680	-1.865500	3.335191
1	3.644083	-3.023279	3.667498
6	2.125962	-4.282310	1.230725
1	2.227570	-4.949710	0.368100
1	2.295518	-4.886076	2.133881
1	1.088875	-3.930540	1.267371
6	5.134216	-3.606143	1.082122
1	5.204168	-4.465518	1.764977
1	5.382693	-3.959707	0.076578
1	5.905367	-2.886201	1.388177
6	4.442134	-0.789493	-0.499403
1	4.461187	-0.383622	-1.520527
1	5.320040	-1.443888	-0.413032
6	4.543349	0.385676	0.495537
1	5.467634	0.953456	0.330274
1	4.613700	-0.028942	1.509762
6	3.263157	1.320957	0.377041
14	3.557211	2.543907	-1.140351
6	2.691383	4.234615	-0.952703
1	2.955673	4.845491	-1.828179
1	1.600363	4.144359	-0.939070
1	2.999406	4.789113	-0.060306
6	5.423184	2.902267	-1.347043
1	5.544605	3.668473	-2.126451

1	5.900131	3.277130	-0.435339
1	5.973300	2.011521	-1.678338
6	3.022426	1.929036	-2.861028
1	3.613394	1.073067	-3.202169
1	1.964297	1.649560	-2.927535
1	3.191147	2.749565	-3.574617
14	3.205010	2.380109	2.018884
6	1.612132	3.387998	2.273559
1	0.799729	2.755894	2.649760
1	1.797786	4.163820	3.030362
1	1.266191	3.890853	1.365556
6	3.446386	1.379159	3.624859
1	4.432110	0.899465	3.672983
1	3.394287	2.092062	4.461334
1	2.687071	0.612415	3.801631
6	4.685094	3.591567	2.083638
1	4.664063	4.374455	1.318030
1	4.679857	4.088928	3.064541
1	5.640860	3.057641	1.994972
6	-3.081503	1.585716	-0.247531
14	-2.647020	2.606050	-1.848812
6	-2.888480	1.643603	-3.474540
1	-2.672211	2.334183	-4.303184
1	-2.219583	0.784915	-3.580328
1	-3.922195	1.298007	-3.604845
6	-3.746756	4.147400	-2.111394
1	-3.685988	4.892023	-1.311031
1	-3.430607	4.637405	-3.043921
1	-4.801678	3.867547	-2.234795
6	-0.842072	3.220088	-1.814513
1	-0.717207	4.059726	-1.120965
1	-0.113339	2.449353	-1.501869
1	-0.535258	3.555072	-2.815404
14	-3.381216	2.846218	1.232014
6	-2.145559	4.300209	1.248263
1	-2.338190	4.901100	2.148773
1	-1.103278	3.965359	1.301177
1	-2.247661	4.966308	0.384540
6	-5.140094	3.583135	1.093780
1	-5.222710	4.430014	1.790591

1	-5.389156	3.950324	0.093337
1	-5.903265	2.848780	1.385094
6	-3.330052	2.184815	3.019062
1	-4.026493	1.360328	3.197427
1	-2.332472	1.866264	3.336828
1	-3.634175	3.015578	3.673385
6	-4.427359	0.793979	-0.503709
1	-4.440663	0.383947	-1.523083
1	-5.304350	1.450274	-0.425123
6	-4.535550	-0.377515	0.494824
1	-5.462226	-0.941449	0.329525
1	-4.605551	0.039579	1.508072
6	-3.259683	-1.317990	0.378921
14	-3.561020	-2.541265	-1.137680
6	-2.689636	-4.229805	-0.957060
1	-1.598750	-4.138328	-0.952201
1	-2.989941	-4.783994	-0.061891
1	-2.960524	-4.841540	-1.829907
6	-5.427412	-2.906292	-1.330648
1	-5.550694	-3.673580	-2.108745
1	-5.897692	-3.282097	-0.416009
1	-5.982762	-2.017979	-1.659747
6	-3.046459	-1.922673	-2.863319
1	-3.652213	-1.075004	-3.199985
1	-1.993123	-1.628153	-2.938367
1	-3.210632	-2.746107	-3.574664
14	-3.201047	-2.377076	2.020543
6	-4.677421	-3.592678	2.088480
1	-4.652946	-4.378456	1.325937
1	-4.670315	-4.086293	3.071260
1	-5.635201	-3.062862	1.997656
6	-1.606241	-3.382393	2.271118
1	-0.795452	-2.750587	2.651318
1	-1.790105	-4.163252	3.023292
1	-1.258885	-3.879221	1.360219
6	-3.441403	-1.377231	3.627172
1	-4.426926	-0.897192	3.676390
1	-3.389068	-2.090938	4.462908
1	-2.681463	-0.611133	3.803950
1	-0.497652	1.458343	1.673366

1	-1.206097	0.141792	2.585479
1	1.215936	-0.138239	2.585959
1	0.506611	-1.456782	1.678215

Ge=Si=Ge (pro)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.684544	-0.368040	1.686604
6	-0.679876	0.372510	1.685778
32	-1.825156	0.063721	0.063403
14	0.000737	-0.016458	-1.727072
32	1.831097	-0.063011	0.063930
6	3.137523	-1.618601	-0.318594
14	2.660938	-2.631963	-1.908697
6	2.885610	-1.674165	-3.538174
1	2.661557	-2.367352	-4.362577
1	2.209949	-0.819817	-3.634953
1	3.916307	-1.324822	-3.681621
6	3.731335	-4.191197	-2.182575
1	3.681535	-4.924191	-1.370731
1	3.385058	-4.689115	-3.099999
1	4.786181	-3.926278	-2.336182
6	0.839332	-3.197066	-1.816268
1	0.210049	-2.518159	-1.213142
1	0.398375	-3.256798	-2.819198
1	0.748679	-4.184502	-1.347355
14	3.423596	-2.861471	1.169138
6	3.377757	-2.177243	2.948585
1	4.065126	-1.342141	3.113662
1	2.378177	-1.866103	3.267982
1	3.693825	-2.995600	3.612684
6	2.161443	-4.291822	1.191778
1	2.256312	-4.964981	0.332903
1	2.333674	-4.889981	2.098044
1	1.125219	-3.936449	1.230950
6	5.174034	-3.614939	1.029378

1	5.252931	-4.463837	1.723828
1	5.416647	-3.980485	0.026456
1	5.942708	-2.885863	1.319606
6	4.462438	-0.798312	-0.576840
1	4.471380	-0.401673	-1.601804
1	5.351500	-1.438052	-0.488891
6	4.569047	0.390698	0.407405
1	5.503976	0.939798	0.235241
1	4.634821	-0.014665	1.425896
6	3.315764	1.357742	0.288012
14	3.592267	2.547199	-1.252078
6	2.725834	4.239009	-1.084869
1	2.991970	4.839506	-1.966830
1	1.634574	4.146997	-1.074439
1	3.030159	4.805053	-0.198515
6	5.457957	2.893469	-1.470528
1	5.583842	3.647258	-2.260898
1	5.937492	3.277454	-0.563725
1	6.001267	1.993839	-1.788808
6	3.032873	1.897735	-2.951135
1	3.632786	1.048685	-3.294359
1	1.979905	1.593820	-2.985867
1	3.166361	2.710169	-3.681066
14	3.249202	2.426604	1.919049
6	1.646705	3.426455	2.149795
1	0.838946	2.794749	2.537216
1	1.821638	4.219594	2.890949
1	1.297789	3.906811	1.230662
6	3.481326	1.434357	3.531751
1	4.464301	0.949736	3.586341
1	3.428429	2.150982	4.364917
1	2.717753	0.671917	3.709600
6	4.725632	3.640740	1.975959
1	4.705945	4.411074	1.197676
1	4.717460	4.152807	2.949015
1	5.681357	3.105014	1.897399
6	-3.130498	1.621874	-0.317249
14	-2.668903	2.640955	-1.909017
6	-2.885719	1.677288	-3.535940
1	-2.667431	2.368566	-4.363377

1	-2.203837	0.827220	-3.630089
1	-3.913469	1.318940	-3.678010
6	-3.761699	4.186632	-2.171878
1	-3.704672	4.924114	-1.364375
1	-3.438150	4.683561	-3.097933
1	-4.816190	3.909082	-2.304014
6	-0.860762	3.242576	-1.848326
1	-0.722899	4.056047	-1.128308
1	-0.146118	2.447260	-1.568530
1	-0.549093	3.603888	-2.837443
14	-3.427895	2.856701	1.177197
6	-2.180306	4.299295	1.217707
1	-2.373280	4.893704	2.122300
1	-1.141192	3.954065	1.274371
1	-2.269401	4.973821	0.359203
6	-5.183787	3.597917	1.038527
1	-5.272355	4.436295	1.744463
1	-5.424269	3.975752	0.039788
1	-5.948295	2.859160	1.314794
6	-3.381622	2.165248	2.953781
1	-4.066790	1.327927	3.115640
1	-2.381526	1.856243	3.273474
1	-3.700972	2.980651	3.619938
6	-4.454383	0.798573	-0.578707
1	-4.458866	0.400056	-1.602808
1	-5.344176	1.437737	-0.495229
6	-4.563300	-0.389505	0.406666
1	-5.498564	-0.937684	0.233228
1	-4.630373	0.015914	1.424976
6	-3.310815	-1.357016	0.288318
14	-3.590217	-2.548099	-1.250891
6	-2.717275	-4.237017	-1.087846
1	-1.626338	-4.143151	-1.092096
1	-3.008714	-4.799657	-0.195142
1	-2.993954	-4.841977	-1.963528
6	-5.455634	-2.903173	-1.458665
1	-5.581556	-3.657717	-2.248354
1	-5.928623	-3.289624	-0.549553
1	-6.005281	-2.006571	-1.774522
6	-3.045997	-1.896094	-2.954006

1	-3.656791	-1.053608	-3.294749
1	-1.996492	-1.581377	-2.994616
1	-3.175935	-2.710780	-3.682068
14	-3.239149	-2.426737	1.918589
6	-4.706145	-3.651885	1.978484
1	-4.679976	-4.424489	1.202722
1	-4.692780	-4.160902	2.953105
1	-5.666532	-3.124925	1.898876
6	-1.629566	-3.416049	2.144154
1	-0.831864	-2.784322	2.551732
1	-1.802027	-4.226448	2.866886
1	-1.267663	-3.873466	1.218369
6	-3.475195	-1.438020	3.532728
1	-4.461745	-0.961047	3.590162
1	-3.414985	-2.155401	4.364748
1	-2.717024	-0.670110	3.709868
1	-0.512025	1.457867	1.726123
1	-1.237930	0.113027	2.592762
1	1.242235	-0.108015	2.593588
1	0.514312	-1.452835	1.728994

Ge=Ge=Ge (pro)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.693653	-0.351778	1.731593
6	-0.693607	0.351499	1.731776
32	-1.869738	0.059312	0.112100
32	-0.000025	-0.000227	-1.771318
32	1.869844	-0.059150	0.112099
6	3.172598	-1.646556	-0.228555
14	2.692455	-2.676606	-1.806217
6	2.966753	-1.748229	-3.446374
1	2.714410	-2.438520	-4.264896
1	2.338179	-0.860494	-3.560668
1	4.014339	-1.451294	-3.586186
6	3.713927	-4.273664	-2.052388

1	3.630058	-4.995407	-1.233244
1	3.359992	-4.769802	-2.967947
1	4.778802	-4.047297	-2.197707
6	0.853730	-3.192556	-1.739130
1	0.223712	-2.479459	-1.177100
1	0.438170	-3.286228	-2.750632
1	0.728094	-4.157972	-1.233572
14	3.439274	-2.871212	1.276306
6	3.427507	-2.154473	3.042650
1	4.157377	-1.352833	3.190983
1	2.444908	-1.787084	3.355137
1	3.702577	-2.974642	3.722624
6	2.138816	-4.265686	1.330033
1	2.204293	-4.950656	0.477783
1	2.304518	-4.859028	2.240693
1	1.113443	-3.880838	1.376889
6	5.167992	-3.676859	1.140112
1	5.227067	-4.513875	1.850992
1	5.394402	-4.069448	0.143729
1	5.959830	-2.965439	1.411419
6	4.508943	-0.846196	-0.490420
1	4.528794	-0.464348	-1.520504
1	5.390319	-1.495326	-0.388616
6	4.628802	0.355653	0.477686
1	5.573180	0.887555	0.298411
1	4.688722	-0.036104	1.501517
6	3.391219	1.338604	0.343583
14	3.694949	2.512012	-1.201231
6	2.777213	4.180469	-1.086615
1	3.041984	4.773224	-1.974185
1	1.688915	4.056604	-1.093213
1	3.047752	4.771328	-0.205368
6	5.558036	2.903619	-1.369554
1	5.687190	3.656954	-2.160114
1	6.004133	3.303449	-0.452930
1	6.132499	2.016932	-1.669038
6	3.213830	1.825045	-2.910028
1	3.825443	0.965219	-3.202702
1	2.160992	1.527786	-2.985115
1	3.386638	2.618792	-3.651975

14	3.311868	2.423987	1.962156
6	1.685261	3.387799	2.172994
1	0.893024	2.744509	2.573442
1	1.837492	4.203111	2.894608
1	1.326675	3.836386	1.241255
6	3.564897	1.441539	3.576872
1	4.567132	0.998380	3.639675
1	3.473294	2.151634	4.412123
1	2.833208	0.645793	3.742143
6	4.752074	3.682158	2.024347
1	4.704659	4.459775	1.254236
1	4.727113	4.184523	3.002353
1	5.726030	3.181631	1.940376
6	-3.172578	1.646759	-0.228554
14	-2.692715	2.676766	-1.806406
6	-2.966306	1.747528	-3.446159
1	-2.713640	2.437285	-4.265038
1	-2.337556	0.859815	-3.559505
1	-4.013770	1.450368	-3.586312
6	-3.714605	4.273509	-2.052865
1	-3.630863	4.995200	-1.233677
1	-3.360651	4.769697	-2.968383
1	-4.779417	4.046947	-2.198262
6	-0.854245	3.193490	-1.739688
1	-0.728459	4.157641	-1.231638
1	-0.223162	2.479080	-1.180416
1	-0.439799	3.290020	-2.751458
14	-3.439380	2.871531	1.276266
6	-2.139053	4.266086	1.330022
1	-2.304867	4.859484	2.240622
1	-1.113655	3.881378	1.376952
1	-2.204578	4.950992	0.477739
6	-5.168059	3.677131	1.139732
1	-5.227527	4.513767	1.851023
1	-5.393940	4.070233	0.143442
1	-5.960024	2.965576	1.410258
6	-3.427745	2.154681	3.042530
1	-4.157768	1.353194	3.190814
1	-2.445229	1.787080	3.354934
1	-3.702619	2.974822	3.722628

6	-4.509019	0.846310	-0.490429
1	-4.528995	0.464631	-1.520539
1	-5.390447	1.495326	-0.388407
6	-4.628800	-0.355772	0.477494
1	-5.573085	-0.887762	0.298010
1	-4.688971	0.035868	1.501342
6	-3.390993	-1.338571	0.343434
14	-3.694480	-2.512330	-1.201307
6	-2.776837	-4.180799	-1.086048
1	-1.688537	-4.056879	-1.090671
1	-3.048837	-4.772314	-0.205670
1	-3.040004	-4.773063	-1.974432
6	-5.557553	-2.903850	-1.369924
1	-5.686546	-3.658000	-2.159743
1	-6.004088	-3.302666	-0.453078
1	-6.131780	-2.017411	-1.670557
6	-3.213096	-1.825863	-2.910222
1	-3.824048	-0.965539	-3.202724
1	-2.160018	-1.529617	-2.985729
1	-3.386868	-2.619517	-3.652060
14	-3.311959	-2.423849	1.962236
6	-4.752197	-3.682008	2.024384
1	-4.704703	-4.459631	1.254286
1	-4.727277	-4.184379	3.002396
1	-5.726166	-3.181540	1.940352
6	-1.685610	-3.387853	2.173759
1	-0.892601	-2.744102	2.571908
1	-1.837599	-4.201375	2.897472
1	-1.328199	-3.838889	1.242752
6	-3.565197	-1.441112	3.576749
1	-4.567573	-0.998319	3.639594
1	-3.473244	-2.150992	4.412154
1	-2.833794	-0.645087	3.741784
1	-0.551832	1.439748	1.793641
1	-1.243487	0.061066	2.636253
1	1.243605	-0.061953	2.636244
1	0.551983	-1.440090	1.792751

Sn=Sn=Sn (pro)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.692431	-0.346346	1.950146
6	-0.692114	0.346193	1.950520
50	-1.933380	0.036204	0.177683
50	-0.000151	-0.000619	-2.025466
50	1.933287	-0.035995	0.177337
6	3.344097	-1.724068	-0.151932
14	2.844326	-2.741886	-1.725994
6	3.133334	-1.808189	-3.364044
1	2.846067	-2.479673	-4.186715
1	2.542590	-0.893076	-3.471934
1	4.189978	-1.548965	-3.510175
6	3.816668	-4.365442	-1.983054
1	3.713583	-5.080016	-1.159392
1	3.443609	-4.854303	-2.894945
1	4.886746	-4.169434	-2.131873
6	0.989651	-3.235140	-1.679341
1	0.359093	-2.529965	-1.108809
1	0.585782	-3.317567	-2.697658
1	0.848272	-4.207314	-1.190603
14	3.564296	-2.925800	1.359531
6	3.529780	-2.167708	3.108308
1	4.262734	-1.367353	3.250949
1	2.543310	-1.782822	3.387030
1	3.779610	-2.970302	3.818213
6	2.211536	-4.272447	1.413669
1	2.255750	-4.969847	0.569733
1	2.341361	-4.861764	2.332620
1	1.201231	-3.844238	1.444443
6	5.272714	-3.771968	1.251958
1	5.320424	-4.594026	1.980370
1	5.487361	-4.187485	0.261897
1	6.076130	-3.066361	1.503942
6	4.657873	-0.874815	-0.401747
1	4.673045	-0.505506	-1.437082

1	5.556521	-1.500460	-0.291023
6	4.789953	0.354806	0.548951
1	5.754118	0.847284	0.354204
1	4.846474	-0.022201	1.579220
6	3.599303	1.399354	0.424507
14	3.871936	2.560496	-1.117754
6	2.871206	4.183296	-1.016975
1	3.101902	4.785076	-1.907954
1	1.789260	3.998193	-1.024478
1	3.102843	4.795048	-0.138420
6	5.721155	2.998578	-1.284014
1	5.842600	3.749965	-2.077179
1	6.152892	3.406845	-0.364282
1	6.310227	2.118561	-1.575761
6	3.408228	1.857227	-2.827668
1	3.980757	0.962937	-3.095940
1	2.342891	1.612332	-2.918746
1	3.628504	2.629488	-3.579666
14	3.473079	2.469644	2.041731
6	1.803089	3.372684	2.225675
1	1.028446	2.693701	2.603052
1	1.907525	4.183985	2.960723
1	1.441328	3.819893	1.294075
6	3.694124	1.464616	3.646494
1	4.694765	1.022519	3.732854
1	3.569595	2.155640	4.493372
1	2.959348	0.663133	3.769083
6	4.865723	3.773984	2.138353
1	4.801988	4.544746	1.361924
1	4.809353	4.279596	3.113169
1	5.856121	3.304400	2.068681
6	-3.344034	1.724346	-0.152143
14	-2.844132	2.741786	-1.726427
6	-3.132560	1.807377	-3.364141
1	-2.845173	2.478485	-4.187070
1	-2.541360	0.892468	-3.471190
1	-4.189039	1.547673	-3.510540
6	-3.816623	4.365197	-1.983987
1	-3.713732	5.079771	-1.160310
1	-3.443343	4.853962	-2.895829

1	-4.886648	4.169082	-2.133043
6	-0.989558	3.235446	-1.680297
1	-0.847905	4.206541	-1.189520
1	-0.357959	2.529167	-1.112270
1	-0.586869	3.320221	-2.698886
14	-3.564438	2.926370	1.359042
6	-2.211707	4.273029	1.413053
1	-2.341688	4.862599	2.331816
1	-1.201400	3.844853	1.444088
1	-2.255841	4.970185	0.568908
6	-5.272775	3.772549	1.250823
1	-5.320943	4.594298	1.979549
1	-5.486682	4.188477	0.260773
1	-6.076387	3.066868	1.501957
6	-3.530130	2.168519	3.107919
1	-4.263304	1.368376	3.250630
1	-2.543755	1.783410	3.386668
1	-3.779749	2.971241	3.817749
6	-4.657691	0.874920	-0.402143
1	-4.672465	0.505500	-1.437433
1	-5.556458	1.500448	-0.291724
6	-4.789938	-0.354678	0.548585
1	-5.754082	-0.847154	0.353688
1	-4.846593	0.022403	1.578832
6	-3.599280	-1.399263	0.424454
14	-3.871405	-2.560834	-1.117651
6	-2.870780	-4.183659	-1.015876
1	-1.788834	-3.998484	-1.022010
1	-3.103414	-4.795718	-0.137775
1	-3.100317	-4.785249	-1.907288
6	-5.720627	-2.998749	-1.284357
1	-5.841800	-3.751135	-2.076614
1	-6.152987	-3.405708	-0.364340
1	-6.309319	-2.118962	-1.577577
6	-3.407223	-1.858575	-2.827862
1	-3.978073	-0.963150	-3.095890
1	-2.341422	-1.615988	-2.919713
1	-3.629609	-2.630503	-3.579585
14	-3.473531	-2.469190	2.041952
6	-4.866158	-3.773540	2.138459

1	-4.802279	-4.544198	1.361943
1	-4.809857	-4.279223	3.113240
1	-5.856572	-3.304002	2.068690
6	-1.803665	-3.372242	2.226625
1	-1.028504	-2.692820	2.602125
1	-1.907896	-4.182059	2.963335
1	-1.442743	-3.821389	1.295650
6	-3.694920	-1.463630	3.646326
1	-4.695778	-1.022015	3.732630
1	-3.569899	-2.154227	4.493477
1	-2.960549	-0.661711	3.768445
1	-0.570107	1.436815	2.027742
1	-1.263862	0.036966	2.836032
1	1.264406	-0.037427	2.835605
1	0.570511	-1.437001	2.026937

Pb=Pb=Pb (pro)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.716778	-0.276670	2.098171
6	-0.716372	0.276200	2.098659
82	-2.010315	0.000827	0.231468
82	-0.000054	-0.002036	-2.038096
82	2.010547	-0.001547	0.230559
6	3.552572	-1.733303	0.050832
14	3.116405	-2.845817	-1.474620
6	3.467872	-1.997120	-3.144982
1	3.192277	-2.694988	-3.949028
1	2.902079	-1.073064	-3.301674
1	4.532857	-1.763067	-3.270356
6	4.110097	-4.476690	-1.583685
1	3.959294	-5.139221	-0.724138
1	3.793783	-5.023315	-2.484003
1	5.187003	-4.284303	-1.678027
6	1.269792	-3.362345	-1.498599
1	0.589467	-2.555776	-1.172797

1	0.976788	-3.667928	-2.512741
1	1.072276	-4.206660	-0.827262
14	3.753619	-2.823820	1.645949
6	3.717593	-1.943420	3.335749
1	4.517850	-1.204048	3.447278
1	2.763105	-1.452996	3.551169
1	3.873132	-2.709510	4.110038
6	2.404228	-4.168088	1.767475
1	2.464197	-4.912552	0.965069
1	2.522545	-4.703821	2.720150
1	1.392046	-3.743014	1.757229
6	5.461534	-3.683777	1.622288
1	5.505352	-4.428162	2.430574
1	5.671229	-4.199816	0.680012
1	6.271048	-2.963144	1.800890
6	4.844953	-0.864463	-0.207418
1	4.892078	-0.561029	-1.261421
1	5.753648	-1.461145	-0.027197
6	4.941497	0.425919	0.669221
1	5.919641	0.894911	0.473108
1	4.965286	0.115801	1.722117
6	3.781084	1.472918	0.443869
14	4.083198	2.524062	-1.163154
6	2.922318	4.034314	-1.262458
1	3.100425	4.555796	-2.213642
1	1.864426	3.739465	-1.244869
1	3.083074	4.757644	-0.455426
6	5.891943	3.138327	-1.223752
1	6.018448	3.802515	-2.090928
1	6.189758	3.695267	-0.329789
1	6.592592	2.301927	-1.350765
6	3.849759	1.642245	-2.838595
1	4.529736	0.795068	-2.977183
1	2.825684	1.284764	-3.001125
1	4.070494	2.371522	-3.632294
14	3.562587	2.631411	1.987519
6	1.819662	3.395015	2.077278
1	1.059132	2.628994	2.270610
1	1.774224	4.118894	2.903481
1	1.544432	3.923635	1.158274

6	3.857556	1.725652	3.637419
1	4.900575	1.401470	3.748607
1	3.645908	2.427747	4.457099
1	3.217205	0.850225	3.780165
6	4.818663	4.073152	2.035771
1	4.703519	4.781905	1.207973
1	4.674044	4.631886	2.972034
1	5.853980	3.707529	2.028756
6	-3.550089	1.734459	0.050399
14	-3.112598	2.843498	-1.476224
6	-3.460553	1.991040	-3.145471
1	-3.183722	2.687403	-3.950310
1	-2.893859	1.066652	-3.298736
1	-4.525452	1.755994	-3.272172
6	-4.106940	4.473629	-1.590593
1	-3.958170	5.137954	-0.731918
1	-3.789060	5.018288	-2.491487
1	-5.183739	4.280150	-1.686562
6	-1.266042	3.360212	-1.497560
1	-1.069897	4.205086	-0.826432
1	-0.586301	2.553825	-1.169807
1	-0.971639	3.664764	-2.511506
14	-3.749456	2.825939	1.644196
6	-2.400030	4.170516	1.762135
1	-2.516883	4.706629	2.714723
1	-1.387802	3.745289	1.750148
1	-2.461773	4.914348	0.959145
6	-5.457792	3.685242	1.622589
1	-5.500188	4.430684	2.429931
1	-5.669220	4.199648	0.679593
1	-6.266719	2.964162	1.803574
6	-3.709677	1.947329	3.334883
1	-4.508982	1.206883	3.448315
1	-2.753988	1.458243	3.548905
1	-3.865034	2.714173	4.108373
6	-4.842231	0.866235	-0.206877
1	-4.888025	0.561388	-1.260883
1	-5.750710	1.464360	-0.028429
6	-4.940152	-0.422086	0.671115
1	-5.919909	-0.889137	0.477181

1	-4.961005	-0.110581	1.724010
6	-3.783082	-1.471392	0.445099
14	-4.087927	-2.520678	-1.162236
6	-2.932923	-4.035528	-1.260815
1	-1.873836	-3.744757	-1.242685
1	-3.097172	-4.757964	-0.453595
1	-3.112802	-4.556289	-2.212047
6	-5.899061	-3.127872	-1.224718
1	-6.027044	-3.791555	-2.092069
1	-6.199941	-3.683492	-0.330774
1	-6.596250	-2.288387	-1.352507
6	-3.849568	-1.639785	-2.837515
1	-4.526406	-0.789707	-2.976468
1	-2.823781	-1.286048	-2.999051
1	-4.072514	-2.368311	-3.631282
14	-3.567147	-2.630082	1.988214
6	-4.828478	-4.067212	2.038012
1	-4.716977	-4.776322	1.209899
1	-4.684688	-4.626308	2.974158
1	-5.862560	-3.697525	2.032192
6	-1.826932	-3.399950	2.075763
1	-1.063622	-2.636539	2.268242
1	-1.783369	-4.123975	2.901875
1	-1.554899	-3.929426	1.156266
6	-3.857018	-1.723380	3.638549
1	-4.898972	-1.395358	3.750619
1	-3.647011	-2.426326	4.457864
1	-3.213326	-0.850014	3.780395
1	-0.717654	1.365264	2.247997
1	-1.298627	-0.169106	2.918583
1	1.298882	0.168964	2.917844
1	0.718134	-1.365564	2.248141

