

Supplementary Materials

Mechanistic Investigations and Molecular Properties of 1,2- Bis(ferrocenyl)dimetallenes Including Group 14 Elements

Hsu-Cheng Hua and Ming-Der Su*

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

*E-mail: midesu@mail.ncyu.edu.tw

Details of the present computational approach are as follows:

All the geometries were fully optimized at the M06-2X/Def2-SVPD level of theory.¹ Frequency calculations were performed on all structures, in order to confirm that the reactants and products had no imaginary frequencies and that the transition states possessed only one imaginary frequency. The relative energies were thus corrected for vibrational zero-point energies (ZPE, not scaled). The thermodynamic corrections to 298 K, ZPE corrections, heat capacity corrections and entropy corrections (ΔS) obtained were applied at the M06-2X/Def2-SVPD level. The relative free energy (ΔG) at 298 K was also calculated at the same level of theory. UV-vis data, Raman data, Nature Bond Orbital (NBO)² and Wiberg bond index³ the natural resonance theory (NRT),⁴ and calculations on the model complexes were performed using the NBO program (Version 3.1) in the GAUSSIAN 09 program package.⁵

References:

- (1) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.
- (2) Glendening, E. D.; Reed, A. E.; Carpenter, J.; Weinhold, F. NBO Version 3.1.
- (3) Wiberg, K. B. *Tetrahedron* **1968**, 1083.
- (4) (a) Glendening, E.D.; Weinhold, F. *J. Comp. Chem.* 1998, *19*, 593. (b) *ibid.*, *J. Comp. Chem.* **1998**, *19*, 610. (c) Glendening, E.D.; Badenhoop, J. K.; Weinhold, F. *J. Comp. Chem.* **1998**, *19*, 628.
- (5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.;

Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, Liashenko, G.; Piskorz, A.; Komaromi, P.; I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S. and Pople, J. A. Gaussian, Inc., Wallingford CT, 2013.

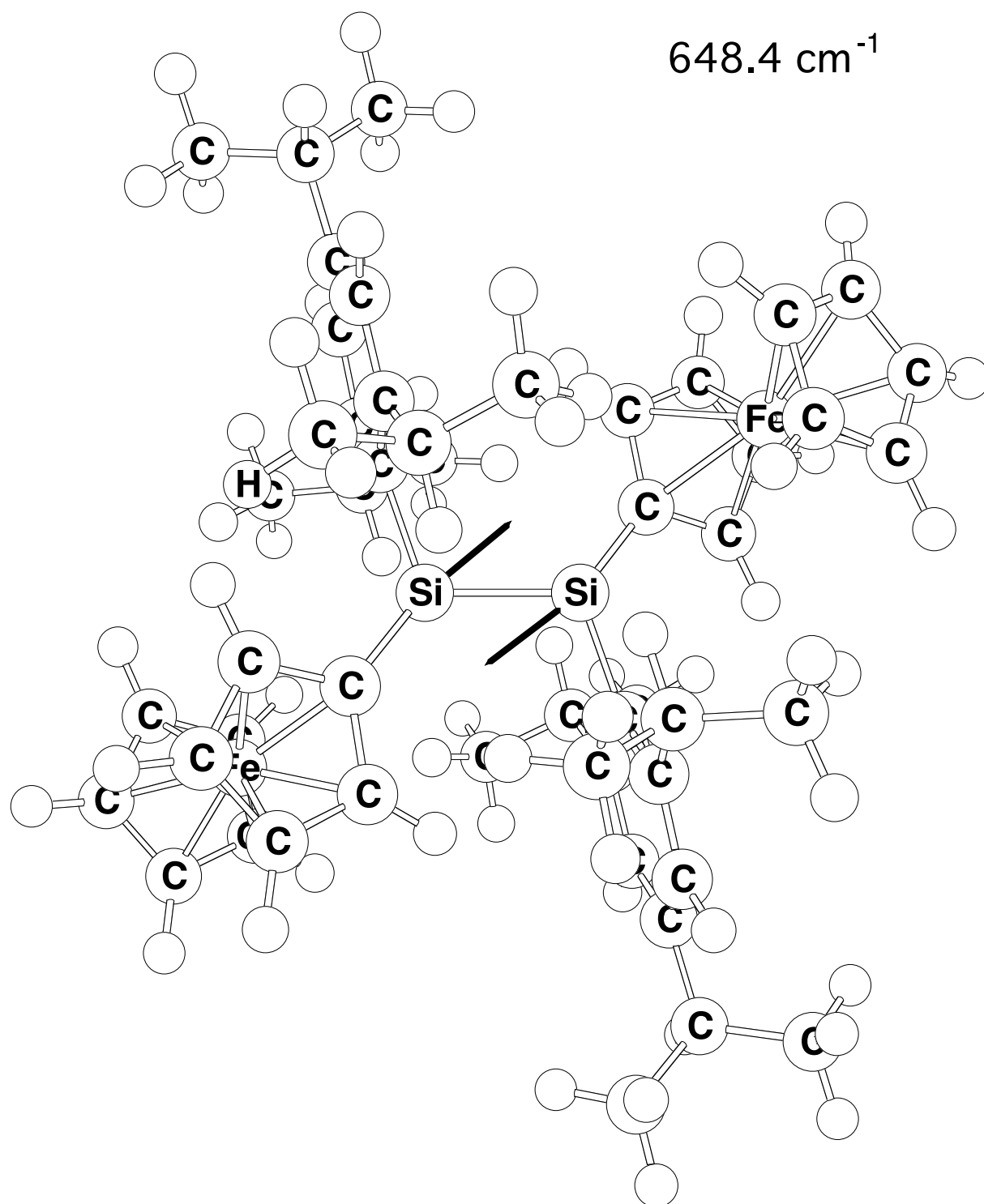


Figure A. Raman Spectra at 648.4 cm^{-1} , computed at the M06-2X/Def2-SVPD level of theory.

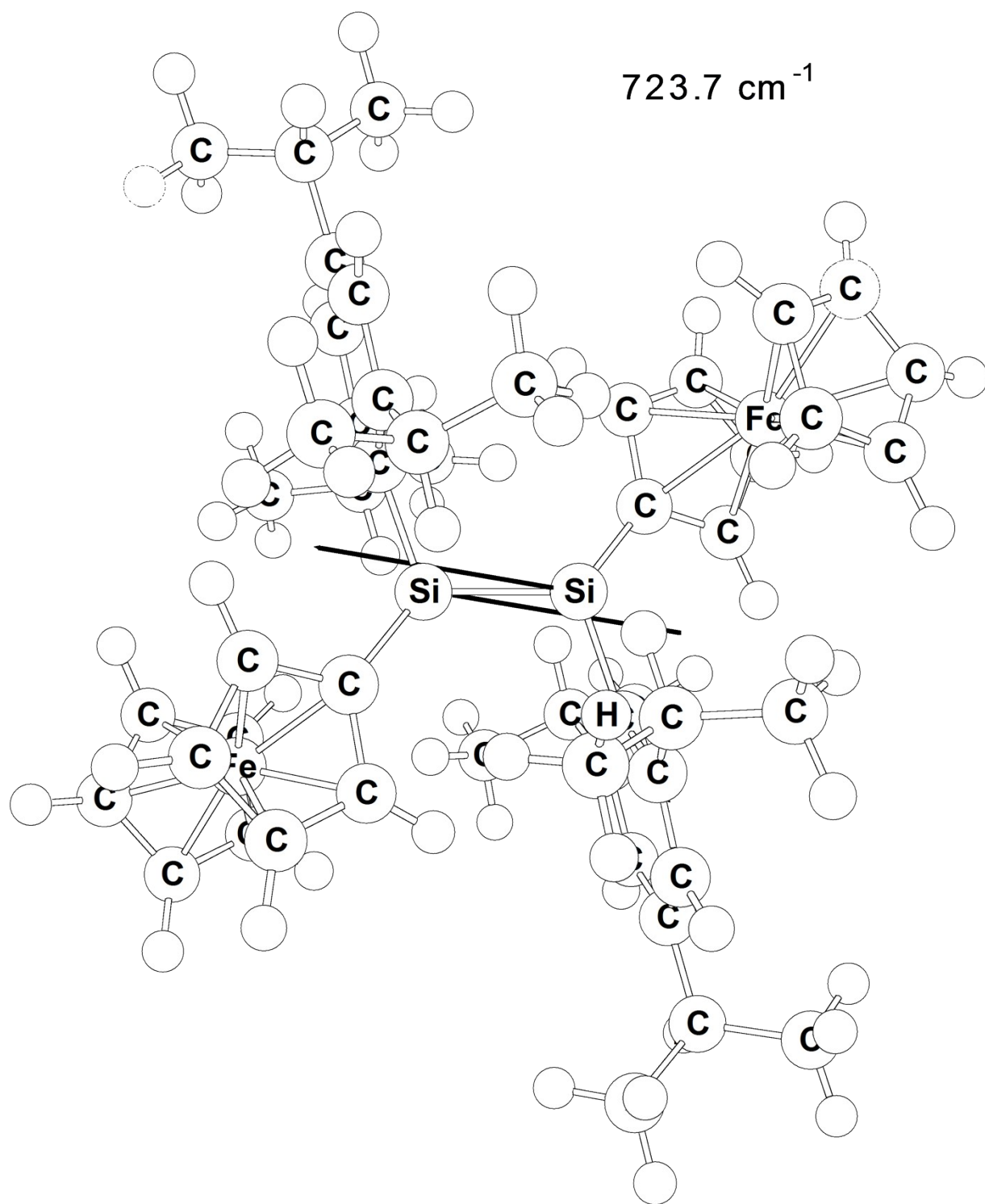


Figure B. Raman Spectra at 723.7 cm^{-1} , computed at the M06-2X/Def2-SVPD level of theory.

(All geometries were calculated M06-2X/Def2-SVPD)

(1) (*E*)-(Tip)(Fc)C=C(Fc)(Tip)-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.075101	-0.669301	-0.339579
6	0.086579	0.664692	0.328727
6	1.112903	-1.576083	-0.358899
6	1.943262	-1.624382	-1.497631
6	1.434882	-2.352220	0.775574
6	3.112870	-2.390013	-1.456368
6	2.616553	-3.097253	0.774362
6	3.479414	-3.118780	-0.324686
1	3.769781	-2.413560	-2.332689
1	2.876521	-3.677506	1.666448
6	-1.100995	1.571736	0.352875
6	-1.427488	2.347370	-0.781250
6	-1.927479	1.621369	1.494783
6	-2.611385	3.088970	-0.777431
6	-3.099286	2.383748	1.455560
6	-3.471679	3.108924	0.323641
1	-2.875637	3.667626	-1.669207
1	-3.753253	2.407648	2.334048
6	1.631531	-0.815087	-2.747060
6	1.624637	-1.666559	-4.019349
6	2.602057	0.362238	-2.867956
1	0.622016	-0.394721	-2.628530
1	0.916483	-2.507780	-3.933512
1	1.320948	-1.052068	-4.884387
1	2.624658	-2.080293	-4.238563
1	2.607279	0.946375	-1.933084
1	3.632785	0.008469	-3.055639
1	2.312031	1.029776	-3.699913
6	4.770831	-3.914739	-0.291350
6	4.511366	-5.410169	-0.081505
6	5.731565	-3.368734	0.770276
1	5.252926	-3.793070	-1.277105
1	3.834321	-5.807782	-0.855249
1	5.456719	-5.978008	-0.121170

1	4.047895	-5.595983	0.903038
1	5.943281	-2.300155	0.599872
1	5.296952	-3.470670	1.780090
1	6.687227	-3.920370	0.754494
6	0.536572	-2.400750	2.005122
6	1.167178	-1.715799	3.223630
6	0.162641	-3.847609	2.346999
1	-0.396705	-1.865047	1.758241
1	1.400902	-0.657765	3.025549
1	0.477538	-1.764351	4.085162
1	2.106531	-2.221104	3.513281
1	-0.317520	-4.343610	1.487521
1	1.053409	-4.435769	2.627589
1	-0.532158	-3.877657	3.204125
6	-1.609489	0.817928	2.746866
6	-2.569510	-0.367586	2.868366
6	-1.614154	1.670447	4.018750
1	-0.595980	0.406399	2.631248
1	-2.567564	-0.952112	1.934011
1	-2.275209	-1.031551	3.701687
1	-3.603523	-0.022254	3.053644
1	-0.917808	2.521610	3.934453
1	-2.619666	2.070560	4.237975
1	-1.302529	1.060015	4.883803
6	-4.765775	3.900688	0.293048
6	-5.727224	3.351768	-0.766401
6	-4.511339	5.396928	0.082927
1	-5.245306	3.777353	1.279849
1	-5.935298	2.282541	-0.595521
1	-6.684560	3.900436	-0.748313
1	-5.295437	3.455128	-1.777278
1	-3.834187	5.796456	0.855595
1	-4.050045	5.584198	-0.902356
1	-5.458356	5.961877	0.124297
6	-0.532087	2.399609	-2.013261
6	-0.179194	3.848870	-2.367686
6	-1.154853	1.700217	-3.227815
1	0.409026	1.878462	-1.764029
1	0.285837	4.362872	-1.510799
1	0.521538	3.880841	-3.219824

1	-1.076967	4.419150	-2.662315
1	-1.366836	0.637976	-3.029045
1	-2.105514	2.186981	-3.512379
1	-0.470574	1.762573	-4.092789
6	1.239720	1.110058	0.993448
6	2.602108	0.579349	1.107646
6	1.254155	2.314254	1.831905
6	3.276699	1.273577	2.138256
1	3.015084	-0.269863	0.569917
6	2.442795	2.337015	2.591374
1	0.417863	3.003409	1.933029
1	4.285154	1.057677	2.489349
1	2.699688	3.073727	3.351723
26	2.939705	2.633350	0.548926
6	4.012677	4.528053	0.449927
6	4.883735	3.487123	0.044227
6	2.913160	4.560518	-0.454629
1	4.143394	5.172177	1.318510
6	4.323129	2.869491	-1.109185
1	5.803807	3.187955	0.544708
6	3.115380	3.546233	-1.427869
1	2.072235	5.251033	-0.407252
1	4.748028	2.027481	-1.653684
1	2.451686	3.311039	-2.257720
6	-1.225278	-1.121874	-0.999214
6	-2.586112	-0.588250	-1.133703
6	-1.241361	-2.345374	-1.811691
6	-3.252643	-1.296005	-2.160491
1	-2.998666	0.273890	-0.616501
6	-2.421264	-2.373972	-2.583903
1	-0.409320	-3.042774	-1.890776
1	-4.255036	-1.079500	-2.528250
1	-2.675223	-3.123646	-3.332561
26	-2.948208	-2.626307	-0.543720
6	-3.149265	-3.524203	1.439030
6	-4.336312	-2.813441	1.116752
6	-2.978039	-4.549701	0.471707
1	-2.478579	-3.305190	2.267637
6	-4.915253	-3.420679	-0.033052
1	-4.735905	-1.955784	1.655935

6	-4.076908	-4.490530	-0.432243
1	-2.158998	-5.266500	0.430447
1	-5.825926	-3.096668	-0.535240
1	-4.227755	-5.136190	-1.296354

(E)-(Tip)(Fc)C=C(Fc)(Tip)-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.075101	-0.669301	-0.339579
6	0.086579	0.664692	0.328727
6	1.112903	-1.576083	-0.358899
6	1.943262	-1.624382	-1.497631
6	1.434882	-2.352220	0.775574
6	3.112870	-2.390013	-1.456368
6	2.616553	-3.097253	0.774362
6	3.479414	-3.118780	-0.324686
1	3.769781	-2.413560	-2.332689
1	2.876521	-3.677506	1.666448
6	-1.100995	1.571736	0.352875
6	-1.427488	2.347370	-0.781250
6	-1.927479	1.621369	1.494783
6	-2.611385	3.088970	-0.777431
6	-3.099286	2.383748	1.455560
6	-3.471679	3.108924	0.323641
1	-2.875637	3.667626	-1.669207
1	-3.753253	2.407648	2.334048
6	1.631531	-0.815087	-2.747060
6	1.624637	-1.666559	-4.019349
6	2.602057	0.362238	-2.867956
1	0.622016	-0.394721	-2.628530
1	0.916483	-2.507780	-3.933512
1	1.320948	-1.052068	-4.884387
1	2.624658	-2.080293	-4.238563
1	2.607279	0.946375	-1.933084
1	3.632785	0.008469	-3.055639
1	2.312031	1.029776	-3.699913
6	4.770831	-3.914739	-0.291350
6	4.511366	-5.410169	-0.081505

6	5.731565	-3.368734	0.770276
1	5.252926	-3.793070	-1.277105
1	3.834321	-5.807782	-0.855249
1	5.456719	-5.978008	-0.121170
1	4.047895	-5.595983	0.903038
1	5.943281	-2.300155	0.599872
1	5.296952	-3.470670	1.780090
1	6.687227	-3.920370	0.754494
6	0.536572	-2.400750	2.005122
6	1.167178	-1.715799	3.223630
6	0.162641	-3.847609	2.346999
1	-0.396705	-1.865047	1.758241
1	1.400902	-0.657765	3.025549
1	0.477538	-1.764351	4.085162
1	2.106531	-2.221104	3.513281
1	-0.317520	-4.343610	1.487521
1	1.053409	-4.435769	2.627589
1	-0.532158	-3.877657	3.204125
6	-1.609489	0.817928	2.746866
6	-2.569510	-0.367586	2.868366
6	-1.614154	1.670447	4.018750
1	-0.595980	0.406399	2.631248
1	-2.567564	-0.952112	1.934011
1	-2.275209	-1.031551	3.701687
1	-3.603523	-0.022254	3.053644
1	-0.917808	2.521610	3.934453
1	-2.619666	2.070560	4.237975
1	-1.302529	1.060015	4.883803
6	-4.765775	3.900688	0.293048
6	-5.727224	3.351768	-0.766401
6	-4.511339	5.396928	0.082927
1	-5.245306	3.777353	1.279849
1	-5.935298	2.282541	-0.595521
1	-6.684560	3.900436	-0.748313
1	-5.295437	3.455128	-1.777278
1	-3.834187	5.796456	0.855595
1	-4.050045	5.584198	-0.902356
1	-5.458356	5.961877	0.124297
6	-0.532087	2.399609	-2.013261
6	-0.179194	3.848870	-2.367686

6	-1.154853	1.700217	-3.227815
1	0.409026	1.878462	-1.764029
1	0.285837	4.362872	-1.510799
1	0.521538	3.880841	-3.219824
1	-1.076967	4.419150	-2.662315
1	-1.366836	0.637976	-3.029045
1	-2.105514	2.186981	-3.512379
1	-0.470574	1.762573	-4.092789
6	1.239720	1.110058	0.993448
6	2.602108	0.579349	1.107646
6	1.254155	2.314254	1.831905
6	3.276699	1.273577	2.138256
1	3.015084	-0.269863	0.569917
6	2.442795	2.337015	2.591374
1	0.417863	3.003409	1.933029
1	4.285154	1.057677	2.489349
1	2.699688	3.073727	3.351723
26	2.939705	2.633350	0.548926
6	4.012677	4.528053	0.449927
6	4.883735	3.487123	0.044227
6	2.913160	4.560518	-0.454629
1	4.143394	5.172177	1.318510
6	4.323129	2.869491	-1.109185
1	5.803807	3.187955	0.544708
6	3.115380	3.546233	-1.427869
1	2.072235	5.251033	-0.407252
1	4.748028	2.027481	-1.653684
1	2.451686	3.311039	-2.257720
6	-1.225278	-1.121874	-0.999214
6	-2.586112	-0.588250	-1.133703
6	-1.241361	-2.345374	-1.811691
6	-3.252643	-1.296005	-2.160491
1	-2.998666	0.273890	-0.616501
6	-2.421264	-2.373972	-2.583903
1	-0.409320	-3.042774	-1.890776
1	-4.255036	-1.079500	-2.528250
1	-2.675223	-3.123646	-3.332561
26	-2.948208	-2.626307	-0.543720
6	-3.149265	-3.524203	1.439030
6	-4.336312	-2.813441	1.116752

6	-2.978039	-4.549701	0.471707
1	-2.478579	-3.305190	2.267637
6	-4.915253	-3.420679	-0.033052
1	-4.735905	-1.955784	1.655935
6	-4.076908	-4.490530	-0.432243
1	-2.158998	-5.266500	0.430447
1	-5.825926	-3.096668	-0.535240
1	-4.227755	-5.136190	-1.296354

(E)-(Tip)(Fc)Si=Si(Fc)(Tip)-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-0.140526	-1.039426	-0.091169
14	0.143750	1.050834	0.072166
6	1.506307	-1.855401	-0.290251
6	2.259175	-1.735989	-1.477308
6	2.057873	-2.393191	0.889549
6	3.561897	-2.238607	-1.471144
6	3.362516	-2.876287	0.852062
6	4.110486	-2.825272	-0.328923
1	4.174780	-2.175730	-2.377442
1	3.801466	-3.313190	1.755503
6	-1.501869	1.866351	0.285140
6	-2.063841	2.401556	-0.891083
6	-2.247467	1.741831	1.476401
6	-3.371614	2.875589	-0.846033
6	-3.553366	2.236133	1.477928
6	-4.112591	2.819223	0.339046
1	-3.818657	3.309672	-1.746856
1	-4.160814	2.168253	2.387596
6	1.715382	-1.052903	-2.732908
6	1.575278	-2.014355	-3.915822
6	2.548962	0.174130	-3.124382
1	0.706973	-0.674751	-2.502399
1	0.893633	-2.844110	-3.670591
1	1.156287	-1.479932	-4.786565
1	2.550549	-2.437887	-4.211750
1	2.600409	0.898124	-2.291908

1	3.580193	-0.104095	-3.407039
1	2.093210	0.680827	-3.995067
6	5.495137	-3.427967	-0.360975
6	5.409638	-4.927963	-0.062345
6	6.428175	-2.691520	0.602301
1	5.886528	-3.303702	-1.385189
1	4.716259	-5.420473	-0.764681
1	6.396683	-5.411640	-0.143604
1	5.024794	-5.099375	0.957755
1	6.468990	-1.617797	0.353517
1	6.063940	-2.780003	1.640428
1	7.450322	-3.102148	0.560113
6	1.238437	-2.451661	2.175456
6	1.831192	-1.621122	3.315903
6	0.927433	-3.889453	2.584438
1	0.258533	-1.979157	1.958597
1	1.916328	-0.559030	3.026541
1	1.175735	-1.679853	4.203154
1	2.832729	-1.981958	3.608862
1	0.419271	-4.412856	1.756273
1	1.843941	-4.449045	2.837107
1	0.259999	-3.902814	3.463942
6	-1.694191	1.059377	2.728361
6	-2.514368	-0.178339	3.114646
6	-1.565154	2.015748	3.916702
1	-0.681737	0.693858	2.495282
1	-2.557540	-0.899430	2.279233
1	-2.053935	-0.683510	3.983861
1	-3.548807	0.087836	3.397472
1	-0.896746	2.857304	3.675635
1	-2.545831	2.422933	4.217707
1	-1.136379	1.482116	4.783154
6	-5.500897	3.413195	0.379355
6	-6.434772	2.672682	-0.579978
6	-5.425623	4.914038	0.082270
1	-5.885981	3.285144	1.405501
1	-6.468885	1.598515	-0.332028
1	-7.458838	3.077949	-0.532451
1	-6.076149	2.764008	-1.619802
1	-4.731411	5.409532	0.781658

1	-5.046854	5.088750	-0.939513
1	-6.414935	5.392067	0.169051
6	-1.252145	2.467050	-2.181548
6	-0.953100	3.906948	-2.591782
6	-1.843971	1.632353	-3.319376
1	-0.268074	2.001693	-1.969768
1	-0.447411	4.434670	-1.765029
1	-0.287028	3.924602	-3.472190
1	-1.874088	4.459584	-2.843357
1	-1.915455	0.568847	-3.031630
1	-2.851356	1.982649	-3.604932
1	-1.195243	1.699350	-4.210929
6	1.467233	1.737893	1.123763
6	2.806343	1.290304	1.327479
6	1.290900	2.947686	1.858499
6	3.438910	2.212259	2.200778
1	3.246103	0.399396	0.873034
6	2.506113	3.237612	2.524319
1	0.371369	3.534679	1.857194
1	4.471474	2.158974	2.540567
1	2.693870	4.106258	3.152385
26	2.824920	3.203596	0.407940
6	3.596816	5.089813	-0.107884
6	4.552829	4.079347	-0.405964
6	2.440810	4.846536	-0.898993
1	3.700977	5.873902	0.640396
6	3.986268	3.213348	-1.381506
1	5.522362	3.950285	0.072722
6	2.681329	3.688211	-1.686705
1	1.524190	5.434542	-0.893004
1	4.458020	2.327344	-1.804659
1	1.986998	3.240873	-2.399211
6	-1.456119	-1.750927	-1.135429
6	-2.793395	-1.307874	-1.359910
6	-1.272120	-2.973681	-1.846772
6	-3.416961	-2.245234	-2.223000
1	-3.237142	-0.408995	-0.925453
6	-2.480720	-3.275827	-2.519012
1	-0.351691	-3.559203	-1.827811
1	-4.446343	-2.198788	-2.573182

1	-2.661839	-4.155698	-3.133270
26	-2.822158	-3.205266	-0.407541
6	-2.692778	-3.677213	1.691451
6	-3.987702	-3.180005	1.379709
6	-2.472052	-4.845402	0.912401
1	-1.992516	-3.238484	2.403495
6	-4.568053	-4.041919	0.408844
1	-4.443648	-2.282296	1.795629
6	-3.630615	-5.072334	0.120069
1	-1.566383	-5.450290	0.912943
1	-5.533801	-3.897848	-0.073179
1	-3.748100	-5.859362	-0.623172

(E)-(Tip)(Fc)Si=Si(Fc)(Tip)-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-0.079685	-1.159103	-0.011537
14	0.071925	1.158658	0.007278
6	1.681302	-1.783284	-0.242056
6	2.388357	-1.593963	-1.451127
6	2.358931	-2.284490	0.893091
6	3.736537	-1.962209	-1.513777
6	3.707632	-2.627545	0.791146
6	4.409390	-2.486004	-0.409396
1	4.290015	-1.826991	-2.449979
1	4.225560	-3.019293	1.673568
6	-1.684772	1.790381	0.247869
6	-2.365191	2.295584	-0.883986
6	-2.388282	1.598861	1.458653
6	-3.714503	2.635126	-0.778322
6	-3.736812	1.965136	1.525363
6	-4.413497	2.488717	0.423206
1	-4.235202	3.027877	-1.658666
1	-4.287602	1.828278	2.462934
6	1.753974	-0.943194	-2.676748
6	1.770999	-1.856235	-3.907036
6	2.422360	0.402488	-2.989227
1	0.695264	-0.733566	-2.449423

1	1.252768	-2.807740	-3.706862
1	1.262499	-1.363488	-4.753540
1	2.804039	-2.086842	-4.220966
1	2.415038	1.063257	-2.104204
1	3.471780	0.261298	-3.304617
1	1.889483	0.915640	-3.810074
6	5.863766	-2.903327	-0.505292
6	6.012626	-4.405498	-0.241349
6	6.747568	-2.079592	0.436050
1	6.193807	-2.706269	-1.539971
1	5.382684	-4.989563	-0.932300
1	7.060620	-4.726230	-0.367050
1	5.702172	-4.653627	0.788458
1	6.662985	-1.002612	0.215398
1	6.451007	-2.232721	1.488213
1	7.806259	-2.373732	0.336431
6	1.651393	-2.455264	2.231346
6	2.265847	-1.590346	3.333666
6	1.547237	-3.928845	2.628823
1	0.612636	-2.097777	2.102195
1	2.258356	-0.524752	3.044409
1	1.686585	-1.697007	4.267577
1	3.309784	-1.879608	3.547188
1	1.047454	-4.506390	1.831991
1	2.543215	-4.373563	2.799436
1	0.958614	-4.038785	3.556349
6	-1.748245	0.951555	2.683108
6	-2.418312	-0.390125	3.008634
6	-1.754087	1.872216	3.908051
1	-0.691850	0.736834	2.449449
1	-2.417434	-1.056479	2.127683
1	-1.881733	-0.898760	3.829833
1	-3.465388	-0.244454	3.329741
1	-1.235634	2.821449	3.698115
1	-2.784479	2.106968	4.227682
1	-1.240315	1.383763	4.753859
6	-5.869297	2.900359	0.522355
6	-6.751583	2.071799	-0.416250
6	-6.025432	4.401549	0.257326
1	-6.196038	2.702689	1.557962

1	-6.661828	0.995409	-0.194740
1	-7.811358	2.361361	-0.314705
1	-6.457869	2.225192	-1.469178
1	-5.396403	4.989095	0.946145
1	-5.718678	4.650086	-0.773478
1	-7.074536	4.717722	0.385259
6	-1.660535	2.473950	-2.222851
6	-1.576021	3.947630	-2.624534
6	-2.264003	1.598336	-3.322842
1	-0.617080	2.130772	-2.093209
1	-1.086219	4.534846	-1.828665
1	-0.986585	4.062240	-3.550950
1	-2.577307	4.378422	-2.799544
1	-2.238037	0.533057	-3.033477
1	-3.313486	1.870161	-3.532263
1	-1.690113	1.714083	-4.258989
6	1.318945	1.870630	1.175228
6	2.703612	1.527251	1.316172
6	1.112326	3.065941	1.939186
6	3.319664	2.478048	2.172475
1	3.198190	0.682033	0.831028
6	2.335487	3.429105	2.558126
1	0.170632	3.613124	2.001324
1	4.369606	2.492814	2.462494
1	2.498202	4.298447	3.194172
26	2.569156	3.481098	0.414824
6	3.168001	5.464562	-0.162194
6	4.188319	4.543833	-0.517985
6	1.990562	5.114287	-0.879394
1	3.259559	6.276842	0.557618
6	3.642639	3.623833	-1.455768
1	5.200907	4.522601	-0.117458
6	2.286593	3.982562	-1.685236
1	1.028773	5.621579	-0.815413
1	4.167897	2.784571	-1.910069
1	1.587633	3.463081	-2.341819
6	-1.312868	-1.879996	-1.188950
6	-2.697730	-1.543937	-1.344358
6	-1.094070	-3.079568	-1.942750
6	-3.301895	-2.503226	-2.199693

1	-3.200594	-0.698277	-0.868668
6	-2.310128	-3.452522	-2.569860
1	-0.149071	-3.622285	-1.993645
1	-4.349169	-2.524783	-2.498760
1	-2.463213	-4.326862	-3.201451
26	-2.563274	-3.490135	-0.427857
6	-2.286939	-3.983780	1.675204
6	-3.639456	-3.614259	1.442711
6	-2.000148	-5.122098	0.875182
1	-1.584118	-3.467440	2.330119
6	-4.192358	-4.533928	0.508856
1	-4.158249	-2.768595	1.892508
6	-3.180071	-5.465641	0.158790
1	-1.042956	-5.638530	0.815116
1	-5.204437	-4.505767	0.107451
1	-3.278321	-6.280787	-0.556874

(E)-(Tip)(Fc)Ge=Ge(Fc)(Tip)-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-0.214060	-1.109948	-0.018607
32	0.199237	1.102513	0.017799
6	1.506089	-1.956516	-0.274796
6	2.234821	-1.834633	-1.474752
6	2.098115	-2.469724	0.895207
6	3.547471	-2.315200	-1.494447
6	3.412401	-2.926523	0.835002
6	4.136584	-2.877930	-0.360778
1	4.137061	-2.247732	-2.415950
1	3.879471	-3.338908	1.735951
6	-1.508944	1.967092	0.283900
6	-2.099136	2.485631	-0.884599
6	-2.236268	1.845707	1.484561
6	-3.412846	2.943841	-0.823464
6	-3.547886	2.328968	1.505457
6	-4.136970	2.893020	0.372400
1	-3.879779	3.358132	-1.723608
1	-4.137015	2.262050	2.427308

6	1.669590	-1.148311	-2.717646
6	1.577599	-2.078094	-3.929630
6	2.456915	0.123701	-3.057468
1	0.643445	-0.821966	-2.490166
1	0.936786	-2.947240	-3.711215
1	1.133416	-1.537471	-4.783764
1	2.570485	-2.446755	-4.239582
1	2.480009	0.811090	-2.192746
1	3.498432	-0.107052	-3.344492
1	1.984566	0.651037	-3.906624
6	5.531233	-3.459137	-0.417705
6	5.473752	-4.960582	-0.116725
6	6.478875	-2.715899	0.526470
1	5.901914	-3.330161	-1.449190
1	4.772796	-5.464133	-0.803408
1	6.465966	-5.430228	-0.218777
1	5.113933	-5.136417	0.911999
1	6.513060	-1.642318	0.276088
1	6.138235	-2.805459	1.572562
1	7.501554	-3.123597	0.463639
6	1.321219	-2.521363	2.207107
6	1.942997	-1.658454	3.307368
6	1.039327	-3.954571	2.652422
1	0.328525	-2.068568	2.019557
1	2.016034	-0.604932	2.984144
1	1.314119	-1.691629	4.214773
1	2.954616	-2.005300	3.581135
1	0.514159	-4.500046	1.849350
1	1.967439	-4.501049	2.890507
1	0.395199	-3.957177	3.549244
6	-1.668678	1.161959	2.727921
6	-2.466846	-0.097315	3.088927
6	-1.555396	2.102096	3.930294
1	-0.648187	0.822016	2.494144
1	-2.503746	-0.795309	2.233320
1	-1.993435	-0.618945	3.940886
1	-3.503328	0.147780	3.382149
1	-0.907624	2.962496	3.698676
1	-2.541802	2.483999	4.244961
1	-1.109394	1.564652	4.785490

6	-5.532432	3.472359	0.430056
6	-6.479948	2.725749	-0.511706
6	-5.478181	4.973400	0.126718
1	-5.901713	3.344189	1.462148
1	-6.511503	1.652416	-0.259840
1	-7.503423	3.131334	-0.447785
1	-6.141141	2.814592	-1.558470
1	-4.777133	5.479284	0.811592
1	-5.120296	5.148409	-0.902809
1	-6.471118	5.441357	0.229556
6	-1.320854	2.538871	-2.195819
6	-1.052423	3.971947	-2.649467
6	-1.932302	1.663659	-3.292317
1	-0.323531	2.097018	-2.004908
1	-0.533813	4.527648	-1.849321
1	-0.406945	3.974819	-3.545306
1	-1.985302	4.507878	-2.892783
1	-1.992395	0.610482	-2.965133
1	-2.948324	1.997351	-3.566395
1	-1.304441	1.700740	-4.200324
6	1.556865	1.780494	1.165575
6	2.899106	1.319577	1.309121
6	1.428196	2.992092	1.904761
6	3.584013	2.237108	2.147214
1	3.312819	0.424317	0.838386
6	2.677452	3.272604	2.510856
1	0.521741	3.597948	1.944782
1	4.631166	2.175514	2.438539
1	2.908248	4.141637	3.124420
26	2.898363	3.235230	0.384538
6	3.629847	5.125979	-0.204100
6	4.580321	4.119633	-0.530326
6	2.438574	4.856737	-0.931239
1	3.767351	5.930401	0.516716
6	3.975510	3.229094	-1.459327
1	5.576974	4.016066	-0.103861
6	2.652573	3.686170	-1.708430
1	1.517668	5.436567	-0.890855
1	4.433719	2.339262	-1.889056
1	1.929862	3.220067	-2.379908

6	-1.551319	-1.801030	-1.182685
6	-2.894075	-1.347695	-1.343278
6	-1.410002	-3.018826	-1.909192
6	-3.567267	-2.276146	-2.178693
1	-3.316428	-0.450989	-0.883373
6	-2.652687	-3.310866	-2.523753
1	-0.499945	-3.620067	-1.937229
1	-4.612025	-2.222081	-2.479968
1	-2.873975	-4.186388	-3.131512
26	-2.893598	-3.252282	-0.399440
6	-2.651862	-3.686001	1.697298
6	-3.970640	-3.219194	1.444217
6	-2.448814	-4.865535	0.930815
1	-1.924170	-3.220562	2.364009
6	-4.583762	-4.112395	0.523274
1	-4.421188	-2.321973	1.866529
6	-3.642700	-5.130433	0.206171
1	-1.533169	-5.454076	0.895656
1	-5.579681	-4.003686	0.096365
1	-3.787617	-5.939781	-0.507566

(E)-(Tip)(Fc)Ge=Ge(Fc)(Tip)-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-0.187319	-1.198933	0.009501
32	0.166159	1.191117	-0.018638
6	1.618173	-1.912453	-0.246282
6	2.321389	-1.756752	-1.458702
6	2.274573	-2.406888	0.900045
6	3.656296	-2.173361	-1.516460
6	3.609849	-2.797678	0.802966
6	4.309400	-2.705985	-0.404376
1	4.213730	-2.074032	-2.454968
1	4.116990	-3.188986	1.691787
6	-1.624406	1.932465	0.254598
6	-2.277873	2.445130	-0.885418
6	-2.325685	1.772210	1.467497
6	-3.612464	2.837189	-0.784510

6	-3.659090	2.192919	1.529746
6	-4.312337	2.733843	0.421582
1	-4.119107	3.236872	-1.669923
1	-4.215682	2.089712	2.468363
6	1.705031	-1.094109	-2.688124
6	1.664972	-2.021003	-3.907457
6	2.427340	0.217003	-3.028801
1	0.659283	-0.833009	-2.454257
1	1.100133	-2.941868	-3.691190
1	1.174263	-1.512106	-4.755112
1	2.681610	-2.307842	-4.228262
1	2.459312	0.892569	-2.155809
1	3.466111	0.027903	-3.353599
1	1.906441	0.739200	-3.851728
6	5.740938	-3.192877	-0.497413
6	5.808665	-4.698005	-0.215497
6	6.664859	-2.402788	0.433521
1	6.078762	-3.025535	-1.534839
1	5.138054	-5.252274	-0.892868
1	6.834656	-5.081555	-0.346015
1	5.492676	-4.915057	0.819766
1	6.631705	-1.325776	0.198999
1	6.361323	-2.527628	1.487456
1	7.707866	-2.749206	0.337597
6	1.557114	-2.513815	2.240126
6	2.200645	-1.648494	3.325275
6	1.371692	-3.969743	2.669215
1	0.536777	-2.110418	2.101021
1	2.242605	-0.591868	3.006871
1	1.606730	-1.702405	4.254608
1	3.228282	-1.976903	3.559162
1	0.845859	-4.534709	1.879959
1	2.340318	-4.464940	2.856532
1	0.770299	-4.026885	3.593383
6	-1.705961	1.108118	2.694634
6	-2.436171	-0.193988	3.051753
6	-1.646416	2.043278	3.907135
1	-0.664438	0.836088	2.453558
1	-2.476240	-0.878560	2.186176
1	-1.914965	-0.711048	3.877614

1	-3.471875	0.005302	3.380051
1	-1.074948	2.957213	3.679371
1	-2.657541	2.342350	4.234232
1	-1.153034	1.535997	4.754227
6	-5.745444	3.215869	0.516742
6	-6.666940	2.420287	-0.412165
6	-5.820719	4.720182	0.232984
1	-6.081062	3.047952	1.554773
1	-6.629235	1.343818	-0.175826
1	-7.711324	2.762573	-0.316268
1	-6.364380	2.544439	-1.466494
1	-5.151016	5.278519	0.907893
1	-5.508527	4.937416	-0.803357
1	-6.848155	5.099121	0.365417
6	-1.560883	2.561880	-2.224942
6	-1.428368	4.015016	-2.681115
6	-2.169584	1.653054	-3.294845
1	-0.526489	2.200268	-2.076320
1	-0.927044	4.614357	-1.901647
1	-0.824503	4.074621	-3.603450
1	-2.412428	4.471962	-2.883797
1	-2.167578	0.600406	-2.960179
1	-3.211185	1.934810	-3.528257
1	-1.581738	1.716235	-4.227489
6	1.497010	1.861675	1.203979
6	2.863203	1.455741	1.319937
6	1.352263	3.072693	1.950256
6	3.537489	2.393018	2.148006
1	3.308529	0.581893	0.838032
6	2.603603	3.392077	2.537502
1	0.436435	3.661909	2.016109
1	4.592552	2.366949	2.417146
1	2.818106	4.264698	3.153166
26	2.788323	3.393840	0.393283
6	3.417152	5.335958	-0.251230
6	4.405930	4.378617	-0.602932
6	2.215064	4.996066	-0.931452
1	3.543073	6.162272	0.446795
6	3.814968	3.446392	-1.500555
1	5.425352	4.340635	-0.221772

6	2.463480	3.833360	-1.708692
1	1.266303	5.526367	-0.859897
1	4.305075	2.577622	-1.938181
1	1.737152	3.314350	-2.335594
6	-1.494578	-1.888443	-1.228499
6	-2.863966	-1.497362	-1.357604
6	-1.333474	-3.106150	-1.960163
6	-3.524067	-2.449964	-2.179103
1	-3.321845	-0.624062	-0.887085
6	-2.578045	-3.444239	-2.551283
1	-0.411403	-3.686754	-2.014571
1	-4.577586	-2.436823	-2.455171
1	-2.780450	-4.325273	-3.158967
26	-2.776506	-3.422369	-0.407780
6	-2.444770	-3.842239	1.697517
6	-3.794607	-3.448709	1.491373
6	-2.207345	-5.014394	0.931053
1	-1.711581	-3.321074	2.314802
6	-4.395635	-4.386212	0.605950
1	-4.277637	-2.572794	1.922539
6	-3.414749	-5.353535	0.259732
1	-1.262732	-5.552434	0.861448
1	-5.416604	-4.345525	0.229218
1	-3.549311	-6.186323	-0.428893

(E)-(Tip)(Fc)Sn=Sn(Fc)(Tip)-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-0.521456	-1.209362	0.153075
50	0.498826	1.200377	-0.156416
6	1.278651	-2.289997	-0.269515
6	1.999110	-2.208630	-1.477235
6	1.861234	-2.828420	0.893271
6	3.266574	-2.797744	-1.522697
6	3.134407	-3.385991	0.813428
6	3.826508	-3.411534	-0.401258
1	3.841408	-2.781381	-2.456084
1	3.588513	-3.824606	1.708667

6	-1.270057	2.316874	0.286754
6	-1.849609	2.863277	-0.873762
6	-1.989871	2.230271	1.493874
6	-3.123263	3.418911	-0.792883
6	-3.256986	2.820028	1.541243
6	-3.816713	3.436827	0.421358
1	-3.577391	3.860492	-1.686678
1	-3.832401	2.800222	2.474160
6	1.485940	-1.452444	-2.704833
6	1.260185	-2.351318	-3.922885
6	2.409625	-0.281648	-3.073614
1	0.508680	-1.013793	-2.448359
1	0.532397	-3.147167	-3.698948
1	0.862191	-1.753512	-4.761932
1	2.200402	-2.821951	-4.258591
1	2.567832	0.391444	-2.212772
1	3.398894	-0.635125	-3.413769
1	1.965480	0.313701	-3.893163
6	5.151327	-4.131984	-0.487885
6	4.937308	-5.618033	-0.180402
6	6.189113	-3.491464	0.435520
1	5.510631	-4.043513	-1.527523
1	4.169325	-6.041493	-0.849356
1	5.868611	-6.195275	-0.300959
1	4.580898	-5.750060	0.856048
1	6.332456	-2.428570	0.178245
1	5.856992	-3.539063	1.487016
1	7.160995	-4.006471	0.359560
6	1.127585	-2.787841	2.232426
6	1.843880	-1.933005	3.280687
6	0.723873	-4.172379	2.730458
1	0.160628	-2.267108	2.081381
1	1.990802	-0.902635	2.908750
1	1.239341	-1.874940	4.203270
1	2.833191	-2.345496	3.542792
1	0.122671	-4.682367	1.957306
1	1.598952	-4.802493	2.958489
1	0.107320	-4.083255	3.642163
6	-1.473193	1.472597	2.719134
6	-2.402675	0.312009	3.104125

6	-1.227408	2.376277	3.929854
1	-0.501995	1.023950	2.455499
1	-2.568279	-0.368339	2.250469
1	-1.957789	-0.277711	3.927213
1	-3.387441	0.675109	3.447052
1	-0.496575	3.165771	3.694118
1	-2.160735	2.855942	4.271856
1	-0.825078	1.780300	4.768099
6	-5.144733	4.151188	0.508259
6	-6.180205	3.503066	-0.412601
6	-4.938654	5.637497	0.197276
1	-5.502310	4.062786	1.548456
1	-6.318127	2.440156	-0.152446
1	-7.154552	4.013455	-0.337126
1	-5.849186	3.549494	-1.464535
1	-4.170927	6.065850	0.863396
1	-4.585544	5.769149	-0.840324
1	-5.872340	6.210544	0.318956
6	-1.114554	2.825736	-2.212629
6	-0.747140	4.212305	-2.731682
6	-1.809610	1.939773	-3.249984
1	-0.132822	2.334293	-2.054383
1	-0.161556	4.750316	-1.966148
1	-0.126700	4.124134	-3.640803
1	-1.638261	4.814583	-2.972439
1	-1.927262	0.908449	-2.870190
1	-2.811326	2.322599	-3.510323
1	-1.208126	1.890018	-4.175045
6	1.947877	1.672649	1.274165
6	3.229787	1.057855	1.356639
6	2.001907	2.902832	1.983949
6	4.065096	1.902183	2.130553
1	3.505326	0.113805	0.878134
6	3.307487	3.044653	2.514979
1	1.177140	3.615126	2.044250
1	5.109853	1.716920	2.370960
1	3.670834	3.889067	3.096573
26	3.392187	2.935710	0.373712
6	4.268811	4.716734	-0.339924
6	5.087855	3.605044	-0.684172

6	3.011905	4.551339	-0.981925
1	4.533862	5.526067	0.337829
6	4.336176	2.752893	-1.538259
1	6.094354	3.410638	-0.317949
6	3.055288	3.340592	-1.726281
1	2.158228	5.224286	-0.911399
1	4.668878	1.806655	-1.963531
1	2.254166	2.939335	-2.350701
6	-1.929853	-1.724437	-1.303150
6	-3.211488	-1.117363	-1.429701
6	-1.965069	-2.975148	-1.977034
6	-4.028240	-1.986622	-2.195620
1	-3.499533	-0.162254	-0.981683
6	-3.259252	-3.137206	-2.530158
1	-1.135478	-3.684135	-2.003103
1	-5.068401	-1.812229	-2.462608
1	-3.607828	-3.999156	-3.094752
26	-3.391106	-2.962848	-0.394394
6	-3.080293	-3.324661	1.717963
6	-4.343133	-2.706653	1.506057
6	-3.065004	-4.553576	1.002983
1	-2.272294	-2.930531	2.338106
6	-5.112060	-3.558285	0.667112
1	-4.653288	-1.742120	1.906780
6	-4.321661	-4.700088	0.355737
1	-2.229745	-5.251215	0.955213
1	-6.110753	-3.345614	0.289768
1	-4.604489	-5.517869	-0.304445

(E)-(Tip)(Fc)Sn=Sn(Fc)(Tip)-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-0.542707	-1.283316	0.109704
50	0.495100	1.245868	-0.115713
6	1.315642	-2.320475	-0.234212
6	2.017171	-2.252498	-1.452895
6	1.922233	-2.864381	0.914573
6	3.285508	-2.840172	-1.524350

6	3.194932	-3.422316	0.808160
6	3.873947	-3.446489	-0.414316
1	3.839133	-2.823421	-2.470534
1	3.665470	-3.856253	1.697486
6	-1.296144	2.376866	0.270983
6	-1.881306	2.970656	-0.864338
6	-2.002321	2.294958	1.485539
6	-3.152211	3.531637	-0.755097
6	-3.265555	2.893090	1.562603
6	-3.844572	3.522210	0.460037
1	-3.614203	3.989294	-1.636938
1	-3.824772	2.862690	2.505184
6	1.479651	-1.504230	-2.671819
6	1.247966	-2.410164	-3.884948
6	2.395436	-0.331030	-3.054007
1	0.496769	-1.075868	-2.408068
1	0.539068	-3.220012	-3.650187
1	0.830897	-1.823279	-4.721929
1	2.193049	-2.865310	-4.228986
1	2.596795	0.326109	-2.189626
1	3.366956	-0.691322	-3.436068
1	1.927017	0.279696	-3.847469
6	5.210992	-4.146707	-0.522110
6	5.035565	-5.639190	-0.220045
6	6.257845	-3.498612	0.386908
1	5.553939	-4.046783	-1.566418
1	4.269258	-6.079487	-0.879633
1	5.979702	-6.191851	-0.358615
1	4.701422	-5.786485	0.821732
1	6.390447	-2.433712	0.132687
1	5.947132	-3.555044	1.444518
1	7.232540	-4.005763	0.290972
6	1.226699	-2.828764	2.270788
6	1.982074	-1.984669	3.298995
6	0.856585	-4.222563	2.775647
1	0.257351	-2.312343	2.136013
1	2.134468	-0.958110	2.919877
1	1.402358	-1.918702	4.236596
1	2.971722	-2.410514	3.537288
1	0.239913	-4.744078	2.022626

1	1.750116	-4.838825	2.972848
1	0.271104	-4.150043	3.708936
6	-1.467796	1.532716	2.697169
6	-2.394647	0.372438	3.089453
6	-1.210669	2.436722	3.906961
1	-0.492960	1.090731	2.424917
1	-2.603392	-0.288355	2.229513
1	-1.930611	-0.237004	3.886254
1	-3.361472	0.744499	3.471821
1	-0.495516	3.238101	3.662539
1	-2.145934	2.904277	4.260911
1	-0.790337	1.846176	4.739708
6	-5.190749	4.205672	0.564639
6	-6.225580	3.536171	-0.343574
6	-5.039623	5.698946	0.255492
1	-5.533857	4.104105	1.608690
1	-6.343629	2.471048	-0.083040
1	-7.208084	4.029418	-0.254476
1	-5.911545	3.590062	-1.400454
1	-4.278241	6.154201	0.910557
1	-4.711560	5.847066	-0.787976
1	-5.991947	6.237162	0.394233
6	-1.173633	2.957500	-2.214742
6	-0.948948	4.351789	-2.796622
6	-1.835098	1.989134	-3.199962
1	-0.154945	2.559016	-2.047530
1	-0.401834	4.979814	-2.072510
1	-0.343204	4.282612	-3.717067
1	-1.896634	4.858525	-3.046147
1	-1.885610	0.968634	-2.777360
1	-2.864866	2.301744	-3.446332
1	-1.255997	1.938006	-4.138984
6	2.033548	1.690772	1.274511
6	3.320395	1.077554	1.331937
6	2.118067	2.926912	1.980640
6	4.181185	1.921752	2.082996
1	3.593790	0.132308	0.856755
6	3.437738	3.065557	2.483831
1	1.309339	3.653959	2.069575
1	5.232187	1.735888	2.298146

1	3.819157	3.909337	3.056772
26	3.479653	2.961326	0.346215
6	4.304383	4.757543	-0.415049
6	5.141253	3.661112	-0.762312
6	3.035787	4.551572	-1.022541
1	4.570830	5.587937	0.236505
6	4.389231	2.777799	-1.584380
1	6.163892	3.502299	-0.424634
6	3.092246	3.332817	-1.749991
1	2.166666	5.203115	-0.937656
1	4.733609	1.832627	-2.002487
1	2.281912	2.897089	-2.335624
6	-2.014960	-1.781087	-1.333971
6	-3.302716	-1.177880	-1.447499
6	-2.076951	-3.045011	-1.991218
6	-4.140980	-2.054366	-2.186068
1	-3.591702	-0.218195	-1.012963
6	-3.382778	-3.209609	-2.521851
1	-1.261971	-3.769392	-2.033604
1	-5.186670	-1.881875	-2.435444
1	-3.746055	-4.076319	-3.071749
26	-3.482347	-3.018498	-0.390694
6	-3.114829	-3.348009	1.718001
6	-4.383982	-2.737297	1.533433
6	-3.114256	-4.587210	1.024343
1	-2.284292	-2.936240	2.292341
6	-5.175360	-3.607200	0.734438
1	-4.685347	-1.766179	1.924759
6	-4.390385	-4.750791	0.419720
1	-2.276094	-5.280389	0.960926
1	-6.189214	-3.410358	0.390498
1	-4.695313	-5.586226	-0.208026

(E)-(Tip)(Fc)Pb=Pb(Fc)(Tip)-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-0.924776	-1.095921	0.197626
82	0.890433	1.084189	-0.187676

6	0.680841	-2.638295	-0.258495
6	1.395543	-2.713394	-1.469609
6	1.158323	-3.309347	0.884374
6	2.509583	-3.559355	-1.541871
6	2.286888	-4.124040	0.782586
6	2.950181	-4.288753	-0.437028
1	3.060790	-3.654019	-2.484951
1	2.652503	-4.652199	1.670751
6	-0.655261	2.672047	0.289731
6	-1.116558	3.355505	-0.852071
6	-1.377712	2.740906	1.495333
6	-2.245541	4.169151	-0.756264
6	-2.490049	3.589865	1.563834
6	-2.920949	4.324144	0.458477
1	-2.604666	4.701699	-1.644342
1	-3.048468	3.681111	2.502973
6	1.050451	-1.857415	-2.687250
6	0.613036	-2.680100	-3.901567
6	2.216534	-0.934145	-3.071472
1	0.197015	-1.212606	-2.419123
1	-0.265306	-3.301731	-3.666895
1	0.343695	-2.009015	-4.736066
1	1.425033	-3.342408	-4.249006
1	2.580037	-0.357242	-2.202977
1	3.069691	-1.511208	-3.469474
1	1.902104	-0.218436	-3.853126
6	4.101330	-5.265851	-0.551324
6	3.604391	-6.684717	-0.252691
6	5.273014	-4.872501	0.351917
1	4.453406	-5.240425	-1.597291
1	2.759438	-6.944815	-0.911760
1	4.405327	-7.429315	-0.395410
1	3.248459	-6.758741	0.789769
1	5.638436	-3.862215	0.103029
1	4.967936	-4.868212	1.412798
1	6.110015	-5.582896	0.242665
6	0.497996	-3.133811	2.249616
6	1.416897	-2.412390	3.240741
6	-0.083793	-4.432690	2.805798
1	-0.375962	-2.469329	2.129878

1	1.745809	-1.439052	2.834026
1	0.889729	-2.224592	4.192749
1	2.319671	-3.008029	3.461214
1	-0.789729	-4.870848	2.079414
1	0.700009	-5.179295	3.016474
1	-0.632079	-4.233796	3.743329
6	-1.035644	1.880588	2.710737
6	-2.208470	0.973399	3.110312
6	-0.574858	2.702156	3.917261
1	-0.194299	1.221965	2.435231
1	-2.580139	0.391889	2.248801
1	-1.895629	0.262213	3.896564
1	-3.053785	1.561654	3.508425
1	0.307726	3.313206	3.670971
1	-1.375962	3.375638	4.268562
1	-0.305134	2.031780	4.752160
6	-4.078359	5.294616	0.564005
6	-5.243772	4.886703	-0.341137
6	-3.590874	6.715136	0.258408
1	-4.433921	5.272372	1.608819
1	-5.602026	3.874993	-0.087562
1	-6.086780	5.591078	-0.239309
1	-4.934484	4.878347	-1.400836
1	-2.747894	6.984017	0.916456
1	-3.234963	6.786535	-0.784220
1	-4.396783	7.455073	0.396823
6	-0.443308	3.177307	-2.210698
6	0.078358	4.482750	-2.808829
6	-1.326793	2.385930	-3.181149
1	0.464373	2.563116	-2.067638
1	0.761917	4.977391	-2.097990
1	0.637097	4.276295	-3.738439
1	-0.737942	5.184605	-3.047499
1	-1.611279	1.408505	-2.750833
1	-2.256788	2.934193	-3.411901
1	-0.794256	2.199032	-4.130387
6	2.446599	1.239546	1.363951
6	3.559391	0.344649	1.390299
6	2.839500	2.426551	2.044890
6	4.616160	0.969229	2.101159

1	3.590929	-0.640746	0.917763
6	4.171580	2.259781	2.503585
1	2.223947	3.321718	2.146309
1	5.601838	0.545796	2.288844
1	4.759442	2.996381	3.049035
26	4.112546	2.121109	0.365279
6	5.307572	3.667306	-0.449321
6	5.860407	2.401687	-0.792423
6	4.010860	3.750490	-1.023133
1	5.776018	4.425033	0.176340
6	4.905560	1.701906	-1.577385
1	6.828470	2.017158	-0.476171
6	3.765011	2.538341	-1.726486
1	3.319945	4.588397	-0.935999
1	5.016448	0.697760	-1.985138
1	2.874081	2.300759	-2.311310
6	-2.432854	-1.297307	-1.397401
6	-3.547616	-0.408133	-1.476527
6	-2.808650	-2.507739	-2.045714
6	-4.588034	-1.059555	-2.187673
1	-3.592705	0.591970	-1.036914
6	-4.131968	-2.361391	-2.536774
1	-2.186589	-3.402227	-2.107781
1	-5.570469	-0.645099	-2.409284
1	-4.706058	-3.117612	-3.069829
26	-4.118250	-2.147860	-0.403257
6	-3.793530	-2.525900	1.700545
6	-4.903510	-1.653750	1.526099
6	-4.078915	-3.745069	1.025204
1	-2.897081	-2.306854	2.284264
6	-5.879475	-2.338599	0.754152
1	-4.981727	-0.637046	1.909619
6	-5.369909	-3.630714	0.444020
1	-3.416730	-4.607628	0.960411
1	-6.832707	-1.928305	0.425247
1	-5.862195	-4.386638	-0.165226

(E)-(Tip)(Fc)Pb=Pb(Fc)(Tip)-Triplet

Atomic

Coordinates (Angstroms)

Number	X	Y	Z
82	-0.828392	-1.199219	0.154412
82	0.800467	1.188298	-0.143892
6	0.859687	-2.653985	-0.231378
6	1.553432	-2.683401	-1.452986
6	1.352750	-3.341873	0.891537
6	2.702568	-3.479244	-1.549792
6	2.515824	-4.103150	0.760858
6	3.189619	-4.201458	-0.460266
1	3.245885	-3.532981	-2.500445
1	2.908828	-4.632538	1.636175
6	-0.841355	2.685523	0.261417
6	-1.317448	3.389734	-0.858333
6	-1.538764	2.713522	1.479955
6	-2.477392	4.155499	-0.730815
6	-2.684046	3.515331	1.574743
6	-3.161665	4.244388	0.485522
1	-2.861759	4.693478	-1.604537
1	-3.232401	3.567190	2.522664
6	1.142983	-1.840723	-2.657393
6	0.732786	-2.689590	-3.864338
6	2.253897	-0.855779	-3.051751
1	0.256805	-1.242960	-2.378817
1	-0.103379	-3.362033	-3.614749
1	0.413144	-2.039965	-4.697608
1	1.576950	-3.305899	-4.219816
1	2.613732	-0.280178	-2.180416
1	3.121267	-1.388086	-3.480532
1	1.888201	-0.142000	-3.811717
6	4.411980	-5.087132	-0.589485
6	4.040820	-6.546626	-0.304985
6	5.553500	-4.611107	0.313679
1	4.756762	-5.020725	-1.636025
1	3.219106	-6.874632	-0.962887
1	4.904686	-7.214664	-0.460561
1	3.701358	-6.665144	0.738860
1	5.834155	-3.570610	0.079499
1	5.257173	-4.649250	1.376466
1	6.444870	-5.249161	0.187675

6	0.696002	-3.224894	2.261396
6	1.547661	-2.375874	3.211439
6	0.312024	-4.577590	2.862313
1	-0.257930	-2.683529	2.131561
1	1.753245	-1.380246	2.776970
1	1.029898	-2.230511	4.175734
1	2.519616	-2.859794	3.413371
1	-0.343288	-5.132791	2.169302
1	1.196774	-5.202509	3.073388
1	-0.234587	-4.431275	3.809996
6	-1.131323	1.868580	2.683508
6	-2.247852	0.894789	3.088174
6	-0.704738	2.717891	3.884527
1	-0.252673	1.261697	2.400535
1	-2.613576	0.315932	2.221559
1	-1.884759	0.183994	3.852015
1	-3.110147	1.435727	3.516289
1	0.134740	3.382866	3.625994
1	-1.541141	3.342649	4.243529
1	-0.384038	2.068615	4.717686
6	-4.388502	5.124832	0.607929
6	-5.524895	4.635035	-0.294662
6	-4.026732	6.584823	0.314856
1	-4.735017	5.062350	1.654153
1	-5.798852	3.594165	-0.054156
1	-6.420953	5.267787	-0.175185
1	-5.225804	4.667843	-1.356900
1	-3.206665	6.921725	0.970306
1	-3.688936	6.699944	-0.729868
1	-4.894743	7.248176	0.467166
6	-0.647272	3.273771	-2.221764
6	-0.313435	4.624645	-2.854584
6	-1.459786	2.370699	-3.157181
1	0.327677	2.776851	-2.071746
1	0.310288	5.225297	-2.170626
1	0.250663	4.473909	-3.791211
1	-1.219576	5.206658	-3.094999
1	-1.633094	1.377068	-2.703738
1	-2.447910	2.814334	-3.372990
1	-0.932493	2.223483	-4.116036

6	2.451870	1.363639	1.339923
6	3.605064	0.524260	1.363052
6	2.787956	2.568429	2.024141
6	4.633475	1.197375	2.077543
1	3.686967	-0.458485	0.893569
6	4.127968	2.461488	2.486899
1	2.136983	3.436351	2.139443
1	5.638617	0.821070	2.263630
1	4.677955	3.222233	3.039617
26	4.084525	2.338819	0.353526
6	5.170609	3.962780	-0.476726
6	5.805361	2.737513	-0.820643
6	3.864787	3.953795	-1.038278
1	5.596069	4.755540	0.136439
6	4.892500	1.971057	-1.594485
1	6.802599	2.424927	-0.515874
6	3.698244	2.726942	-1.735420
1	3.116393	4.740261	-0.943423
1	5.067006	0.974118	-1.997253
1	2.811373	2.419299	-2.289509
6	-2.438567	-1.420972	-1.370631
6	-3.595441	-0.589742	-1.448448
6	-2.752500	-2.648313	-2.024766
6	-4.602436	-1.290085	-2.167361
1	-3.696049	0.405820	-1.010821
6	-4.080984	-2.563500	-2.524145
1	-2.093540	-3.514905	-2.099248
1	-5.604242	-0.924751	-2.389644
1	-4.612863	-3.343800	-3.067235
26	-4.092462	-2.372194	-0.394714
6	-3.735157	-2.728574	1.705272
6	-4.903202	-1.937520	1.538854
6	-3.935929	-3.963574	1.032078
1	-2.843084	-2.439171	2.260858
6	-5.834607	-2.690365	0.773754
1	-5.049082	-0.927422	1.919733
6	-5.237129	-3.942387	0.460447
1	-3.212239	-4.774938	0.958540
1	-6.819214	-2.352645	0.454944
1	-5.682755	-4.733760	-0.140005

4-C-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.289047	0.372969	-1.341291
6	-1.012473	0.236288	-0.716119
6	-1.775055	1.361038	-0.280915
6	-1.606970	-1.057288	-0.644466
6	-3.051059	1.148382	0.247832
6	-2.863247	-1.212042	-0.066204
6	-3.606736	-0.121982	0.396045
1	-3.644637	2.014420	0.560481
1	-3.282389	-2.220357	0.022036
6	-1.336555	2.803223	-0.514781
6	-1.341225	3.638191	0.769862
6	-2.216657	3.454712	-1.591060
1	-0.307897	2.803534	-0.900916
1	-0.683456	3.197367	1.537413
1	-0.985195	4.661794	0.561004
1	-2.356540	3.717856	1.196181
1	-2.200411	2.864630	-2.522459
1	-3.265552	3.528514	-1.253912
1	-1.858938	4.474032	-1.817894
6	-4.978862	-0.314145	1.012814
6	-4.915060	-1.192046	2.267894
6	-5.973206	-0.885043	-0.004961
1	-5.340904	0.683244	1.317474
1	-4.208657	-0.778330	3.006340
1	-5.909355	-1.269027	2.740808
1	-4.582827	-2.214459	2.016800
1	-6.039479	-0.241572	-0.897571
1	-5.659204	-1.890483	-0.335727
1	-6.980131	-0.973679	0.438484
6	-0.845139	-2.283237	-1.114406
6	-1.664594	-3.149586	-2.074190
6	-0.360812	-3.100727	0.088549
1	0.037627	-1.912348	-1.665098
1	-2.008210	-2.560053	-2.939649

1	-1.052423	-3.988348	-2.447753
1	-2.551425	-3.581891	-1.579387
1	0.227148	-2.470207	0.776390
1	-1.220010	-3.502771	0.654639
1	0.264786	-3.953454	-0.229962
6	1.281759	1.065245	-0.592701
6	2.513237	1.569536	-1.169121
6	1.359914	1.330373	0.831423
6	3.283347	2.141591	-0.144802
1	2.756645	1.504003	-2.228576
6	2.580186	1.972272	1.095491
1	0.608034	1.026932	1.560548
1	4.264987	2.601270	-0.254283
1	2.953828	2.266927	2.076209
26	2.969156	0.040992	0.219540
6	2.957028	-2.052475	-0.169489
6	4.139986	-1.474798	-0.701036
6	2.948831	-1.831506	1.235263
1	2.173960	-2.541083	-0.747601
6	4.867834	-0.898210	0.376718
1	4.422429	-1.452451	-1.752565
6	4.132781	-1.118490	1.571433
1	2.169648	-2.140130	1.930659
1	5.809569	-0.356488	0.296132
1	4.413136	-0.776650	2.567008

4-C-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.203112	0.461109	-1.077455
6	-1.149877	0.270339	-0.663843
6	-1.955877	1.375267	-0.261834
6	-1.707012	-1.040744	-0.634535
6	-3.235024	1.128456	0.238195
6	-2.991329	-1.226584	-0.135009
6	-3.768951	-0.158213	0.329556
1	-3.850142	1.974077	0.565056
1	-3.397706	-2.242258	-0.083925

6	-1.491457	2.814673	-0.419582
6	-1.491235	3.577896	0.908611
6	-2.348456	3.536833	-1.468038
1	-0.457863	2.804182	-0.794689
1	-0.857369	3.074436	1.657138
1	-1.102033	4.600171	0.762666
1	-2.510688	3.662125	1.324095
1	-2.335309	2.994983	-2.428193
1	-3.398595	3.615045	-1.136423
1	-1.968461	4.558739	-1.639836
6	-5.146509	-0.393281	0.918109
6	-5.065690	-1.241572	2.192796
6	-6.100797	-1.023457	-0.101926
1	-5.553442	0.594521	1.196446
1	-4.392547	-0.780631	2.934380
1	-6.063672	-1.355227	2.650034
1	-4.680103	-2.251646	1.968187
1	-6.176626	-0.403375	-1.010112
1	-5.748792	-2.025283	-0.403911
1	-7.110482	-1.136840	0.328810
6	-0.877742	-2.238829	-1.063753
6	-1.639801	-3.186985	-1.993820
6	-0.348923	-2.976123	0.172241
1	-0.007871	-1.852663	-1.622931
1	-2.032498	-2.650106	-2.873432
1	-0.972751	-3.991571	-2.347592
1	-2.490058	-3.667210	-1.479349
1	0.238405	-2.291490	0.807957
1	-1.186062	-3.368719	0.776474
1	0.294225	-3.826814	-0.114973
6	1.340722	1.116342	-0.569604
6	2.527096	1.532418	-1.272735
6	1.563230	1.425009	0.824650
6	3.408680	2.141042	-0.344285
1	2.691282	1.417258	-2.343047
6	2.814827	2.075957	0.946609
1	0.860703	1.200902	1.627477
1	4.385280	2.564241	-0.576554
1	3.257796	2.439372	1.873313
26	3.126058	0.068677	0.195314

6	3.071584	-2.083153	-0.160375
6	4.269946	-1.545216	-0.700573
6	3.074914	-1.838570	1.238497
1	2.275037	-2.566583	-0.725329
6	5.025059	-0.986528	0.367492
1	4.556719	-1.553090	-1.751395
6	4.284850	-1.163623	1.564757
1	2.291697	-2.117752	1.942316
1	5.989678	-0.488843	0.276247
1	4.582714	-0.830311	2.558074

4-Si-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	0.367344	0.684601	-1.843552
6	-1.205886	0.314421	-0.803088
6	-1.993212	1.368361	-0.296990
6	-1.664743	-1.009027	-0.648076
6	-3.189850	1.083440	0.369930
6	-2.867192	-1.262283	0.015332
6	-3.644879	-0.225486	0.538590
1	-3.800199	1.904708	0.762658
1	-3.211365	-2.297062	0.125685
6	-1.593399	2.823606	-0.509023
6	-1.373593	3.564718	0.812348
6	-2.612525	3.554030	-1.391416
1	-0.625690	2.843487	-1.048906
1	-0.598110	3.070857	1.420571
1	-1.055422	4.604480	0.624584
1	-2.306286	3.597287	1.402692
1	-2.744817	3.036080	-2.356102
1	-3.597371	3.601833	-0.894817
1	-2.283040	4.587827	-1.592426
6	-4.962480	-0.513023	1.234492
6	-4.790353	-1.465793	2.422004
6	-5.997492	-1.056342	0.241722
1	-5.340405	0.448013	1.624885
1	-4.051182	-1.076857	3.141813

1	-5.749662	-1.606029	2.949301
1	-4.446347	-2.459306	2.085289
1	-6.140482	-0.360061	-0.601168
1	-5.666645	-2.024874	-0.172883
1	-6.971837	-1.213143	0.736131
6	-0.863790	-2.180488	-1.198106
6	-1.618751	-2.908936	-2.313022
6	-0.434734	-3.140759	-0.085326
1	0.063930	-1.772670	-1.650926
1	-1.883159	-2.213914	-3.126975
1	-1.005441	-3.724027	-2.733900
1	-2.553577	-3.351235	-1.926914
1	0.118466	-2.601116	0.701404
1	-1.314704	-3.614509	0.383386
1	0.209077	-3.945670	-0.480492
6	1.513273	1.272273	-0.479039
6	2.815124	1.825959	-0.740183
6	1.381795	1.215983	0.950584
6	3.450699	2.108336	0.489836
1	3.242401	1.981564	-1.731979
6	2.561881	1.726751	1.539406
1	0.516557	0.812791	1.479976
1	4.452387	2.516986	0.620754
1	2.774678	1.789101	2.606617
26	3.037863	0.012879	0.347627
6	2.875329	-2.024563	-0.271204
6	4.078507	-1.464353	-0.781709
6	2.925808	-1.961007	1.147697
1	2.055212	-2.423309	-0.866352
6	4.874733	-1.059699	0.322827
1	4.332186	-1.345780	-1.834175
6	4.162882	-1.363985	1.514588
1	2.148998	-2.292653	1.835094
1	5.846478	-0.570909	0.265321
1	4.495209	-1.153939	2.530227

4-Si-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

14	0.364344	0.644802	-1.694930
6	-1.290693	0.300492	-0.864581
6	-2.044688	1.376698	-0.335225
6	-1.768701	-1.023079	-0.703645
6	-3.228056	1.104872	0.358479
6	-2.961482	-1.244245	-0.012394
6	-3.705444	-0.194302	0.531191
1	-3.809245	1.936608	0.771517
1	-3.320052	-2.272418	0.110625
6	-1.641158	2.834239	-0.517034
6	-1.479915	3.570554	0.815934
6	-2.634519	3.554834	-1.435936
1	-0.659205	2.859274	-1.019433
1	-0.736962	3.071283	1.459681
1	-1.136054	4.603793	0.638313
1	-2.435356	3.624555	1.367001
1	-2.715502	3.039215	-2.407850
1	-3.641043	3.588068	-0.982635
1	-2.308654	4.593068	-1.619142
6	-5.005613	-0.458259	1.265845
6	-4.800906	-1.379437	2.472933
6	-6.066742	-1.024344	0.315481
1	-5.370155	0.513851	1.640641
1	-4.045588	-0.970602	3.164044
1	-5.746341	-1.507155	3.027370
1	-4.462332	-2.380285	2.152971
1	-6.227911	-0.352597	-0.543561
1	-5.753095	-2.007145	-0.077993
1	-7.028374	-1.159547	0.839483
6	-1.014610	-2.235673	-1.229260
6	-1.831814	-3.015380	-2.263727
6	-0.550687	-3.135034	-0.077945
1	-0.107129	-1.867365	-1.742618
1	-2.129415	-2.363643	-3.102459
1	-1.240350	-3.854473	-2.668427
1	-2.750664	-3.434339	-1.816519
1	0.047052	-2.557527	0.649028
1	-1.411183	-3.572006	0.459730
1	0.069316	-3.966901	-0.455209

6	1.642459	1.325735	-0.547337
6	2.949276	1.837796	-0.821306
6	1.500367	1.305831	0.880479
6	3.583859	2.149926	0.408974
1	3.386163	1.961518	-1.812118
6	2.687912	1.822264	1.461446
1	0.626922	0.936126	1.420085
1	4.589122	2.552934	0.525297
1	2.884528	1.928315	2.527735
26	3.152657	0.024898	0.341980
6	2.903648	-2.062886	-0.237341
6	4.122881	-1.565230	-0.768110
6	2.972632	-1.974483	1.178057
1	2.051667	-2.414140	-0.819341
6	4.953090	-1.182119	0.321260
1	4.372148	-1.480434	-1.825012
6	4.242714	-1.435618	1.523709
1	2.188465	-2.259935	1.878406
1	5.949782	-0.749656	0.244839
1	4.596667	-1.231927	2.533398

4-Ge-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.350960	0.561733	-1.710698
6	-1.275773	0.254744	-0.575456
6	-2.009826	1.331693	-0.039992
6	-1.818042	-1.045150	-0.493960
6	-3.255352	1.093441	0.553828
6	-3.064157	-1.249706	0.102824
6	-3.805508	-0.186659	0.627280
1	-3.830818	1.934685	0.956104
1	-3.475741	-2.264586	0.152398
6	-1.516248	2.768549	-0.151497
6	-1.446094	3.467864	1.209665
6	-2.374214	3.570281	-1.138382
1	-0.483909	2.748869	-0.547907
1	-0.822731	2.898175	1.918760

1	-1.012445	4.476982	1.103841
1	-2.452093	3.578376	1.651917
1	-2.398807	3.085509	-2.129168
1	-3.414177	3.648018	-0.775025
1	-1.976229	4.592554	-1.260128
6	-5.184315	-0.412083	1.220225
6	-5.157859	-1.413104	2.379684
6	-6.177596	-0.851850	0.137906
1	-5.528460	0.557776	1.619848
1	-4.451156	-1.095048	3.163602
1	-6.160048	-1.509383	2.831611
1	-4.850780	-2.414640	2.031150
1	-6.216019	-0.119577	-0.685375
1	-5.880766	-1.825540	-0.290110
1	-7.192850	-0.960139	0.557219
6	-1.059177	-2.246605	-1.041086
6	-1.834348	-2.962011	-2.150218
6	-0.658446	-3.210491	0.079948
1	-0.116312	-1.878155	-1.496538
1	-2.081946	-2.265756	-2.968466
1	-1.242096	-3.794811	-2.566364
1	-2.779324	-3.380100	-1.762203
1	-0.085297	-2.683586	0.861170
1	-1.553591	-3.648065	0.555628
1	-0.042800	-4.039294	-0.310857
6	1.623300	1.203971	-0.362797
6	2.931702	1.657181	-0.744433
6	1.575863	1.267090	1.069150
6	3.660281	1.995343	0.419777
1	3.304000	1.705559	-1.769253
6	2.818302	1.753449	1.545206
1	0.727051	0.958888	1.682107
1	4.689377	2.352147	0.457271
1	3.098886	1.889143	2.589920
26	3.118119	-0.075248	0.476045
6	2.880460	-2.119281	-0.096784
6	4.136592	-1.634483	-0.555701
6	2.860242	-2.017422	1.321277
1	2.071676	-2.497110	-0.722602
6	4.893289	-1.237648	0.579768

1	4.451267	-1.558091	-1.595545
6	4.104937	-1.472583	1.739015
1	2.032516	-2.291016	1.974010
1	5.889879	-0.798394	0.561432
1	4.393870	-1.249585	2.765227

4-Ge-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.349047	0.587922	-1.570906
6	-1.368241	0.263644	-0.660592
6	-2.070166	1.347478	-0.084515
6	-1.910295	-1.040253	-0.587484
6	-3.293632	1.102081	0.547641
6	-3.134359	-1.233846	0.057875
6	-3.847429	-0.175508	0.624918
1	-3.846457	1.939665	0.985714
1	-3.547363	-2.247164	0.114785
6	-1.577391	2.786765	-0.159115
6	-1.586796	3.488735	1.202971
6	-2.389351	3.571540	-1.196182
1	-0.530007	2.777142	-0.502702
1	-1.014284	2.914576	1.951295
1	-1.128287	4.488222	1.115387
1	-2.612914	3.625137	1.587801
1	-2.335095	3.085547	-2.185836
1	-3.452601	3.625085	-0.900298
1	-2.006075	4.601810	-1.292657
6	-5.197068	-0.403398	1.278825
6	-5.112022	-1.400567	2.438892
6	-6.235307	-0.851449	0.242932
1	-5.526249	0.566117	1.691048
1	-4.373865	-1.075466	3.190421
1	-6.092725	-1.501403	2.934807
1	-4.814052	-2.401158	2.080278
1	-6.310277	-0.124256	-0.582278
1	-5.955411	-1.827396	-0.190972
1	-7.230950	-0.958607	0.706965

6	-1.199825	-2.265468	-1.144751
6	-2.051950	-3.009644	-2.177844
6	-0.747642	-3.191203	-0.009444
1	-0.287243	-1.919396	-1.663775
1	-2.342811	-2.340177	-3.005313
1	-1.488406	-3.859185	-2.599920
1	-2.975974	-3.410468	-1.724158
1	-0.119127	-2.640973	0.713466
1	-1.614826	-3.602070	0.539120
1	-0.162705	-4.039890	-0.404679
6	1.773947	1.262080	-0.452922
6	3.096749	1.661340	-0.811130
6	1.683152	1.342212	0.973887
6	3.801014	2.003443	0.374098
1	3.500865	1.688678	-1.822828
6	2.927689	1.807135	1.476825
1	0.810735	1.067314	1.568505
1	4.836522	2.336958	0.428376
1	3.174867	1.962609	2.526408
26	3.220715	-0.078387	0.460068
6	2.883352	-2.162264	-0.064088
6	4.155424	-1.751240	-0.543700
6	2.882863	-2.026002	1.349749
1	2.043385	-2.490162	-0.677164
6	4.946738	-1.372462	0.575900
1	4.464932	-1.718321	-1.587382
6	4.160427	-1.542841	1.745989
1	2.048509	-2.242700	2.015816
1	5.968065	-0.995976	0.538950
1	4.472452	-1.321374	2.765657

4-Sn-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.371058	0.797810	-1.712934
6	-1.393429	0.276166	-0.476178
6	-2.127334	1.279778	0.181537
6	-1.901107	-1.036900	-0.494451

6	-3.349019	0.963852	0.789434
6	-3.124849	-1.324545	0.116430
6	-3.870809	-0.330115	0.756751
1	-3.925601	1.749166	1.291887
1	-3.514188	-2.349001	0.089551
6	-1.643343	2.723893	0.205371
6	-1.515340	3.273561	1.629235
6	-2.534687	3.624476	-0.657729
1	-0.621940	2.749349	-0.226413
1	-0.859653	2.633603	2.242284
1	-1.089717	4.291308	1.615146
1	-2.502279	3.326873	2.121764
1	-2.603001	3.246193	-1.692292
1	-3.558579	3.661550	-0.245838
1	-2.139851	4.654661	-0.687356
6	-5.227399	-0.640711	1.363170
6	-5.154417	-1.755350	2.410831
6	-6.244865	-0.982311	0.267744
1	-5.574342	0.276353	1.870474
1	-4.434117	-1.505942	3.207228
1	-6.143163	-1.917965	2.873297
1	-4.838444	-2.708885	1.953389
1	-6.321981	-0.166104	-0.469499
1	-5.942258	-1.896887	-0.272019
1	-7.245053	-1.157285	0.700978
6	-1.128330	-2.165930	-1.163239
6	-1.895925	-2.778615	-2.337368
6	-0.699748	-3.230406	-0.149688
1	-0.191342	-1.735887	-1.579078
1	-2.159224	-2.008683	-3.081589
1	-1.294157	-3.557008	-2.836683
1	-2.832772	-3.246366	-1.988381
1	-0.135586	-2.771997	0.679717
1	-1.581694	-3.736344	0.280121
1	-0.066577	-3.999083	-0.625838
6	1.729620	1.222178	-0.075379
6	3.069923	1.683671	-0.292532
6	1.583022	1.072877	1.341643
6	3.724713	1.818354	0.957218
1	3.522765	1.876745	-1.267238

6	2.800515	1.439926	1.972472
1	0.687111	0.705960	1.846838
1	4.757260	2.129178	1.116036
1	3.007490	1.408737	3.042404
26	3.136635	-0.214689	0.664275
6	2.848885	-2.160640	-0.177537
6	4.128428	-1.661182	-0.547727
6	2.802086	-2.243516	1.241094
1	2.043381	-2.431102	-0.860947
6	4.872959	-1.440903	0.642474
1	4.470058	-1.463759	-1.562842
6	4.053685	-1.799416	1.747294
1	1.952439	-2.572901	1.837427
1	5.883771	-1.039438	0.698939
1	4.326443	-1.722778	2.798866

4-Sn-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.390241	0.741121	-1.599442
6	-1.494108	0.273503	-0.577802
6	-2.190464	1.307706	0.081785
6	-2.002033	-1.042726	-0.563041
6	-3.395293	1.003996	0.728028
6	-3.207109	-1.295982	0.099770
6	-3.926350	-0.284937	0.740176
1	-3.947350	1.802686	1.235241
1	-3.598131	-2.319434	0.112510
6	-1.714689	2.754682	0.105605
6	-1.652407	3.332675	1.522731
6	-2.578966	3.621406	-0.816009
1	-0.685092	2.786288	-0.289522
1	-1.030782	2.702436	2.180546
1	-1.209724	4.342792	1.498698
1	-2.655658	3.417836	1.975004
1	-2.570697	3.227216	-1.847175
1	-3.626774	3.638800	-0.466081
1	-2.205408	4.659610	-0.837179

6	-5.258582	-0.574898	1.405642
6	-5.137000	-1.637701	2.501859
6	-6.308879	-0.975791	0.362953
1	-5.595144	0.362665	1.881088
1	-4.394776	-1.342320	3.261592
1	-6.108287	-1.787853	3.003495
1	-4.824145	-2.608581	2.080233
1	-6.415772	-0.196922	-0.409795
1	-6.018459	-1.914354	-0.140888
1	-7.292450	-1.134118	0.837701
6	-1.279692	-2.226131	-1.191435
6	-2.125998	-2.926323	-2.258447
6	-0.802310	-3.205742	-0.113845
1	-0.376422	-1.838257	-1.696375
1	-2.427705	-2.219410	-3.049750
1	-1.554145	-3.746194	-2.725597
1	-3.043302	-3.360766	-1.823072
1	-0.184330	-2.685121	0.639019
1	-1.657004	-3.669432	0.410666
1	-0.199288	-4.015351	-0.560522
6	1.893430	1.284272	-0.166236
6	3.242384	1.700899	-0.359166
6	1.689859	1.150988	1.242616
6	3.858817	1.839891	0.914589
1	3.725648	1.871538	-1.320842
6	2.898892	1.500734	1.905090
1	0.771578	0.812572	1.725863
1	4.891840	2.133142	1.097252
1	3.065738	1.487163	2.981534
26	3.238494	-0.197590	0.638670
6	2.855631	-2.171199	-0.143265
6	4.137129	-1.727968	-0.567693
6	2.854545	-2.215781	1.276982
1	2.012038	-2.407904	-0.792461
6	4.931893	-1.506800	0.591453
1	4.449651	-1.568990	-1.598782
6	4.139338	-1.809221	1.731227
1	2.013145	-2.499091	1.908315
1	5.959262	-1.145883	0.603586
1	4.450826	-1.720786	2.770972

4-Sn-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.404586	1.055961	-1.429094
6	-1.456850	0.272026	-0.296200
6	-2.180757	1.119161	0.559828
6	-1.964592	-1.009712	-0.574369
6	-3.389477	0.679957	1.116531
6	-3.177175	-1.421318	-0.011775
6	-3.908524	-0.584822	0.836932
1	-3.956061	1.343130	1.780700
1	-3.566480	-2.420803	-0.239628
6	-1.705099	2.533768	0.867124
6	-1.562645	2.791283	2.369703
6	-2.615887	3.579284	0.212910
1	-0.690827	2.654565	0.435654
1	-0.887192	2.055342	2.834785
1	-1.154413	3.799638	2.553373
1	-2.542358	2.726845	2.874105
1	-2.697643	3.413150	-0.874759
1	-3.633881	3.523110	0.636324
1	-2.231579	4.599697	0.383887
6	-5.242203	-1.027723	1.411535
6	-5.126997	-2.336360	2.199498
6	-6.300531	-1.144066	0.308369
1	-5.571131	-0.240720	2.112672
1	-4.376538	-2.253406	3.002992
1	-6.097008	-2.600970	2.654745
1	-4.828171	-3.170388	1.540852
1	-6.407023	-0.193981	-0.240803
1	-6.018346	-1.924331	-0.420423
1	-7.283208	-1.413724	0.733081
6	-1.207665	-1.982947	-1.468917
6	-2.004795	-2.367538	-2.717995
6	-0.753543	-3.219513	-0.687813
1	-0.283560	-1.474759	-1.819497
1	-2.304641	-1.471844	-3.287217

1	-1.410596	-3.021224	-3.379466
1	-2.923224	-2.913174	-2.440439
1	-0.168859	-2.923200	0.198929
1	-1.625370	-3.799974	-0.338955
1	-0.132549	-3.882370	-1.315392
6	1.735302	1.098285	0.407377
6	3.097842	1.538920	0.394460
6	1.482469	0.619429	1.731360
6	3.664481	1.341311	1.681285
1	3.631205	1.937090	-0.470982
6	2.659842	0.770255	2.512090
1	0.544290	0.174396	2.068862
1	4.690991	1.558783	1.976803
1	2.787119	0.473376	3.553225
26	3.050740	-0.532031	0.869116
6	2.724880	-2.232731	-0.389430
6	4.025486	-1.706290	-0.624175
6	2.649856	-2.627941	0.974385
1	1.925400	-2.321549	-1.125205
6	4.753786	-1.780361	0.592997
1	4.392965	-1.301112	-1.566042
6	3.904073	-2.349333	1.580359
1	1.780856	-3.052088	1.474977
1	5.774772	-1.435286	0.749876
1	4.160106	-2.518388	2.625276

4-Pb-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.378781	0.811398	-1.385752
6	-1.611246	0.241999	-0.389125
6	-2.270572	1.209352	0.387525
6	-2.129218	-1.055238	-0.543822
6	-3.479742	0.848193	0.998238
6	-3.335008	-1.363656	0.096427
6	-4.031463	-0.424407	0.859614
1	-4.015839	1.588782	1.601338
1	-3.742917	-2.375074	-0.008534

6	-1.765349	2.634235	0.577218
6	-1.751058	3.067071	2.046208
6	-2.574808	3.606997	-0.287096
1	-0.720299	2.679116	0.228148
1	-1.178059	2.355226	2.664121
1	-1.278527	4.059402	2.139909
1	-2.769956	3.143073	2.463925
1	-2.513096	3.328243	-1.353487
1	-3.639505	3.597023	0.007911
1	-2.194608	4.636711	-0.174719
6	-5.359843	-0.774462	1.503741
6	-5.229204	-1.941366	2.487391
6	-6.422902	-1.066652	0.438476
1	-5.687700	0.111823	2.074120
1	-4.479149	-1.723168	3.265233
1	-6.195541	-2.140820	2.981169
1	-4.920996	-2.865077	1.967631
1	-6.534857	-0.214576	-0.251836
1	-6.143354	-1.951842	-0.159318
1	-7.401757	-1.267730	0.906525
6	-1.426536	-2.165868	-1.312083
6	-2.313974	-2.781959	-2.397512
6	-0.892992	-3.228189	-0.343716
1	-0.551661	-1.723320	-1.819737
1	-2.664800	-2.011348	-3.105428
1	-1.750385	-3.542543	-2.964389
1	-3.202040	-3.276227	-1.964893
1	-0.235584	-2.767759	0.415660
1	-1.721333	-3.733184	0.185827
1	-0.314631	-3.996884	-0.885170
6	1.935194	1.198295	0.175690
6	3.290426	1.607322	0.047467
6	1.695898	0.913150	1.552583
6	3.882919	1.594908	1.341490
1	3.794945	1.873828	-0.880827
6	2.898439	1.167387	2.271028
1	0.761868	0.542230	1.978711
1	4.916507	1.848627	1.574174
1	3.042839	1.035117	3.342711
26	3.238012	-0.398373	0.831601

6	2.829384	-2.279667	-0.161464
6	4.121860	-1.818090	-0.527455
6	2.815471	-2.475504	1.245547
1	1.986115	-2.425998	-0.836980
6	4.910972	-1.737856	0.653368
1	4.446021	-1.557045	-1.533912
6	4.103640	-2.145293	1.748817
1	1.963697	-2.808867	1.837297
1	5.945536	-1.402469	0.709851
1	4.408940	-2.176415	2.793677

5-C-C-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.290254	-0.227889	0.113461
6	0.611574	-0.701486	1.258359
6	0.857975	0.831866	-0.390717
6	1.142963	1.961294	0.448095
6	1.653902	0.735491	-1.587849
6	2.106111	2.913439	0.067029
6	2.583331	1.739118	-1.903807
6	2.846158	2.846116	-1.102419
1	2.278774	3.764760	0.731459
1	3.134911	1.643950	-2.843484
6	-1.630654	0.601547	0.517316
6	-2.204439	1.530170	-0.406439
6	-2.342880	0.468156	1.751171
6	-3.331577	2.302478	-0.076082
6	-3.453883	1.289644	2.029115
6	-3.979264	2.231368	1.150056
1	-3.710034	3.005781	-0.824482
1	-3.943633	1.185319	3.001680
6	0.485369	2.318028	1.783020
6	-0.309922	3.627931	1.683878
6	1.509770	2.404833	2.921453
1	-0.199717	1.518425	2.056768
1	-1.077856	3.576148	0.895300
1	-0.818215	3.833895	2.642034

1	0.349316	4.487835	1.465872
1	2.003491	1.430399	3.071067
1	2.282341	3.172454	2.736929
1	0.998120	2.678923	3.860371
6	3.877367	3.906719	-1.465605
6	3.533317	4.657387	-2.759165
6	5.299793	3.338488	-1.560141
1	3.872025	4.646055	-0.645658
1	2.539018	5.129821	-2.707170
1	4.280415	5.449645	-2.944227
1	3.547691	3.979880	-3.630979
1	5.604427	2.836556	-0.627423
1	5.383546	2.610907	-2.387155
1	6.018484	4.152332	-1.763513
6	1.596387	-0.328870	-2.690501
6	2.979126	-0.912694	-3.034958
6	0.973729	0.247542	-3.972747
1	0.968888	-1.159694	-2.367218
1	3.536968	-1.218390	-2.134720
1	2.851508	-1.796727	-3.683224
1	3.606996	-0.193306	-3.586303
1	0.014473	0.754503	-3.783043
1	1.649275	0.991655	-4.430222
1	0.799730	-0.554053	-4.710840
6	-2.026487	-0.494112	2.900821
6	-3.274274	-1.267218	3.366318
6	-1.457531	0.261232	4.111211
1	-1.272394	-1.220263	2.562319
1	-3.835869	-1.704197	2.528544
1	-2.982167	-2.078803	4.054036
1	-3.972512	-0.617841	3.922220
1	-0.511888	0.770303	3.873690
1	-2.184887	1.018710	4.459203
1	-1.276190	-0.432790	4.949737
6	-5.181965	3.101575	1.508598
6	-6.408083	2.838402	0.621249
6	-4.864930	4.604087	1.491432
1	-5.467381	2.839947	2.542851
1	-6.720442	1.782100	0.648474
1	-7.258676	3.455366	0.963688

1	-6.207581	3.112102	-0.429753
1	-4.021957	4.856477	2.154572
1	-4.616849	4.948791	0.471881
1	-5.748275	5.178385	1.825151
6	-1.731716	1.789317	-1.833946
6	-1.220212	3.218032	-2.047553
6	-2.864468	1.487230	-2.833051
1	-0.890901	1.126630	-2.046290
1	-0.353056	3.437049	-1.402489
1	-0.913913	3.353115	-3.100093
1	-2.010225	3.959721	-1.832743
1	-3.357159	0.525858	-2.610935
1	-3.642894	2.268587	-2.800600
1	-2.478394	1.455936	-3.867651
6	1.586288	-1.780862	1.084809
6	2.192768	-2.390715	-0.080237
6	2.126668	-2.545142	2.212339
6	3.031854	-3.450583	0.300579
1	2.017217	-2.082333	-1.101181
6	2.972002	-3.568102	1.724692
1	1.911489	-2.376655	3.267322
1	3.647332	-4.056633	-0.366714
1	3.538119	-4.289182	2.317115
26	3.763480	-1.665220	1.216712
6	5.801582	-1.581874	1.889200
6	5.745188	-1.277500	0.504841
6	5.018513	-0.619289	2.584909
1	6.346006	-2.414202	2.336159
6	4.927691	-0.124707	0.338262
1	6.229230	-1.845509	-0.289448
6	4.481566	0.282443	1.625984
1	4.851215	-0.598726	3.660978
1	4.652972	0.345384	-0.605583
1	3.797595	1.105619	1.827677
6	-0.738294	-1.391888	-0.839879
6	-1.248074	-1.356160	-2.181096
6	-0.577852	-2.786396	-0.542325
6	-1.266193	-2.669085	-2.721178
1	-1.520696	-0.487710	-2.763254
6	-0.855465	-3.561669	-1.699600

1	-0.268285	-3.210947	0.408212
1	-1.593811	-2.938268	-3.724774
1	-0.809432	-4.647751	-1.767772
26	-2.627975	-2.591095	-1.120636
6	-4.359590	-1.913492	-0.081291
6	-4.665340	-2.047896	-1.462624
6	-3.982198	-3.197161	0.406559
1	-4.372274	-0.981158	0.484456
6	-4.475606	-3.408107	-1.827722
1	-4.976763	-1.246870	-2.130784
6	-4.055676	-4.117432	-0.672786
1	-3.663799	-3.443912	1.417555
1	-4.610597	-3.832361	-2.822205
1	-3.810966	-5.178466	-0.629601

5-C-C-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.317647	-0.183975	0.051604
6	0.472834	-0.847965	1.153545
6	0.815966	0.852079	-0.446092
6	1.136524	1.922037	0.451061
6	1.616798	0.758809	-1.626916
6	2.122587	2.858125	0.118859
6	2.582253	1.743080	-1.896510
6	2.859267	2.811637	-1.055417
1	2.323267	3.674272	0.819413
1	3.150582	1.658071	-2.826888
6	-1.619466	0.601565	0.499633
6	-2.170179	1.578922	-0.375109
6	-2.299443	0.394885	1.735788
6	-3.275965	2.346105	0.011162
6	-3.380327	1.223616	2.078463
6	-3.891680	2.215452	1.248660
1	-3.655702	3.093261	-0.692761
1	-3.859458	1.082437	3.051338
6	0.505014	2.206609	1.818562
6	-0.264631	3.535522	1.813799

6	1.537756	2.186756	2.953187
1	-0.212419	1.425637	2.059028
1	-1.040121	3.544080	1.030975
1	-0.759341	3.694720	2.788076
1	0.410651	4.391631	1.636254
1	2.004550	1.190258	3.043317
1	2.338751	2.932887	2.809592
1	1.041084	2.420410	3.911335
6	3.905652	3.859623	-1.385367
6	3.545526	4.640212	-2.654221
6	5.309569	3.255810	-1.501778
1	3.917938	4.574652	-0.544126
1	2.550144	5.106540	-2.568848
1	4.287302	5.435813	-2.841851
1	3.535553	3.975359	-3.535769
1	5.598761	2.726328	-0.578976
1	5.361793	2.536261	-2.338349
1	6.053947	4.047756	-1.695307
6	1.552423	-0.291156	-2.743740
6	2.932562	-0.878898	-3.092562
6	0.932178	0.304271	-4.016966
1	0.926843	-1.128543	-2.431969
1	3.493380	-1.180496	-2.192183
1	2.802247	-1.767071	-3.734742
1	3.557960	-0.164241	-3.652968
1	-0.031129	0.801024	-3.821063
1	1.605715	1.062514	-4.453743
1	0.766313	-0.483094	-4.772203
6	-1.971441	-0.651480	2.809575
6	-3.237603	-1.340494	3.351259
6	-1.228775	-0.030965	4.005691
1	-1.338580	-1.435718	2.366580
1	-3.946893	-1.602489	2.551851
1	-2.959472	-2.261707	3.891842
1	-3.775333	-0.697760	4.070687
1	-0.221579	0.331097	3.747110
1	-1.812186	0.822847	4.400919
1	-1.128423	-0.770532	4.818953
6	-5.067651	3.084816	1.658993
6	-6.293646	2.844768	0.769039

6	-4.707017	4.575076	1.671674
1	-5.340085	2.796410	2.689359
1	-6.594275	1.784231	0.772187
1	-7.148360	3.448986	1.120180
1	-6.084000	3.136673	-0.275222
1	-3.838620	4.776205	2.320205
1	-4.463249	4.931370	0.655190
1	-5.560145	5.172858	2.037517
6	-1.686930	1.883826	-1.789394
6	-1.122422	3.299917	-1.943432
6	-2.824328	1.653892	-2.799663
1	-0.868760	1.204750	-2.032891
1	-0.238870	3.453052	-1.301826
1	-0.820412	3.468826	-2.992399
1	-1.879554	4.061413	-1.684814
1	-3.353397	0.706720	-2.601792
1	-3.569818	2.465537	-2.754088
1	-2.429651	1.627776	-3.831191
6	1.511594	-1.817625	1.109133
6	2.135649	-2.371765	-0.070119
6	2.051553	-2.567348	2.219742
6	2.938234	-3.475751	0.301001
1	1.945915	-2.049367	-1.085736
6	2.889381	-3.596652	1.716127
1	1.818955	-2.390426	3.268683
1	3.518247	-4.095691	-0.382397
1	3.436265	-4.326702	2.311431
26	3.733727	-1.704643	1.189448
6	5.800299	-1.641150	1.818456
6	5.721717	-1.320542	0.438008
6	5.048312	-0.669852	2.537943
1	6.321795	-2.496692	2.246725
6	4.927110	-0.146727	0.302368
1	6.173024	-1.887146	-0.376190
6	4.520644	0.261068	1.600950
1	4.894766	-0.656813	3.616210
1	4.649931	0.344593	-0.630604
1	3.875468	1.110174	1.821339
6	-0.787966	-1.331007	-0.909565
6	-1.306408	-1.256844	-2.243040

6	-0.638242	-2.730318	-0.637429
6	-1.350425	-2.559414	-2.804556
1	-1.566920	-0.371102	-2.802855
6	-0.940791	-3.476566	-1.805094
1	-0.322205	-3.171052	0.303028
1	-1.690119	-2.802538	-3.810211
1	-0.908310	-4.561488	-1.891884
26	-2.682645	-2.478100	-1.173140
6	-4.389372	-1.781740	-0.101229
6	-4.718553	-1.918305	-1.476964
6	-4.008323	-3.065746	0.384107
1	-4.391290	-0.847854	0.462232
6	-4.540354	-3.280758	-1.841435
1	-5.033792	-1.115778	-2.141813
6	-4.104194	-3.988657	-0.691055
1	-3.670791	-3.309176	1.389707
1	-4.686377	-3.704730	-2.834231
1	-3.855383	-5.048554	-0.647816

5-Si-Si-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	0.357980	-0.225775	-0.157466
14	-0.954524	-0.916763	-2.076030
6	-0.921165	1.119746	0.449586
6	-1.119777	2.251806	-0.394005
6	-1.702590	1.052095	1.639854
6	-2.018252	3.261454	-0.021952
6	-2.573944	2.094793	1.969533
6	-2.750924	3.214382	1.158226
1	-2.145116	4.128974	-0.677546
1	-3.141616	2.027655	2.903663
6	2.020576	0.673633	-0.570004
6	2.589154	1.547936	0.392897
6	2.700764	0.529012	-1.806517
6	3.739052	2.285081	0.090206
6	3.841197	1.297445	-2.071768
6	4.373484	2.192505	-1.147693

1	4.149278	2.960135	0.849266
1	4.343949	1.192510	-3.038646
6	-0.386589	2.492581	-1.715102
6	0.589586	3.671945	-1.618877
6	-1.345775	2.693953	-2.894456
1	0.217018	1.608062	-1.951735
1	1.336216	3.514611	-0.824334
1	1.131169	3.793566	-2.573607
1	0.052013	4.614216	-1.409847
1	-1.992918	1.813187	-3.043532
1	-1.988834	3.579978	-2.756315
1	-0.770622	2.843462	-3.824522
6	-3.710562	4.322576	1.544607
6	-3.285677	5.002792	2.850570
6	-5.150457	3.805368	1.635522
1	-3.672668	5.078871	0.741547
1	-2.256830	5.392647	2.779637
1	-3.960340	5.842573	3.090200
1	-3.320906	4.291716	3.694416
1	-5.463032	3.329842	0.691029
1	-5.248718	3.055489	2.440396
1	-5.847743	4.630965	1.859162
6	-1.633464	-0.085940	2.654329
6	-3.008953	-0.665317	3.011337
6	-0.913385	0.367016	3.932157
1	-1.050330	-0.904950	2.219133
1	-3.557621	-0.990225	2.111652
1	-2.882230	-1.540749	3.671739
1	-3.637387	0.064455	3.550617
1	0.068122	0.818576	3.710462
1	-1.512514	1.126356	4.466098
1	-0.753986	-0.487016	4.613028
6	2.280262	-0.434942	-2.913351
6	3.441526	-1.301131	-3.421218
6	1.647676	0.308416	-4.096783
1	1.536271	-1.136175	-2.493794
1	4.000842	-1.767881	-2.595210
1	3.051963	-2.100009	-4.075719
1	4.154695	-0.709094	-4.019387
1	0.763481	0.893261	-3.798803

1	2.387226	1.000144	-4.538590
1	1.327427	-0.403258	-4.876925
6	5.606485	3.012818	-1.473938
6	6.782742	2.643242	-0.563867
6	5.312608	4.515329	-1.415883
1	5.893286	2.765765	-2.511054
1	7.010196	1.566420	-0.627973
1	7.687398	3.208098	-0.847398
1	6.552911	2.878924	0.490022
1	4.469980	4.780276	-2.075716
1	5.050002	4.826356	-0.389620
1	6.196703	5.097237	-1.728286
6	2.026806	1.718087	1.799895
6	1.462670	3.120321	2.055107
6	3.079973	1.359469	2.856341
1	1.189347	1.016043	1.919340
1	0.617408	3.342881	1.383292
1	1.100500	3.202213	3.095349
1	2.239754	3.891279	1.905605
1	3.536886	0.378102	2.644114
1	3.888352	2.110373	2.887826
1	2.622109	1.323615	3.861351
6	-2.076407	-2.235070	-1.365884
6	-2.521642	-2.529714	-0.030687
6	-2.943343	-2.986254	-2.242808
6	-3.612810	-3.423537	-0.091630
1	-2.092250	-2.113553	0.879297
6	-3.868795	-3.715172	-1.465663
1	-2.900754	-2.962339	-3.332572
1	-4.181603	-3.802950	0.757176
1	-4.660690	-4.360566	-1.845102
26	-4.108854	-1.610677	-1.130708
6	-6.063743	-1.064778	-1.747859
6	-5.922041	-0.816468	-0.355018
6	-5.111071	-0.265329	-2.437167
1	-6.756854	-1.771139	-2.203556
6	-4.885171	0.141941	-0.182633
1	-6.492249	-1.295515	0.439938
6	-4.385107	0.481667	-1.467733
1	-4.948904	-0.247136	-3.514092

1	-4.516985	0.543973	0.760878
1	-3.572941	1.182613	-1.661835
6	0.764634	-1.635315	1.051495
6	1.277793	-1.612820	2.392441
6	0.476532	-3.010338	0.770185
6	1.263466	-2.928819	2.920702
1	1.615524	-0.737556	2.941143
6	0.774687	-3.799362	1.910214
1	0.087830	-3.391583	-0.173346
1	1.610802	-3.223535	3.910266
1	0.678715	-4.881746	1.982755
26	2.552164	-2.846990	1.235000
6	4.225400	-2.116434	0.127591
6	4.606324	-2.326515	1.480075
6	3.802311	-3.367308	-0.405432
1	4.223203	-1.155540	-0.389442
6	4.420219	-3.703014	1.784193
1	4.961197	-1.560925	2.168650
6	3.925999	-4.346477	0.618218
1	3.423731	-3.546890	-1.410872
1	4.597060	-4.175397	2.749784
1	3.657939	-5.398957	0.533789

5-Si-Si-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	0.413527	-0.205635	-0.129784
14	-0.789354	-1.195612	-1.898388
6	-0.881313	1.119947	0.449519
6	-1.073220	2.241813	-0.406718
6	-1.674743	1.054383	1.628646
6	-1.967567	3.257205	-0.049243
6	-2.551580	2.099766	1.940367
6	-2.712678	3.217344	1.125098
1	-2.088970	4.118869	-0.713955
1	-3.134893	2.035410	2.864772
6	2.064330	0.670620	-0.581403
6	2.617047	1.552690	0.382143

6	2.753622	0.515494	-1.811570
6	3.764804	2.294053	0.083207
6	3.886424	1.294027	-2.073893
6	4.405622	2.198630	-1.150691
1	4.168793	2.971880	0.842896
1	4.399706	1.182281	-3.033921
6	-0.352780	2.444563	-1.738607
6	0.616199	3.632418	-1.693524
6	-1.329450	2.586677	-2.912401
1	0.252830	1.556759	-1.950388
1	1.370793	3.504827	-0.900339
1	1.149025	3.725613	-2.656419
1	0.076676	4.578636	-1.509702
1	-1.969859	1.692555	-3.010089
1	-1.983088	3.468764	-2.799413
1	-0.769125	2.709104	-3.855657
6	-3.669073	4.332511	1.498618
6	-3.249168	5.013164	2.805996
6	-5.112995	3.825376	1.578662
1	-3.618993	5.085994	0.693535
1	-2.216609	5.394514	2.742019
1	-3.918934	5.858756	3.038626
1	-3.296333	4.304015	3.650874
1	-5.419830	3.346650	0.633903
1	-5.223763	3.080002	2.386069
1	-5.806396	4.656892	1.792324
6	-1.621021	-0.080909	2.647000
6	-3.004072	-0.638990	3.008421
6	-0.893730	0.368650	3.921652
1	-1.052862	-0.911785	2.213823
1	-3.561705	-0.952162	2.110300
1	-2.887810	-1.518075	3.665853
1	-3.618881	0.098537	3.552821
1	0.093003	0.807587	3.697751
1	-1.483814	1.138331	4.450854
1	-0.744721	-0.483457	4.607145
6	2.355392	-0.483616	-2.893908
6	3.547742	-1.268571	-3.457639
6	1.600004	0.191874	-4.048054
1	1.692786	-1.234678	-2.433158

1	4.185333	-1.678098	-2.656362
1	3.177308	-2.109264	-4.069847
1	4.181590	-0.643298	-4.110771
1	0.687921	0.712349	-3.711054
1	2.252092	0.937980	-4.539461
1	1.300266	-0.555282	-4.804111
6	5.640304	3.018388	-1.468605
6	6.810526	2.636928	-0.555583
6	5.347977	4.520425	-1.400172
1	5.930047	2.777201	-2.506180
1	7.033606	1.559617	-0.627532
1	7.718924	3.200288	-0.829341
1	6.575504	2.864268	0.498995
1	4.507641	4.790647	-2.060837
1	5.081870	4.823562	-0.372501
1	6.233437	5.103926	-1.704934
6	2.046890	1.719626	1.786665
6	1.470501	3.117048	2.038897
6	3.096182	1.366002	2.848344
1	1.213944	1.012157	1.907972
1	0.630902	3.335353	1.358957
1	1.096401	3.192938	3.075175
1	2.244192	3.892993	1.899649
1	3.561414	0.388430	2.637308
1	3.898056	2.123055	2.887201
1	2.631049	1.324526	3.849587
6	-2.199712	-2.286065	-1.386150
6	-2.636090	-2.529345	-0.042323
6	-3.097874	-3.004425	-2.239712
6	-3.756703	-3.398637	-0.074718
1	-2.171105	-2.122904	0.854502
6	-4.043052	-3.691616	-1.435596
1	-3.063063	-3.011302	-3.329234
1	-4.311632	-3.757679	0.791124
1	-4.859118	-4.315301	-1.798347
26	-4.232156	-1.565292	-1.111283
6	-6.139146	-0.865148	-1.803702
6	-6.066494	-0.681505	-0.396721
6	-5.108338	-0.086166	-2.402769
1	-6.841643	-1.511029	-2.329308

6	-4.991540	0.210689	-0.127094
1	-6.704651	-1.159678	0.345370
6	-4.403983	0.582808	-1.364931
1	-4.888217	-0.029663	-3.468211
1	-4.659501	0.552631	0.853052
1	-3.539202	1.238674	-1.477119
6	0.783667	-1.631801	1.060409
6	1.298343	-1.615078	2.400812
6	0.477031	-3.002680	0.776566
6	1.276038	-2.932464	2.923509
1	1.646319	-0.744509	2.950209
6	0.774274	-3.795117	1.912937
1	0.086331	-3.380343	-0.168432
1	1.626896	-3.233147	3.910024
1	0.669059	-4.876803	1.982472
26	2.557270	-2.848587	1.226244
6	4.225558	-2.110162	0.116713
6	4.616765	-2.344684	1.461983
6	3.789564	-3.348301	-0.433958
1	4.224990	-1.141490	-0.384493
6	4.424839	-3.724692	1.744371
1	4.982239	-1.593282	2.160407
6	3.916441	-4.345165	0.572001
1	3.397103	-3.504486	-1.438283
1	4.607233	-4.214622	2.699926
1	3.639475	-5.393791	0.472242

5-Ge-Ge-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.377254	-0.224713	-0.107879
32	-1.001837	-0.986015	-2.089224
6	-0.915661	1.209303	0.495756
6	-1.095124	2.319410	-0.373301
6	-1.675060	1.179463	1.696517
6	-1.970860	3.354164	-0.017246
6	-2.524733	2.244252	2.011394
6	-2.691617	3.345106	1.172101

1	-2.089465	4.208440	-0.691944
1	-3.081288	2.211530	2.954387
6	2.103040	0.701374	-0.533359
6	2.657322	1.588059	0.422614
6	2.779736	0.542341	-1.765856
6	3.804090	2.327296	0.112596
6	3.916716	1.312761	-2.039464
6	4.440601	2.221731	-1.123563
1	4.211474	3.013388	0.863410
1	4.422804	1.195899	-3.003215
6	-0.364829	2.503366	-1.704083
6	0.635544	3.665037	-1.653213
6	-1.327121	2.683036	-2.884473
1	0.223002	1.601102	-1.912874
1	1.386808	3.516624	-0.861115
1	1.171162	3.744434	-2.615714
1	0.119558	4.624323	-1.469386
1	-2.000813	1.816341	-2.998395
1	-1.946522	3.589528	-2.773898
1	-0.756340	2.782964	-3.823886
6	-3.629918	4.476750	1.541648
6	-3.183211	5.174247	2.830887
6	-5.076938	3.983934	1.652192
1	-3.585481	5.216048	0.723231
1	-2.148404	5.544643	2.743533
1	-3.841525	6.029499	3.060656
1	-3.222434	4.478875	3.687541
1	-5.402554	3.493737	0.719584
1	-5.181295	3.251832	2.472538
1	-5.760422	4.824264	1.862982
6	-1.595178	0.061222	2.730844
6	-2.965232	-0.511307	3.116553
6	-0.855262	0.534001	3.989524
1	-1.016177	-0.764674	2.301586
1	-3.517179	-0.872765	2.233322
1	-2.830768	-1.360870	3.808470
1	-3.594158	0.235908	3.631035
1	0.124819	0.976374	3.744360
1	-1.443374	1.304904	4.518977
1	-0.689563	-0.309186	4.682235

6	2.359634	-0.444375	-2.852196
6	3.526144	-1.306000	-3.354900
6	1.706374	0.272561	-4.040508
1	1.628071	-1.144287	-2.411250
1	4.100598	-1.745327	-2.524386
1	3.142013	-2.125085	-3.986845
1	4.223759	-0.717957	-3.974651
1	0.826429	0.862641	-3.739899
1	2.436374	0.958221	-4.506643
1	1.375862	-0.453987	-4.802493
6	5.670206	3.045296	-1.453944
6	6.845733	2.684193	-0.539672
6	5.368287	4.546440	-1.402237
1	5.958812	2.794008	-2.489563
1	7.073865	1.606968	-0.595392
1	7.750487	3.247628	-0.825745
1	6.613671	2.927125	0.512126
1	4.526453	4.804173	-2.066031
1	5.098966	4.858152	-0.377933
1	6.250152	5.132817	-1.712507
6	2.084868	1.766599	1.824611
6	1.504323	3.165166	2.063036
6	3.132888	1.426716	2.891571
1	1.254645	1.055700	1.947163
1	0.659656	3.372907	1.385782
1	1.135811	3.253270	3.100502
1	2.274358	3.942345	1.909839
1	3.596891	0.445944	2.692639
1	3.935452	2.183771	2.921900
1	2.667526	1.397799	3.893277
6	-2.172561	-2.287621	-1.220667
6	-2.556144	-2.479477	0.148899
6	-3.113436	-3.041801	-2.006565
6	-3.688847	-3.323961	0.196436
1	-2.061527	-2.032866	1.010085
6	-4.030501	-3.679613	-1.142014
1	-3.128773	-3.080899	-3.096665
1	-4.225793	-3.627964	1.094739
1	-4.870509	-4.305757	-1.441541
26	-4.160139	-1.549576	-0.918321

6	-6.093716	-0.929470	-1.533930
6	-5.930238	-0.653639	-0.148376
6	-5.113154	-0.189510	-2.249138
1	-6.820448	-1.615517	-1.967360
6	-4.852741	0.262786	-0.007389
1	-6.514693	-1.086153	0.662551
6	-4.348253	0.549546	-1.303219
1	-4.957902	-0.204471	-3.327146
1	-4.462033	0.674285	0.922420
1	-3.515212	1.220383	-1.516082
6	0.790918	-1.651318	1.190617
6	1.318103	-1.590745	2.522019
6	0.508176	-3.030506	0.939716
6	1.329556	-2.897674	3.075420
1	1.654517	-0.698751	3.045185
6	0.834000	-3.793236	2.091023
1	0.107377	-3.432517	0.009253
1	1.695816	-3.169150	4.064794
1	0.750730	-4.874821	2.187833
26	2.589140	-2.833270	1.364490
6	4.239673	-2.090178	0.225392
6	4.646580	-2.300045	1.570054
6	3.812736	-3.341351	-0.301619
1	4.226356	-1.129181	-0.290476
6	4.473796	-3.677726	1.875075
1	5.012016	-1.533829	2.252230
6	3.960745	-4.321802	0.717593
1	3.415610	-3.518336	-1.300327
1	4.672482	-4.150926	2.835729
1	3.696223	-5.375066	0.635431

5-Ge-Ge-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.453435	-0.183055	-0.050953
32	-0.814034	-1.299718	-1.852676
6	-0.869560	1.220062	0.497880
6	-1.046984	2.311874	-0.391715

6	-1.643960	1.192066	1.686382
6	-1.923406	3.350270	-0.055688
6	-2.502741	2.257680	1.977006
6	-2.655994	3.352242	1.127724
1	-2.042431	4.192107	-0.746010
1	-3.078269	2.228380	2.908129
6	2.160846	0.712826	-0.546977
6	2.700060	1.629087	0.387658
6	2.838351	0.523096	-1.775053
6	3.834929	2.377223	0.056147
6	3.959206	1.306942	-2.070270
6	4.468787	2.249193	-1.178564
1	4.237124	3.082547	0.791513
1	4.471430	1.167748	-3.027182
6	-0.336628	2.447640	-1.736110
6	0.632488	3.635323	-1.761314
6	-1.326675	2.521321	-2.904651
1	0.270170	1.551076	-1.905695
1	1.391061	3.548353	-0.965837
1	1.161176	3.673260	-2.730177
1	0.096472	4.591679	-1.627817
1	-1.953386	1.613299	-2.951512
1	-1.993684	3.396873	-2.822234
1	-0.779312	2.607467	-3.859564
6	-3.598374	4.487275	1.475724
6	-3.171233	5.192032	2.767712
6	-5.047504	3.996872	1.564863
1	-3.539135	5.221699	0.653865
1	-2.133591	5.558066	2.696373
1	-3.830036	6.051416	2.979796
1	-3.228712	4.503484	3.628827
1	-5.357620	3.500508	0.630311
1	-5.166159	3.269740	2.387689
1	-5.732976	4.839455	1.759661
6	-1.582656	0.075627	2.723638
6	-2.965124	-0.457472	3.121229
6	-0.820710	0.535613	3.973601
1	-1.033690	-0.770363	2.291862
1	-3.545494	-0.771782	2.238227
1	-2.848943	-1.330724	3.786173

1	-3.556231	0.296324	3.669564
1	0.171904	0.944491	3.720498
1	-1.382527	1.330920	4.495551
1	-0.678305	-0.304783	4.674664
6	2.437605	-0.529326	-2.803673
6	3.636343	-1.288387	-3.387820
6	1.608864	0.068880	-3.948541
1	1.823659	-1.282867	-2.284193
1	4.327117	-1.634127	-2.601109
1	3.277730	-2.170168	-3.946246
1	4.210338	-0.666321	-4.095891
1	0.695718	0.572353	-3.591867
1	2.209641	0.813561	-4.501915
1	1.300975	-0.721396	-4.655972
6	5.695733	3.069815	-1.524389
6	6.877076	2.702092	-0.619706
6	5.401191	4.571875	-1.471231
1	5.973585	2.815504	-2.562057
1	7.101157	1.624291	-0.680815
1	7.781569	3.263681	-0.909622
1	6.651971	2.941494	0.434431
1	4.553053	4.832746	-2.125625
1	5.146218	4.887390	-0.444505
1	6.282131	5.153148	-1.792720
6	2.136457	1.820621	1.791755
6	1.544332	3.216114	2.016556
6	3.195975	1.501875	2.854378
1	1.314188	1.103751	1.936976
1	0.705040	3.413551	1.329813
1	1.165930	3.307485	3.050027
1	2.310853	3.996860	1.865312
1	3.667264	0.522487	2.665659
1	3.992234	2.265685	2.867180
1	2.737956	1.483114	3.859484
6	-2.338647	-2.322300	-1.236832
6	-2.743376	-2.487513	0.125871
6	-3.292482	-3.022368	-2.037253
6	-3.912700	-3.293059	0.157733
1	-2.234119	-2.070113	0.994261
6	-4.250975	-3.624986	-1.181390

1	-3.287193	-3.076185	-3.126013
1	-4.462865	-3.585384	1.051337
1	-5.108333	-4.218468	-1.496994
26	-4.328118	-1.470723	-0.940483
6	-6.199013	-0.672738	-1.664075
6	-6.133679	-0.473669	-0.259180
6	-5.124929	0.046472	-2.260751
1	-6.929169	-1.285568	-2.191319
6	-5.019490	0.367518	0.011311
1	-6.806616	-0.904756	0.480952
6	-4.399996	0.693580	-1.223977
1	-4.890981	0.080316	-3.324350
1	-4.686455	0.709176	0.991141
1	-3.505643	1.308863	-1.335794
6	0.820234	-1.618038	1.237302
6	1.378210	-1.552212	2.555703
6	0.485125	-2.989997	1.011202
6	1.366785	-2.852110	3.123918
1	1.758794	-0.664066	3.054577
6	0.819920	-3.744489	2.164135
1	0.056889	-3.394332	0.093135
1	1.751329	-3.121885	4.106777
1	0.706614	-4.821636	2.277056
26	2.584119	-2.834040	1.374575
6	4.224442	-2.107276	0.212013
6	4.657584	-2.358108	1.541519
6	3.752536	-3.334244	-0.333453
1	4.224395	-1.135589	-0.283317
6	4.457086	-3.737752	1.819082
1	5.055412	-1.616708	2.233188
6	3.899652	-4.341425	0.659618
1	3.324639	-3.474967	-1.326065
1	4.666822	-4.238345	2.763338
1	3.604561	-5.385048	0.560556

5-Sn-Sn-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

50	0.382463	-0.229922	-0.062631
50	-1.133930	-1.110031	-2.292063
6	-0.922011	1.395769	0.577394
6	-1.072357	2.466289	-0.335068
6	-1.632723	1.424477	1.799448
6	-1.912111	3.536528	-0.007006
6	-2.447677	2.520477	2.090258
6	-2.604884	3.582764	1.199306
1	-2.026995	4.366999	-0.711549
1	-2.983936	2.543359	3.045240
6	2.264204	0.729736	-0.530174
6	2.820535	1.646149	0.388560
6	2.902718	0.511879	-1.767775
6	3.966141	2.362191	0.030890
6	4.040243	1.255705	-2.091660
6	4.578299	2.191580	-1.212066
1	4.393244	3.075958	0.743845
1	4.531829	1.097956	-3.057030
6	-0.346991	2.551489	-1.679491
6	0.695358	3.675433	-1.706318
6	-1.312149	2.684610	-2.862812
1	0.216838	1.622472	-1.843547
1	1.453920	3.535794	-0.919035
1	1.218647	3.682393	-2.679070
1	0.219335	4.661686	-1.564723
1	-2.016626	1.835290	-2.918527
1	-1.907413	3.611225	-2.801141
1	-0.749946	2.708134	-3.812606
6	-3.513804	4.743114	1.538915
6	-3.021374	5.476691	2.789591
6	-4.962498	4.269676	1.692946
1	-3.472945	5.447601	0.690484
1	-1.979346	5.813796	2.661149
1	-3.650857	6.356437	3.004356
1	-3.053546	4.812265	3.670579
1	-5.302863	3.743140	0.785442
1	-5.057006	3.569236	2.541502
1	-5.637943	5.121419	1.879766
6	-1.526105	0.330960	2.858076
6	-2.884228	-0.228150	3.297777

6	-0.737340	0.821892	4.078940
1	-0.964535	-0.510384	2.430563
1	-3.449651	-0.633594	2.442123
1	-2.733774	-1.045017	4.025089
1	-3.505164	0.541965	3.788122
1	0.247012	1.227642	3.789081
1	-1.288419	1.623814	4.601963
1	-0.572061	-0.005059	4.791424
6	2.427330	-0.515383	-2.791478
6	3.547943	-1.438615	-3.280992
6	1.742825	0.159253	-3.986707
1	1.696114	-1.174231	-2.291420
1	4.116305	-1.864886	-2.439012
1	3.118933	-2.269116	-3.868204
1	4.255172	-0.903720	-3.935903
1	0.893616	0.792399	-3.679108
1	2.466334	0.804377	-4.514695
1	1.359071	-0.591081	-4.700116
6	5.811173	2.981672	-1.590368
6	6.986274	2.627042	-0.674965
6	5.521264	4.484697	-1.591967
1	6.080440	2.685688	-2.619085
1	7.180930	1.541785	-0.693451
1	7.903302	3.153546	-0.988368
1	6.767691	2.911481	0.369085
1	4.669007	4.717470	-2.252121
1	5.265733	4.835343	-0.577036
1	6.399813	5.054235	-1.938465
6	2.247437	1.872116	1.786058
6	1.676489	3.281507	1.984373
6	3.285480	1.550762	2.867112
1	1.410096	1.169973	1.933374
1	0.826706	3.472767	1.308568
1	1.315913	3.405809	3.021142
1	2.449729	4.048645	1.800327
1	3.719034	0.548362	2.711701
1	4.108284	2.286476	2.863917
1	2.819135	1.578571	3.868502
6	-2.323149	-2.379694	-1.040452
6	-2.616790	-2.427267	0.362379

6	-3.352655	-3.133661	-1.691495
6	-3.790306	-3.198688	0.554949
1	-2.051031	-1.937014	1.156976
6	-4.245868	-3.638913	-0.721587
1	-3.437261	-3.252646	-2.773495
1	-4.277671	-3.399605	1.508571
1	-5.135006	-4.235704	-0.919305
26	-4.233199	-1.489505	-0.663990
6	-6.141464	-0.792395	-1.262870
6	-5.927947	-0.458942	0.103702
6	-5.145833	-0.136703	-2.036420
1	-6.907756	-1.464510	-1.646282
6	-4.804458	0.407912	0.173802
1	-6.509911	-0.823381	0.948946
6	-4.321143	0.607946	-1.145783
1	-5.020766	-0.205683	-3.116402
1	-4.373733	0.849080	1.071990
1	-3.473839	1.243987	-1.405710
6	0.814182	-1.677890	1.446319
6	1.376868	-1.538283	2.752158
6	0.520789	-3.062041	1.270587
6	1.414589	-2.817629	3.367794
1	1.728966	-0.612126	3.205716
6	0.888910	-3.763276	2.447317
1	0.087808	-3.500637	0.370129
1	1.810723	-3.037779	4.357775
1	0.805975	-4.837520	2.601599
26	2.613375	-2.827016	1.605905
6	4.223385	-2.114119	0.378861
6	4.675985	-2.281121	1.714645
6	3.776711	-3.379879	-0.092162
1	4.198103	-1.171180	-0.169130
6	4.512629	-3.647921	2.070334
1	5.064857	-1.492145	2.356736
6	3.958247	-4.327974	0.952407
1	3.346453	-3.585776	-1.071821
1	4.738666	-4.088109	3.040260
1	3.684132	-5.381060	0.913549

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.450232	-0.150518	-0.002848
50	-0.904532	-1.445319	-2.084788
6	-0.921302	1.440546	0.530951
6	-1.051177	2.490870	-0.405424
6	-1.648409	1.485596	1.742078
6	-1.884832	3.572736	-0.104571
6	-2.462809	2.590150	1.999403
6	-2.595228	3.640870	1.091046
1	-1.986571	4.390339	-0.825771
1	-3.017354	2.629141	2.942837
6	2.323362	0.746723	-0.557502
6	2.872090	1.686141	0.339606
6	2.963896	0.479471	-1.783879
6	4.024000	2.383766	-0.033039
6	4.104656	1.207769	-2.122024
6	4.640387	2.168014	-1.266922
1	4.453718	3.113806	0.661474
1	4.603863	1.013023	-3.076409
6	-0.322782	2.526828	-1.747105
6	0.714721	3.652537	-1.820043
6	-1.294438	2.591592	-2.929596
1	0.239760	1.591312	-1.871369
1	1.474374	3.548099	-1.027700
1	1.238311	3.621394	-2.792049
1	0.237632	4.643108	-1.718907
1	-1.972141	1.720129	-2.933762
1	-1.909500	3.507104	-2.900977
1	-0.734499	2.590639	-3.881170
6	-3.501841	4.811008	1.401290
6	-3.018728	5.562136	2.645572
6	-4.953502	4.344197	1.546590
1	-3.448216	5.501529	0.542259
1	-1.972932	5.890552	2.524621
1	-3.644316	6.449812	2.838187
1	-3.066504	4.913634	3.537714
1	-5.282220	3.797471	0.646815

1	-5.060784	3.662710	2.408933
1	-5.629199	5.201197	1.706038
6	-1.563416	0.408665	2.818863
6	-2.933259	-0.111753	3.268205
6	-0.762315	0.904794	4.030062
1	-1.026391	-0.455574	2.405187
1	-3.513308	-0.499904	2.414586
1	-2.799766	-0.932856	3.993851
1	-3.529573	0.673884	3.764224
1	0.233253	1.279815	3.735239
1	-1.293935	1.731741	4.534056
1	-0.619503	0.089866	4.760965
6	2.486646	-0.596202	-2.749618
6	3.610177	-1.488274	-3.284119
6	1.685794	-0.007273	-3.917852
1	1.828212	-1.271337	-2.183149
1	4.250616	-1.862801	-2.469070
1	3.168672	-2.357187	-3.802966
1	4.248427	-0.957951	-4.010142
1	0.825240	0.594890	-3.579525
1	2.330145	0.648356	-4.529546
1	1.298403	-0.812102	-4.569200
6	5.887152	2.926639	-1.657955
6	7.047325	2.562615	-0.727535
6	5.620800	4.432791	-1.694130
1	6.154730	2.602455	-2.678424
1	7.215449	1.472628	-0.726810
1	7.979031	3.061651	-1.041519
1	6.825807	2.868370	0.309837
1	4.772867	4.660901	-2.361617
1	5.367509	4.810491	-0.688433
1	6.507292	4.981964	-2.052106
6	2.288505	1.945303	1.727491
6	1.721910	3.360089	1.891799
6	3.309462	1.632082	2.826405
1	1.444190	1.252257	1.889542
1	0.883342	3.542507	1.199710
1	1.346603	3.504344	2.920440
1	2.501645	4.119362	1.704525
1	3.723747	0.617377	2.701755

1	4.146459	2.351037	2.811519
1	2.832496	1.695292	3.820949
6	-2.503278	-2.417016	-1.068638
6	-2.805377	-2.439524	0.327508
6	-3.539910	-3.127678	-1.733464
6	-4.010627	-3.173074	0.509765
1	-2.222290	-1.974263	1.125564
6	-4.463056	-3.599957	-0.767404
1	-3.603391	-3.264102	-2.814052
1	-4.506157	-3.362133	1.460947
1	-5.363094	-4.175532	-0.976143
26	-4.400948	-1.421287	-0.712411
6	-6.241271	-0.579177	-1.435944
6	-6.127549	-0.298959	-0.047291
6	-5.156123	0.056715	-2.102725
1	-7.004002	-1.198993	-1.905219
6	-4.974113	0.510527	0.141551
1	-6.790634	-0.662210	0.736525
6	-4.376955	0.733496	-1.126471
1	-4.947873	0.017344	-3.171696
1	-4.601772	0.902616	1.087705
1	-3.465428	1.308328	-1.298534
6	0.785946	-1.622418	1.495421
6	1.346776	-1.472000	2.801204
6	0.451546	-2.998696	1.338676
6	1.348557	-2.741512	3.435761
1	1.722483	-0.547071	3.237876
6	0.800240	-3.687060	2.528258
1	0.015930	-3.441733	0.440911
1	1.735317	-2.956594	4.430564
1	0.687547	-4.755898	2.700169
26	2.557178	-2.800702	1.667569
6	4.181374	-2.130273	0.425737
6	4.632240	-2.287401	1.763634
6	3.711888	-3.393627	-0.029304
1	4.175079	-1.196249	-0.137604
6	4.446640	-3.646570	2.136503
1	5.033734	-1.496781	2.395978
6	3.879283	-4.331126	1.027394
1	3.274028	-3.601817	-1.005764

1	4.664140	-4.076982	3.112820
1	3.585842	-5.379438	1.003737

5-Pb-pb-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.409439	-0.217879	0.046556
82	-1.279957	-1.279208	-2.144612
6	-0.817957	1.629141	0.619605
6	-0.962995	2.623084	-0.372607
6	-1.473372	1.791460	1.859440
6	-1.748800	3.753315	-0.106603
6	-2.233637	2.943030	2.088732
6	-2.390037	3.933542	1.117083
1	-1.861113	4.525992	-0.875588
1	-2.726613	3.068164	3.059752
6	2.399237	0.712836	-0.546331
6	2.998261	1.689125	0.277024
6	2.996044	0.392471	-1.781670
6	4.143769	2.357424	-0.171708
6	4.137216	1.088672	-2.198153
6	4.719994	2.081504	-1.413518
1	4.603332	3.116733	0.471736
1	4.596693	0.848503	-3.163181
6	-0.280167	2.557252	-1.738874
6	0.794142	3.638667	-1.900305
6	-1.277074	2.609067	-2.901874
1	0.250333	1.597888	-1.820556
1	1.568165	3.545426	-1.121139
1	1.291996	3.538472	-2.881205
1	0.353539	4.649536	-1.838542
1	-2.007672	1.780662	-2.855769
1	-1.848695	3.552852	-2.907223
1	-0.745591	2.531774	-3.866432
6	-3.242005	5.157377	1.388073
6	-2.684880	5.978104	2.555462
6	-4.703960	4.765742	1.627579
1	-3.203934	5.787395	0.482435

1	-1.636294	6.264590	2.370971
1	-3.276517	6.896870	2.708249
1	-2.715309	5.397648	3.494020
1	-5.100277	4.182906	0.779352
1	-4.798865	4.144418	2.535582
1	-5.334427	5.661044	1.763738
6	-1.356805	0.781561	2.995137
6	-2.711761	0.305686	3.531309
6	-0.495471	1.336779	4.136040
1	-0.840190	-0.107335	2.607182
1	-3.315904	-0.165680	2.737519
1	-2.558302	-0.440968	4.329829
1	-3.297317	1.137079	3.962256
1	0.490090	1.669976	3.767389
1	-0.986916	2.204774	4.611306
1	-0.331451	0.565644	4.908736
6	2.465326	-0.698503	-2.706387
6	3.553262	-1.672906	-3.172167
6	1.735997	-0.095938	-3.913636
1	1.743668	-1.300746	-2.128102
1	4.140971	-2.055498	-2.321762
1	3.094544	-2.532279	-3.691892
1	4.250550	-1.194477	-3.879930
1	0.913161	0.572905	-3.605383
1	2.439623	0.503318	-4.517972
1	1.314772	-0.884842	-4.562392
6	5.959295	2.814630	-1.886609
6	7.159546	2.504198	-0.986536
6	5.711334	4.321875	-1.993805
1	6.190828	2.437960	-2.898291
1	7.338623	1.417578	-0.933077
1	8.073614	2.991332	-1.366884
1	6.982081	2.867217	0.040916
1	4.849250	4.533059	-2.648185
1	5.496792	4.757093	-1.002284
1	6.596543	4.836626	-2.404646
6	2.475058	2.032183	1.668728
6	1.949577	3.468780	1.772080
6	3.536705	1.764589	2.741586
1	1.626822	1.362237	1.885379

1	1.098199	3.636938	1.092506
1	1.604863	3.679106	2.800087
1	2.742807	4.197231	1.525592
1	3.925111	0.734986	2.663989
1	4.387697	2.461536	2.646766
1	3.105786	1.900570	3.749888
6	-2.507663	-2.418275	-0.651622
6	-2.684285	-2.262195	0.762052
6	-3.650592	-3.146155	-1.119419
6	-3.900099	-2.885831	1.144037
1	-2.012450	-1.734220	1.442683
6	-4.499093	-3.437625	-0.023875
1	-3.851332	-3.403408	-2.161822
1	-4.316899	-2.916723	2.151089
1	-5.452471	-3.963834	-0.069255
26	-4.303095	-1.315592	-0.256301
6	-6.173267	-0.524855	-0.869213
6	-5.886224	-0.081729	0.451702
6	-5.157772	-0.028551	-1.730131
1	-7.004508	-1.163586	-1.164582
6	-4.696328	0.693112	0.406581
1	-6.466704	-0.311279	1.344350
6	-4.245016	0.727114	-0.938841
1	-5.085992	-0.204440	-2.803114
1	-4.199805	1.183108	1.243400
1	-3.362813	1.271084	-1.279293
6	0.873084	-1.545796	1.784842
6	1.517206	-1.284587	3.031471
6	0.544862	-2.933259	1.772071
6	1.575823	-2.496373	3.774923
1	1.917727	-0.325683	3.361030
6	0.977036	-3.519498	2.992466
1	0.049907	-3.458554	0.952995
1	2.031940	-2.623536	4.756153
1	0.888865	-4.569965	3.266317
26	2.658353	-2.718112	1.954936
6	4.213949	-2.131259	0.597660
6	4.740397	-2.238147	1.912608
6	3.703693	-3.406698	0.227695
1	4.182756	-1.221663	-0.003810

6	4.560052	-3.576781	2.354907
1	5.187438	-1.428216	2.487067
6	3.920292	-4.300473	1.312655
1	3.211291	-3.652421	-0.713001
1	4.834581	-3.970848	3.332280
1	3.617746	-5.345894	1.350930

5-Pb-Pb-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.420404	-0.194320	0.051726
82	-1.114032	-1.541154	-2.116462
6	-0.858066	1.643716	0.565141
6	-1.001523	2.615918	-0.446669
6	-1.539553	1.819280	1.788732
6	-1.809204	3.739513	-0.218062
6	-2.326382	2.960144	1.979689
6	-2.480972	3.930576	0.987608
1	-1.919312	4.494980	-1.004555
1	-2.840377	3.095106	2.938424
6	2.412296	0.757693	-0.549948
6	2.982469	1.772544	0.246597
6	3.039103	0.405938	-1.762624
6	4.123388	2.447517	-0.207439
6	4.174556	1.107439	-2.184668
6	4.726529	2.139497	-1.428312
1	4.560124	3.235378	0.417341
1	4.655769	0.839165	-3.131328
6	-0.312047	2.518748	-1.805529
6	0.691933	3.653391	-2.034861
6	-1.320574	2.425860	-2.955666
1	0.282210	1.594461	-1.830726
1	1.468803	3.649991	-1.251971
1	1.196957	3.524925	-3.008607
1	0.195799	4.639937	-2.031625
1	-1.986449	1.549839	-2.837621
1	-1.964092	3.321304	-3.006194
1	-0.799229	2.328815	-3.924025

6	-3.362283	5.142527	1.219931
6	-2.841817	6.001076	2.377443
6	-4.819496	4.726551	1.448835
1	-3.324446	5.753665	0.301465
1	-1.798279	6.310958	2.202523
1	-3.458789	6.907475	2.501927
1	-2.872344	5.440007	3.327776
1	-5.193311	4.115411	0.610310
1	-4.915323	4.126298	2.371016
1	-5.469061	5.612338	1.555189
6	-1.420779	0.838799	2.948243
6	-2.774975	0.364965	3.485570
6	-0.569982	1.431910	4.078065
1	-0.894157	-0.054345	2.584523
1	-3.379667	-0.101440	2.689183
1	-2.622110	-0.383185	4.282759
1	-3.359476	1.196043	3.918535
1	0.413072	1.766035	3.703598
1	-1.072631	2.307484	4.527084
1	-0.400143	0.683509	4.871482
6	2.542661	-0.724605	-2.657978
6	3.658055	-1.666195	-3.125485
6	1.772091	-0.172438	-3.863648
1	1.855204	-1.343060	-2.055456
1	4.276778	-2.008886	-2.279509
1	3.221295	-2.552775	-3.618039
1	4.321630	-1.178883	-3.859633
1	0.927769	0.468008	-3.553032
1	2.442916	0.446415	-4.485396
1	1.373150	-0.987033	-4.494372
6	5.964531	2.872003	-1.907928
6	7.158718	2.596298	-0.988363
6	5.708736	4.374105	-2.059235
1	6.209658	2.469808	-2.906598
1	7.347082	1.513187	-0.903767
1	8.072133	3.080996	-1.373849
1	6.968593	2.986016	0.027005
1	4.851997	4.562464	-2.727368
1	5.483304	4.836002	-1.082374
1	6.595116	4.881904	-2.476398

6	2.438704	2.143874	1.622560
6	1.896440	3.575939	1.682942
6	3.490202	1.910417	2.713027
1	1.594698	1.470287	1.845523
1	1.053804	3.714824	0.985571
1	1.533632	3.807799	2.700028
1	2.684696	4.307564	1.429706
1	3.882440	0.880307	2.667207
1	4.340347	2.606868	2.607467
1	3.049061	2.071763	3.713039
6	-2.502566	-2.469382	-0.614271
6	-2.727377	-2.300689	0.787430
6	-3.637029	-3.193332	-1.102934
6	-3.925554	-2.980923	1.156615
1	-2.070342	-1.769812	1.481022
6	-4.488433	-3.538761	-0.018396
1	-3.812635	-3.465651	-2.147011
1	-4.338418	-3.046401	2.163496
1	-5.412816	-4.112660	-0.085414
26	-4.419844	-1.290428	-0.240866
6	-6.311837	-0.412624	-0.943357
6	-6.131337	0.033265	0.385906
6	-5.246835	0.130013	-1.739776
1	-7.123171	-1.038861	-1.313093
6	-4.934563	0.804496	0.422841
1	-6.762120	-0.210706	1.239814
6	-4.425355	0.914928	-0.898635
1	-5.124078	-0.013561	-2.813520
1	-4.502939	1.288421	1.299503
1	-3.528056	1.472944	-1.172405
6	0.878949	-1.459746	1.846624
6	1.506039	-1.165268	3.095090
6	0.566517	-2.851481	1.862138
6	1.571625	-2.360339	3.864906
1	1.889719	-0.194423	3.408694
6	0.993840	-3.406859	3.098885
1	0.085994	-3.402556	1.051279
1	2.015974	-2.461427	4.854656
1	0.913410	-4.451657	3.396397
26	2.689141	-2.605870	2.050742

6	4.257493	-2.045949	0.676822
6	4.774373	-2.089379	1.999645
6	3.776547	-3.344913	0.353830
1	4.214266	-1.161409	0.039989
6	4.617275	-3.412690	2.493577
1	5.201649	-1.248606	2.544171
6	4.000289	-4.189952	1.476434
1	3.301323	-3.637697	-0.582331
1	4.890721	-3.762187	3.488147
1	3.719611	-5.239353	1.553878

6-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.115941	0.177784	0.623712
6	1.406196	0.136760	0.249440
6	2.114858	1.324916	-0.079249
6	2.145873	-1.080955	0.198148
6	3.506433	1.294012	-0.237545
6	3.535521	-1.049798	0.036031
6	4.252793	0.127205	-0.148948
1	4.030817	2.228370	-0.462482
1	4.078386	-2.000626	0.028615
6	1.486457	2.682483	-0.400153
6	1.715247	3.037389	-1.876718
6	1.991957	3.806196	0.513808
1	0.405435	2.620308	-0.279591
1	1.325388	2.242049	-2.534885
1	1.197074	3.980801	-2.125243
1	2.787211	3.172916	-2.100673
1	1.838844	3.565131	1.579358
1	3.070074	3.989316	0.367868
1	1.462811	4.749894	0.294009
6	5.760231	0.128233	-0.314065
6	6.191582	-0.658600	-1.557062
6	6.464485	-0.400137	0.939437
1	6.068690	1.178636	-0.458281
1	5.704512	-0.265276	-2.464369

1	7.284992	-0.599859	-1.694787
1	5.920907	-1.724922	-1.462158
1	6.179041	0.182138	1.830744
1	6.196409	-1.455234	1.124362
1	7.560653	-0.345298	0.823368
6	1.562566	-2.497546	0.185335
6	2.080676	-3.368307	1.336721
6	1.834763	-3.169845	-1.168693
1	0.477705	-2.450756	0.278397
1	1.901734	-2.896048	2.317403
1	1.580719	-4.352526	1.330759
1	3.165840	-3.546955	1.249027
1	1.453038	-2.549659	-1.997358
1	2.913677	-3.328599	-1.334472
1	1.338315	-4.155719	-1.211230
6	-0.906230	0.084859	-0.684730
6	-1.409004	1.163356	-1.475598
6	-1.143025	-1.107404	-1.437095
6	-1.934024	0.642875	-2.689149
1	-1.424060	2.217375	-1.204767
6	-1.767001	-0.764443	-2.665816
1	-0.909780	-2.124267	-1.127316
1	-2.412149	1.222589	-3.477172
1	-2.092854	-1.465601	-3.432619
26	-3.018690	-0.173637	-1.056881
6	-4.214387	-0.168947	0.723612
6	-4.686889	0.826122	-0.174086
6	-4.322810	-1.430370	0.076598
1	-3.807732	0.009813	1.717732
6	-5.094527	0.179977	-1.373171
1	-4.714066	1.898191	0.017163
6	-4.869013	-1.214765	-1.218774
1	-4.022668	-2.392399	0.491041
1	-5.485914	0.669357	-2.264300
1	-5.055669	-1.979556	-1.971894
6	-0.510520	1.460936	1.438406
1	0.385713	1.970939	1.832328
1	-1.057920	2.201896	0.834195
6	-0.541658	-0.956950	1.622970
1	-1.103379	-1.765352	1.123260

1	0.337823	-1.418249	2.102881
6	-1.377102	1.013186	2.582367
6	-1.394137	-0.318258	2.683975
6	-2.072460	2.031612	3.430337
6	-2.102921	-1.175358	3.685661
1	-2.624601	1.576370	4.266745
1	-1.347589	2.751860	3.851106
1	-2.788850	2.617768	2.824783
1	-2.820802	-1.852681	3.185435
1	-1.384667	-1.817410	4.227484
1	-2.655108	-0.581444	4.430195

6-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-0.141404	0.606436	0.047917
6	1.714479	0.183967	-0.065579
6	2.429511	0.388086	-1.269673
6	2.423653	-0.326321	1.051327
6	3.818528	0.213641	-1.295191
6	3.810165	-0.487291	0.984247
6	4.534238	-0.196812	-0.173160
1	4.365212	0.389758	-2.228219
1	4.344074	-0.869069	1.861844
6	1.749947	0.711954	-2.596338
6	1.920895	-0.447562	-3.587031
6	2.245666	2.027859	-3.205294
1	0.667727	0.809724	-2.423905
1	1.527517	-1.387065	-3.163713
1	1.380226	-0.234838	-4.525936
1	2.984137	-0.604693	-3.837858
1	2.129529	2.868497	-2.500962
1	3.314601	1.962187	-3.472856
1	1.685142	2.264824	-4.126129
6	6.041267	-0.363123	-0.218070
6	6.454148	-1.820407	0.016588
6	6.735939	0.572558	0.776425
1	6.368646	-0.080150	-1.233704

1	5.970727	-2.491389	-0.712256
1	7.547734	-1.934443	-0.076405
1	6.165129	-2.154016	1.028567
1	6.458981	1.623553	0.592556
1	6.451690	0.324490	1.814068
1	7.832723	0.482023	0.695738
6	1.735629	-0.804530	2.325876
6	2.212801	-0.049135	3.570736
6	1.917201	-2.317889	2.504923
1	0.653592	-0.634427	2.225294
1	2.096098	1.041165	3.453437
1	1.642371	-0.366564	4.460861
1	3.280370	-0.250294	3.768213
1	1.553490	-2.866373	1.619571
1	2.979606	-2.577740	2.651846
1	1.358437	-2.671082	3.389645
6	-1.133239	-0.896115	-0.458226
6	-1.693621	-1.174855	-1.743717
6	-1.408965	-2.037798	0.358399
6	-2.305236	-2.455738	-1.712661
1	-1.682418	-0.501761	-2.601971
6	-2.127538	-2.991406	-0.408667
1	-1.139513	-2.148359	1.410058
1	-2.842446	-2.930912	-2.532352
1	-2.504914	-3.949116	-0.052373
26	-3.247828	-1.180958	-0.285313
6	-4.227413	0.536318	0.527408
6	-4.771149	0.236029	-0.750952
6	-4.449362	-0.585285	1.371895
1	-3.707287	1.455779	0.797302
6	-5.331995	-1.069150	-0.696001
1	-4.742752	0.884429	-1.625550
6	-5.132628	-1.577097	0.616368
1	-4.131656	-0.678809	2.409601
1	-5.804685	-1.600036	-1.521125
1	-5.425517	-2.564389	0.970795
6	-0.688473	2.154439	-0.915124
1	0.163240	2.731736	-1.321086
1	-1.337098	1.914270	-1.780334
6	-0.715602	1.298485	1.726364

1	-1.382659	0.595977	2.265334
1	0.120967	1.522653	2.414019
6	-1.443051	2.993349	0.099415
6	-1.453301	2.578985	1.382665
6	-2.103047	4.234210	-0.435195
6	-2.127253	3.275561	2.533046
1	-2.617837	4.826066	0.335374
1	-1.353030	4.884221	-0.922151
1	-2.842120	3.968575	-1.213598
1	-2.886206	2.613154	2.991006
1	-1.389266	3.501452	3.324621
1	-2.622524	4.216241	2.251234

6-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.155854	0.555810	-0.010351
6	-1.786792	0.125004	0.082185
6	-2.510062	0.289115	1.288068
6	-2.490889	-0.335674	-1.059784
6	-3.898079	0.097217	1.301018
6	-3.876934	-0.514733	-1.000066
6	-4.608128	-0.284765	0.165797
1	-4.449295	0.237953	2.237333
1	-4.405544	-0.860021	-1.895523
6	-1.855464	0.600115	2.631685
6	-2.055037	-0.559936	3.617240
6	-2.366317	1.910705	3.242493
1	-0.768812	0.700969	2.481844
1	-1.674601	-1.506490	3.199413
1	-1.523727	-0.356635	4.563285
1	-3.123695	-0.697655	3.857089
1	-2.228968	2.761943	2.554753
1	-3.442697	1.841432	3.478528
1	-1.834484	2.131901	4.184259
6	-6.114064	-0.474194	0.204382
6	-6.514088	-1.924775	-0.087559
6	-6.826617	0.489487	-0.750556

1	-6.443304	-0.236198	1.230909
1	-6.022479	-2.622886	0.609404
1	-7.606534	-2.050901	0.006754
1	-6.230601	-2.213815	-1.114672
1	-6.564801	1.537052	-0.529394
1	-6.545833	0.283303	-1.798227
1	-7.921708	0.379929	-0.667565
6	-1.811821	-0.734862	-2.367600
6	-2.312423	0.083217	-3.563959
6	-1.990468	-2.235534	-2.637819
1	-0.728508	-0.557917	-2.273325
1	-2.188167	1.166516	-3.398476
1	-1.763641	-0.195855	-4.480240
1	-3.384347	-0.106115	-3.749475
1	-1.616153	-2.839090	-1.794442
1	-3.054546	-2.487647	-2.789327
1	-1.443970	-2.530377	-3.550713
6	1.195860	-1.034977	0.437387
6	1.773437	-1.358909	1.703836
6	1.494728	-2.125417	-0.436103
6	2.413421	-2.623898	1.607980
1	1.754565	-0.727825	2.593606
6	2.240201	-3.099382	0.280465
1	1.223723	-2.190156	-1.491032
1	2.963992	-3.128120	2.401374
1	2.634865	-4.030795	-0.123830
26	3.322800	-1.264452	0.241338
6	4.251048	0.503488	-0.515616
6	4.806074	0.181963	0.752986
6	4.508877	-0.584099	-1.394122
1	3.699917	1.413329	-0.756826
6	5.408294	-1.101802	0.657965
1	4.761115	0.802497	1.646963
6	5.224281	-1.575774	-0.669010
1	4.194636	-0.656807	-2.434588
1	5.903131	-1.638851	1.466141
1	5.553520	-2.539875	-1.054483
6	0.777742	2.118189	1.039174
1	-0.035418	2.652089	1.563532
1	1.506304	1.820037	1.818365

6	0.790380	1.376467	-1.698867
1	1.527076	0.721908	-2.205739
1	-0.014355	1.568786	-2.431156
6	1.434642	3.035365	0.023589
6	1.438496	2.683067	-1.279669
6	2.022920	4.301530	0.588388
6	2.039640	3.488041	-2.401849
1	2.471217	4.958730	-0.170308
1	1.243093	4.878213	1.118588
1	2.801872	4.065411	1.336567
1	2.834157	2.908019	-2.907949
1	1.272446	3.702941	-3.167798
1	2.473253	4.445458	-2.079524

6-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-0.194948	0.556782	-0.036093
6	1.977764	0.102483	-0.088220
6	2.694463	0.153615	-1.314894
6	2.686395	-0.262656	1.092940
6	4.081275	-0.066118	-1.316843
6	4.070293	-0.471968	1.031081
6	4.794553	-0.358208	-0.156623
1	4.633305	-0.025785	-2.263488
1	4.607900	-0.755323	1.944028
6	2.046281	0.358160	-2.691197
6	2.189009	-0.895089	-3.573176
6	2.582677	1.571168	-3.468695
1	0.963784	0.523981	-2.545830
1	1.788255	-1.794233	-3.078162
1	1.649241	-0.753236	-4.526489
1	3.247739	-1.086499	-3.824488
1	2.471498	2.513349	-2.907801
1	3.651025	1.449388	-3.722709
1	2.035459	1.672550	-4.423374
6	6.300795	-0.559880	-0.180926
6	6.702071	-1.977534	0.242307

6	7.014466	0.489171	0.679903
1	6.631391	-0.417915	-1.224767
1	6.211613	-2.736431	-0.388807
1	7.794738	-2.111088	0.158707
1	6.420550	-2.173924	1.291508
1	6.752550	1.510716	0.359561
1	6.731604	0.384684	1.741993
1	8.109929	0.372894	0.610088
6	2.033084	-0.536120	2.455262
6	2.560502	0.348463	3.597326
6	2.193179	-2.010328	2.869421
1	0.948962	-0.340319	2.368479
1	2.442312	1.424103	3.389119
1	2.016033	0.116650	4.530771
1	3.630454	0.155730	3.795661
1	1.810583	-2.700342	2.100459
1	3.254726	-2.258388	3.050113
1	1.651415	-2.202907	3.812687
6	-1.305093	-1.259722	-0.367688
6	-1.898771	-1.729143	-1.581026
6	-1.613635	-2.232833	0.632787
6	-2.549090	-2.968501	-1.329047
1	-1.887045	-1.213398	-2.542277
6	-2.372266	-3.280614	0.045016
1	-1.341233	-2.172510	1.687553
1	-3.102713	-3.565216	-2.053621
1	-2.765470	-4.156918	0.559527
26	-3.436048	-1.438001	-0.135682
6	-4.309384	0.437731	0.401490
6	-4.877705	-0.020664	-0.818507
6	-4.596199	-0.527078	1.405995
1	-3.737335	1.358294	0.531581
6	-5.516536	-1.265203	-0.567897
1	-4.815278	0.483809	-1.781662
6	-5.342390	-1.578484	0.807318
1	-4.281935	-0.481186	2.447881
1	-6.026689	-1.884533	-1.304451
1	-5.696281	-2.478639	1.308278
6	-0.985198	2.193535	-1.247959
1	-0.222130	2.691093	-1.873509

1	-1.773282	1.845112	-1.944667
6	-0.993975	1.669968	1.663561
1	-1.783502	1.098338	2.191230
1	-0.233176	1.919310	2.425109
6	-1.573811	3.185309	-0.256537
6	-1.578390	2.945120	1.075539
6	-2.121824	4.435899	-0.904850
6	-2.139378	3.888421	2.114576
1	-2.543439	5.164011	-0.197627
1	-1.323238	4.944757	-1.475103
1	-2.911988	4.179927	-1.634313
1	-2.943704	3.395104	2.691046
1	-1.352807	4.157677	2.842797
1	-2.548151	4.822821	1.704703

6-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-0.191653	0.532668	-0.049452
6	2.085829	0.122531	-0.079376
6	2.799314	0.118022	-1.301973
6	2.785967	-0.197613	1.112520
6	4.174709	-0.165474	-1.298559
6	4.158451	-0.476610	1.053046
6	4.880162	-0.463469	-0.138162
1	4.718037	-0.182881	-2.249402
1	4.682059	-0.742377	1.977752
6	2.182478	0.302515	-2.688812
6	2.268565	-1.012997	-3.480044
6	2.841780	1.420406	-3.511825
1	1.114812	0.561149	-2.572273
1	1.824058	-1.853765	-2.923160
1	1.755093	-0.919209	-4.452275
1	3.324225	-1.265374	-3.686406
1	2.791152	2.401041	-3.010807
1	3.904969	1.195253	-3.707637
1	2.346574	1.505702	-4.495095
6	6.370925	-0.751527	-0.167889

6	6.718130	-2.146062	0.365271
6	7.148735	0.327623	0.593838
1	6.686476	-0.712325	-1.225260
1	6.187434	-2.935856	-0.191041
1	7.803008	-2.329488	0.274277
1	6.453512	-2.244105	1.432634
1	6.920295	1.331817	0.201499
1	6.884126	0.313932	1.665758
1	8.236235	0.158451	0.511120
6	2.157682	-0.365777	2.497074
6	2.811624	0.513931	3.574733
6	2.242161	-1.836077	2.939419
1	1.090233	-0.086808	2.441825
1	2.759535	1.588317	3.333370
1	2.316053	0.350518	4.547921
1	3.875529	0.250650	3.710538
1	1.804596	-2.514425	2.189270
1	3.296685	-2.132011	3.084492
1	1.723149	-1.985809	3.901739
6	-1.313830	-1.394731	-0.334817
6	-1.918529	-1.881021	-1.534510
6	-1.623302	-2.340800	0.687794
6	-2.570993	-3.115403	-1.254697
1	-1.908120	-1.388773	-2.507845
6	-2.388019	-3.400123	0.124209
1	-1.343504	-2.263093	1.739098
1	-3.133400	-3.723195	-1.963429
1	-2.785118	-4.262785	0.658841
26	-3.458006	-1.572039	-0.090244
6	-4.348962	0.322334	0.334611
6	-4.956113	-0.236752	-0.823235
6	-4.580500	-0.566844	1.420307
1	-3.790985	1.259914	0.373319
6	-5.562938	-1.467212	-0.453503
1	-4.943910	0.191638	-1.824385
6	-5.330667	-1.671522	0.933247
1	-4.229750	-0.438005	2.443415
1	-6.095844	-2.145977	-1.118388
1	-5.655643	-2.533789	1.514257
6	-1.222426	2.105337	-1.325535

1	-0.613520	2.542512	-2.133819
1	-2.086887	1.600530	-1.799837
6	-1.170329	1.712406	1.625895
1	-2.011693	1.098525	2.001493
1	-0.516285	1.933666	2.485451
6	-1.691110	3.169917	-0.357318
6	-1.672380	2.988583	0.985217
6	-2.165739	4.434863	-1.039652
6	-2.135582	4.021959	1.989020
1	-2.529391	5.209111	-0.350184
1	-1.342366	4.874191	-1.632000
1	-2.980687	4.211965	-1.751977
1	-2.956458	3.619837	2.610560
1	-1.311328	4.273207	2.680699
1	-2.489860	4.959877	1.539567

7-C-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.524790	0.205961	-0.235202
6	1.028755	-2.030411	0.743132
6	0.563983	1.406042	-0.138219
6	0.847551	2.052596	1.126987
6	1.298007	2.027572	-1.235662
6	1.659577	3.204889	1.234746
6	2.087500	3.187512	-1.050581
6	2.295395	3.831887	0.166389
1	1.801519	3.648167	2.226758
1	2.568763	3.622877	-1.933287
6	-1.929517	0.562608	0.556842
6	-2.666799	1.720710	0.125967
6	-2.576447	-0.131309	1.648997
6	-3.882875	2.121128	0.717078
6	-3.804277	0.320891	2.191674
6	-4.501872	1.446646	1.762932
1	-4.366757	3.023884	0.330823
1	-4.242266	-0.245845	3.021668
6	0.322686	1.600089	2.489378

6	-0.675087	2.616329	3.068144
6	1.451965	1.372295	3.512824
1	-0.192574	0.642612	2.345877
1	-1.517190	2.799578	2.380754
1	-1.081209	2.257075	4.029932
1	-0.175289	3.583823	3.262624
1	2.223833	0.682461	3.136895
1	1.954229	2.314394	3.794544
1	1.036275	0.944148	4.442497
6	3.151623	5.101233	0.333945
6	2.601164	6.326379	-0.418849
6	4.630720	4.908686	-0.047862
1	3.135276	5.358990	1.408631
1	1.569945	6.570365	-0.117597
1	3.230248	7.212609	-0.211830
1	2.614125	6.169761	-1.511596
1	5.104261	4.091224	0.518947
1	4.745800	4.695077	-1.125242
1	5.198834	5.835273	0.159128
6	1.301960	1.610060	-2.712444
6	2.717781	1.448980	-3.300782
6	0.534960	2.627662	-3.576486
1	0.811921	0.638652	-2.808250
1	3.362589	0.815035	-2.670387
1	2.644273	0.984349	-4.299338
1	3.228650	2.418177	-3.438323
1	-0.467119	2.848041	-3.176028
1	1.082437	3.586880	-3.629441
1	0.420344	2.248984	-4.606415
6	-2.068010	-1.370573	2.392285
6	-3.041444	-2.561460	2.299274
6	-1.811904	-1.093403	3.887145
1	-1.120891	-1.667339	1.933270
1	-3.301517	-2.814999	1.259696
1	-2.594081	-3.451957	2.776432
1	-3.987823	-2.354886	2.832331
1	-1.159986	-0.219705	4.049928
1	-2.754669	-0.903243	4.431982
1	-1.339506	-1.974657	4.356950
6	-5.825749	1.901713	2.396138

6	-7.010263	1.887710	1.414111
6	-5.740215	3.289006	3.056217
1	-6.067193	1.181085	3.198218
1	-7.165945	0.892721	0.967742
1	-7.941628	2.173409	1.937413
1	-6.862299	2.614141	0.596012
1	-4.957119	3.331585	3.829895
1	-5.532042	4.077522	2.311929
1	-6.703748	3.542357	3.536171
6	-2.238951	2.655773	-0.996325
6	-1.825324	4.032306	-0.466373
6	-3.343696	2.812201	-2.058180
1	-1.355081	2.225344	-1.471226
1	-0.991019	3.949477	0.250019
1	-1.503143	4.675491	-1.303752
1	-2.671355	4.530990	0.040013
1	-3.787597	1.841911	-2.338548
1	-4.165187	3.453482	-1.696689
1	-2.937115	3.288470	-2.967567
6	2.287481	-2.162636	-0.110549
6	2.673930	-1.700037	-1.411756
6	3.285823	-3.137305	0.262274
6	3.848970	-2.394210	-1.831811
1	2.169231	-0.941406	-2.006270
6	4.218142	-3.294526	-0.798195
1	3.303741	-3.691376	1.200551
1	4.397194	-2.239570	-2.762520
1	5.088464	-3.952403	-0.794241
26	4.328292	-1.316840	-0.088839
6	6.291295	-1.016955	0.707318
6	6.124712	-0.184690	-0.431592
6	5.309735	-0.649240	1.668568
1	7.035600	-1.805914	0.815538
6	5.042122	0.700329	-0.176356
1	6.725774	-0.221872	-1.340214
6	4.535724	0.413396	1.120694
1	5.169580	-1.121024	2.640265
1	4.657969	1.461143	-0.854889
1	3.683213	0.908313	1.582919
6	-0.812542	-0.476593	-1.646410

6	-1.477441	0.119134	-2.794762
6	-0.361678	-1.752014	-2.159912
6	-1.348908	-0.709609	-3.944471
1	-1.974878	1.075680	-2.848939
6	-0.668103	-1.885296	-3.546635
1	0.154056	-2.531619	-1.613720
1	-1.758216	-0.505627	-4.936715
1	-0.464354	-2.752459	-4.179906
26	-2.491929	-1.715814	-2.507142
6	-4.162526	-1.933396	-1.228550
6	-4.603310	-1.426462	-2.482229
6	-3.579486	-3.213798	-1.459018
1	-4.217291	-1.404202	-0.277588
6	-4.293050	-2.387388	-3.482243
1	-5.079634	-0.462322	-2.653680
6	-3.662429	-3.490661	-2.850999
1	-3.129173	-3.871390	-0.717613
1	-4.502781	-2.297408	-4.548411
1	-3.306396	-4.390208	-3.353252
6	0.126533	-3.303890	0.619467
6	1.339967	-1.931673	2.259315
6	0.281956	-4.030486	1.948033
6	0.951373	-3.285120	2.841917
6	-0.244498	-5.427235	2.150021
1	-0.047444	-5.801147	3.167780
1	-1.335316	-5.488491	1.985998
1	0.224834	-6.138934	1.446764
6	1.316466	-3.676280	4.249235
1	0.899781	-2.976042	4.995370
1	0.951049	-4.683336	4.507088
1	2.412073	-3.681501	4.394523
1	-0.943477	-3.097914	0.417446
1	0.471062	-3.956594	-0.205050
1	0.785770	-1.137074	2.793606
1	2.412151	-1.714479	2.427534

7-Si-Si

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

14	-0.433210	0.073078	-0.168925
14	0.812241	-1.787649	0.735642
6	0.784224	1.593850	-0.125493
6	0.992754	2.208950	1.141599
6	1.462560	2.167832	-1.241614
6	1.788847	3.357486	1.253158
6	2.242960	3.318143	-1.073334
6	2.420680	3.940924	0.160210
1	1.920210	3.822069	2.235560
1	2.734143	3.747713	-1.952425
6	-2.107935	0.642498	0.659111
6	-2.768701	1.793639	0.139945
6	-2.733239	-0.011209	1.754067
6	-3.973786	2.237266	0.697924
6	-3.947371	0.465176	2.269610
6	-4.593080	1.587988	1.764160
1	-4.446652	3.131993	0.280367
1	-4.410162	-0.064408	3.108915
6	0.389570	1.710027	2.456612
6	-0.661236	2.687296	3.002122
6	1.467282	1.449366	3.518300
1	-0.114055	0.747008	2.278306
1	-1.486050	2.840033	2.286520
1	-1.091615	2.307407	3.945585
1	-0.200773	3.669077	3.214606
1	2.226056	0.735530	3.159302
1	1.983512	2.379737	3.810100
1	1.009694	1.026516	4.430189
6	3.276143	5.186505	0.306478
6	2.710356	6.365130	-0.494217
6	4.735385	4.918522	-0.080334
1	3.258314	5.467093	1.374111
1	1.671016	6.587683	-0.201314
1	3.318544	7.271439	-0.328730
1	2.719104	6.148138	-1.576798
1	5.159014	4.084315	0.502847
1	4.818380	4.661273	-1.151175
1	5.352632	5.816326	0.097208
6	1.401997	1.646606	-2.677756

6	2.793867	1.425339	-3.289628
6	0.601110	2.597898	-3.580061
1	0.896094	0.674451	-2.681656
1	3.427702	0.795560	-2.644475
1	2.693539	0.925759	-4.269004
1	3.323236	2.378617	-3.461288
1	-0.401176	2.810746	-3.173761
1	1.126137	3.564365	-3.686273
1	0.477862	2.164103	-4.587603
6	-2.176252	-1.239201	2.462600
6	-3.107882	-2.451473	2.348335
6	-1.862682	-0.962012	3.937746
1	-1.234318	-1.515867	1.977689
1	-3.342149	-2.686838	1.297534
1	-2.631825	-3.336074	2.807587
1	-4.063553	-2.269878	2.871023
1	-1.192370	-0.093717	4.055207
1	-2.785484	-0.751508	4.506338
1	-1.377189	-1.844144	4.391603
6	-5.904126	2.078196	2.353328
6	-7.042494	2.044455	1.327208
6	-5.765698	3.477711	2.963802
1	-6.169371	1.382942	3.168884
1	-7.169729	1.035662	0.901516
1	-7.994716	2.344121	1.798475
1	-6.845974	2.743342	0.495434
1	-4.968877	3.505477	3.724910
1	-5.521869	4.225004	2.188471
1	-6.712160	3.785895	3.441018
6	-2.245371	2.640416	-1.016715
6	-1.756606	4.017621	-0.547468
6	-3.301413	2.808617	-2.120931
1	-1.376075	2.131945	-1.456044
1	-0.924201	3.929946	0.170850
1	-1.404264	4.611470	-1.409678
1	-2.577704	4.577204	-0.063623
1	-3.763321	1.844117	-2.390886
1	-4.109748	3.489802	-1.804507
1	-2.845747	3.246389	-3.027231
6	2.380918	-2.159598	-0.225243

6	2.805731	-1.738052	-1.519713
6	3.312795	-3.165810	0.197607
6	3.973123	-2.459881	-1.885075
1	2.309435	-0.982706	-2.127958
6	4.283984	-3.350248	-0.821109
1	3.284063	-3.696496	1.151097
1	4.544308	-2.334551	-2.803972
1	5.137503	-4.026442	-0.779482
26	4.370972	-1.350960	-0.113485
6	6.272587	-1.037058	0.786359
6	6.155267	-0.213618	-0.366051
6	5.248805	-0.663719	1.699737
1	7.002569	-1.832881	0.931326
6	5.060189	0.670982	-0.164595
1	6.782244	-0.266972	-1.255238
6	4.498952	0.391964	1.110483
1	5.064236	-1.124527	2.669651
1	4.696083	1.423479	-0.863372
1	3.629976	0.892398	1.537055
6	-0.840733	-0.591595	-1.904325
6	-1.464303	0.035017	-3.036031
6	-0.412845	-1.879597	-2.370296
6	-1.388488	-0.830947	-4.156092
1	-1.924553	1.017270	-3.061668
6	-0.744004	-2.025318	-3.740668
1	0.084805	-2.643660	-1.775616
1	-1.799352	-0.631387	-5.145027
1	-0.563411	-2.909671	-4.349896
26	-2.533244	-1.740695	-2.618442
6	-4.157092	-1.831740	-1.237282
6	-4.623728	-1.354603	-2.491768
6	-3.627504	-3.137935	-1.438053
1	-4.169419	-1.270810	-0.301690
6	-4.382654	-2.361638	-3.466577
1	-5.070030	-0.378094	-2.675217
6	-3.767671	-3.463703	-2.814746
1	-3.173572	-3.777713	-0.682842
1	-4.605936	-2.290623	-4.530337
1	-3.437806	-4.385715	-3.291713
6	-0.139209	-3.446465	0.744816

6	1.254047	-1.883148	2.586299
6	0.135275	-4.032042	2.117738
6	0.815736	-3.276475	3.007592
6	-0.364284	-5.432835	2.349814
1	-0.174384	-5.806939	3.366324
1	-1.451969	-5.487889	2.161910
1	0.111894	-6.129922	1.636163
6	1.197702	-3.687711	4.404189
1	0.803133	-2.962490	5.139123
1	0.834634	-4.687587	4.682668
1	2.297317	-3.680997	4.518425
1	-1.226698	-3.350974	0.565495
1	0.246882	-4.125161	-0.039937
1	0.766945	-1.122557	3.221825
1	2.344885	-1.753908	2.730643

7-Ge-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-0.448766	0.122871	-0.207767
32	0.794343	-1.799663	0.700324
6	0.835664	1.663452	-0.097614
6	1.030790	2.238325	1.184965
6	1.530642	2.233738	-1.196782
6	1.840538	3.372413	1.328082
6	2.326962	3.366228	-1.000152
6	2.490859	3.962410	0.248961
1	1.967462	3.819004	2.319524
1	2.836529	3.804255	-1.864630
6	-2.158401	0.712204	0.662904
6	-2.788310	1.872569	0.142872
6	-2.772452	0.064086	1.761398
6	-3.981065	2.337990	0.704087
6	-3.974037	0.561363	2.284072
6	-4.600968	1.693229	1.773558
1	-4.440947	3.241038	0.289761
1	-4.443021	0.042765	3.127125
6	0.393821	1.708828	2.470789

6	-0.676825	2.666902	3.009111
6	1.442373	1.420332	3.553125
1	-0.102252	0.749311	2.256632
1	-1.482062	2.830683	2.274591
1	-1.133342	2.259616	3.928595
1	-0.229010	3.645662	3.257819
1	2.214137	0.720727	3.192555
1	1.945029	2.343579	3.887762
1	0.961117	0.966864	4.437664
6	3.350730	5.199116	0.418501
6	2.782839	6.382970	-0.371674
6	4.807066	4.923095	0.029952
1	3.330462	5.465749	1.489579
1	1.739897	6.591550	-0.080770
1	3.382301	7.292695	-0.196322
1	2.795901	6.173453	-1.455669
1	5.219207	4.077128	0.604605
1	4.886131	4.673496	-1.042970
1	5.434372	5.811768	0.215834
6	1.449339	1.721107	-2.632467
6	2.827291	1.488133	-3.267395
6	0.636319	2.677925	-3.515158
1	0.934864	0.752363	-2.629257
1	3.450875	0.822456	-2.649587
1	2.704501	1.020623	-4.259944
1	3.376528	2.434364	-3.415096
1	-0.356387	2.890401	-3.086267
1	1.162994	3.642877	-3.625268
1	0.491334	2.246840	-4.520904
6	-2.216433	-1.175036	2.449266
6	-3.151177	-2.381580	2.315689
6	-1.885527	-0.926279	3.924845
1	-1.278961	-1.446095	1.953340
1	-3.389475	-2.591594	1.260399
1	-2.672830	-3.276215	2.752171
1	-4.103521	-2.209631	2.847099
1	-1.201410	-0.069673	4.047392
1	-2.798412	-0.714528	4.508543
1	-1.404455	-1.822119	4.356104
6	-5.904446	2.202209	2.356984

6	-7.030920	2.173521	1.318795
6	-5.740760	3.602970	2.956192
1	-6.182649	1.515456	3.175371
1	-7.155613	1.163306	0.895247
1	-7.987764	2.480855	1.774482
1	-6.815914	2.866312	0.486477
1	-4.940503	3.618952	3.714239
1	-5.481320	4.337530	2.173806
1	-6.679271	3.934547	3.432598
6	-2.223331	2.697765	-1.007179
6	-1.645914	4.035126	-0.524496
6	-3.264681	2.935066	-2.109375
1	-1.390182	2.139852	-1.457736
1	-0.829705	3.886325	0.201856
1	-1.241110	4.607370	-1.378487
1	-2.432616	4.645442	-0.044791
1	-3.774611	1.997618	-2.388577
1	-4.034086	3.657314	-1.787480
1	-2.781528	3.354491	-3.009782
6	2.405621	-2.159439	-0.328142
6	2.797574	-1.689503	-1.615348
6	3.376156	-3.131295	0.069656
6	3.993517	-2.352191	-2.000706
1	2.261337	-0.945831	-2.204099
6	4.349083	-3.249679	-0.957299
1	3.376466	-3.676894	1.014811
1	4.551613	-2.185260	-2.921169
1	5.230718	-3.889648	-0.935389
26	4.348810	-1.258263	-0.203736
6	6.214909	-0.885830	0.742539
6	6.099599	-0.061377	-0.409752
6	5.159782	-0.545882	1.633463
1	6.962209	-1.662283	0.901275
6	4.975498	0.790189	-0.228826
1	6.745379	-0.093409	-1.286248
6	4.392711	0.489266	1.030888
1	4.964192	-1.013879	2.597729
1	4.604597	1.535818	-0.931233
1	3.499963	0.965663	1.437213
6	-0.866472	-0.524531	-2.023324

6	-1.485090	0.118742	-3.144295
6	-0.460955	-1.817371	-2.488042
6	-1.440524	-0.752034	-4.263425
1	-1.930857	1.108829	-3.158854
6	-0.811282	-1.956460	-3.855041
1	0.027602	-2.589194	-1.893230
1	-1.858437	-0.546463	-5.248192
1	-0.651134	-2.842263	-4.467874
26	-2.579368	-1.639196	-2.697984
6	-4.175077	-1.695647	-1.276688
6	-4.659782	-1.215011	-2.522856
6	-3.671545	-3.010653	-1.483444
1	-4.162785	-1.132790	-0.341933
6	-4.457182	-2.229534	-3.498486
1	-5.092228	-0.231031	-2.699446
6	-3.846473	-3.339444	-2.855449
1	-3.209703	-3.652583	-0.734608
1	-4.699568	-2.157316	-4.557799
1	-3.539147	-4.267974	-3.334466
6	-0.214952	-3.507486	0.746374
6	1.230345	-1.933359	2.625413
6	0.049347	-4.060501	2.133318
6	0.740480	-3.314121	3.024045
6	-0.489013	-5.444403	2.381325
1	-0.318241	-5.813148	3.402851
1	-1.576017	-5.470828	2.183127
1	-0.026001	-6.159534	1.677018
6	1.093594	-3.727388	4.427962
1	0.707493	-2.986870	5.152326
1	0.705499	-4.716544	4.709643
1	2.191753	-3.742565	4.552739
1	-1.299662	-3.384651	0.572413
1	0.151266	-4.207325	-0.027676
1	0.749519	-1.162053	3.252655
1	2.320404	-1.834880	2.789395

7-Sn-Sn

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

50	0.521931	0.218241	0.275394
50	-0.917950	-1.845434	-0.694110
6	-0.837999	1.884703	0.063098
6	-1.005202	2.409477	-1.238093
6	-1.521669	2.467769	1.150970
6	-1.794829	3.551689	-1.411111
6	-2.297394	3.606368	0.930175
6	-2.431206	4.171582	-0.338718
1	-1.915011	3.981031	-2.411168
1	-2.807537	4.072832	1.779315
6	2.354945	0.755122	-0.712160
6	2.999472	1.902729	-0.202293
6	2.909749	0.063237	-1.808252
6	4.193987	2.329101	-0.781187
6	4.117828	0.518809	-2.349592
6	4.774272	1.639822	-1.847611
1	4.687305	3.223224	-0.386956
1	4.568835	-0.020106	-3.189739
6	-0.360327	1.809685	-2.490972
6	0.751606	2.707001	-3.048572
6	-1.395476	1.496913	-3.578674
1	0.106756	0.843675	-2.232179
1	1.556010	2.860931	-2.310756
1	1.202089	2.250158	-3.947623
1	0.345340	3.693349	-3.334273
1	-2.180550	0.816504	-3.207771
1	-1.882316	2.414440	-3.949753
1	-0.906521	1.009415	-4.440551
6	-3.252776	5.426116	-0.531564
6	-2.635239	6.596517	0.239849
6	-4.711800	5.187611	-0.132911
1	-3.226664	5.673194	-1.606867
1	-1.585965	6.754167	-0.061037
1	-3.195911	7.528917	0.059215
1	-2.645815	6.396740	1.325604
1	-5.136232	4.336485	-0.691056
1	-4.788957	4.954346	0.943616
1	-5.326223	6.081747	-0.331400
6	-1.425924	1.934298	2.576865

6	-2.792519	1.723861	3.238402
6	-0.552096	2.841411	3.451527
1	-0.941986	0.947405	2.546534
1	-3.434167	1.063211	2.633736
1	-2.658915	1.256177	4.229331
1	-3.324923	2.678608	3.391694
1	0.447416	2.992452	3.009554
1	-1.021700	3.834710	3.566235
1	-0.419747	2.400846	4.454986
6	2.277241	-1.169750	-2.446813
6	3.147366	-2.421034	-2.291665
6	1.914188	-0.951862	-3.919300
1	1.336409	-1.381350	-1.921810
1	3.374346	-2.623027	-1.231915
1	2.619194	-3.297902	-2.707429
1	4.105834	-2.310813	-2.828080
1	1.246805	-0.082173	-4.045047
1	2.815374	-0.780977	-4.533416
1	1.397031	-1.846152	-4.311238
6	6.089451	2.103090	-2.433051
6	7.198606	2.050994	-1.378460
6	5.951067	3.499805	-3.045191
1	6.353242	1.399647	-3.241486
1	7.278586	1.041037	-0.943039
1	8.173256	2.322524	-1.816957
1	6.988419	2.755475	-0.554834
1	5.147273	3.517555	-3.799758
1	5.699852	4.243550	-2.269022
1	6.892268	3.814104	-3.526189
6	2.429998	2.733637	0.943816
6	1.844671	4.063362	0.451477
6	3.450537	2.962334	2.062038
1	1.596277	2.179131	1.406069
1	1.026888	3.903245	-0.270794
1	1.435738	4.641886	1.299040
1	2.626852	4.671303	-0.036729
1	3.917235	2.011548	2.369905
1	4.249129	3.652802	1.743506
1	2.955787	3.410893	2.941724
6	-2.641129	-2.151438	0.476381

6	-2.976643	-1.597141	1.742553
6	-3.680365	-3.055283	0.116436
6	-4.218452	-2.147435	2.155296
1	-2.375005	-0.871764	2.291453
6	-4.651958	-3.053455	1.149029
1	-3.716076	-3.627749	-0.811483
1	-4.749327	-1.911286	3.075997
1	-5.575335	-3.628194	1.158287
26	-4.480074	-1.086149	0.299718
6	-6.272325	-0.604990	-0.729382
6	-6.138544	0.242043	0.404858
6	-5.170337	-0.358451	-1.593395
1	-7.059108	-1.339607	-0.891972
6	-4.957110	1.014148	0.236748
1	-6.806876	0.273514	1.263767
6	-4.357016	0.641721	-0.994419
1	-4.975704	-0.859090	-2.541225
1	-4.562736	1.758970	0.926979
1	-3.430667	1.058841	-1.392279
6	0.906129	-0.476814	2.254144
6	1.565088	0.146336	3.354742
6	0.468098	-1.759369	2.708659
6	1.529523	-0.736214	4.465682
1	2.037601	1.127336	3.339994
6	0.852958	-1.918202	4.064478
1	-0.052289	-2.512865	2.112698
1	1.973690	-0.551529	5.442228
1	0.678342	-2.802070	4.675442
26	2.591646	-1.642985	2.843450
6	4.128819	-1.737704	1.348596
6	4.672913	-1.275098	2.577080
6	3.594883	-3.037513	1.569870
1	4.109313	-1.175985	0.412861
6	4.477717	-2.286982	3.556988
1	5.139280	-0.303847	2.737034
6	3.810790	-3.376618	2.933780
1	3.089451	-3.662152	0.833864
1	4.756167	-2.222865	4.607708
1	3.491165	-4.296564	3.421104
6	0.154175	-3.702508	-0.804594

6	-1.316471	-2.032764	-2.791923
6	-0.140609	-4.187344	-2.209232
6	-0.812634	-3.429653	-3.111274
6	0.370378	-5.580899	-2.456375
1	0.197374	-5.959859	-3.472209
1	1.454771	-5.616747	-2.245394
1	-0.106473	-6.272654	-1.738186
6	-1.158545	-3.857149	-4.512013
1	-0.748359	-3.128861	-5.235337
1	-0.797764	-4.858731	-4.780455
1	-2.256296	-3.835574	-4.638339
1	1.240523	-3.579058	-0.644407
1	-0.202809	-4.423770	-0.047630
1	-0.789314	-1.273505	-3.397724
1	-2.393092	-1.927671	-3.018951

7-Pb-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.560603	0.285129	0.294818
82	-1.033975	-1.833144	-0.592485
6	-0.748667	2.074298	-0.015369
6	-0.895273	2.538140	-1.337870
6	-1.391822	2.734780	1.049464
6	-1.637236	3.705211	-1.561276
6	-2.119836	3.895288	0.777672
6	-2.240816	4.403817	-0.517424
1	-1.746109	4.089723	-2.581274
1	-2.603353	4.424985	1.605698
6	2.478781	0.727314	-0.757127
6	3.177775	1.862430	-0.299713
6	2.979622	-0.035149	-1.828110
6	4.381108	2.209391	-0.916904
6	4.199292	0.342932	-2.406277
6	4.914798	1.453011	-1.962962
1	4.921093	3.095770	-0.567425
1	4.611585	-0.251798	-3.228991
6	-0.281799	1.844590	-2.555812

6	0.861370	2.664454	-3.166076
6	-1.334627	1.502416	-3.616634
1	0.151030	0.881373	-2.237470
1	1.674442	2.825162	-2.438803
1	1.289711	2.139557	-4.038273
1	0.495680	3.649519	-3.506075
1	-2.135259	0.867059	-3.200729
1	-1.799894	2.411043	-4.034808
1	-0.867184	0.952930	-4.452746
6	-3.010077	5.683690	-0.768117
6	-2.337389	6.865951	-0.062738
6	-4.476056	5.536384	-0.349869
1	-2.982774	5.875077	-1.854818
1	-1.284897	6.964248	-0.377023
1	-2.860111	7.810604	-0.289242
1	-2.348803	6.724962	1.032238
1	-4.945974	4.678673	-0.859235
1	-4.557544	5.366756	0.738203
1	-5.048070	6.447587	-0.593716
6	-1.295709	2.259452	2.494568
6	-2.656621	2.145723	3.189192
6	-0.353127	3.152373	3.309895
1	-0.864253	1.247653	2.494213
1	-3.335550	1.480902	2.631025
1	-2.524668	1.725471	4.201219
1	-3.146460	3.128886	3.299160
1	0.643686	3.221226	2.841335
1	-0.759690	4.176731	3.387185
1	-0.225726	2.749855	4.329778
6	2.277508	-1.264253	-2.395451
6	3.089458	-2.547542	-2.192194
6	1.901414	-1.098939	-3.871477
1	1.337457	-1.399513	-1.843092
1	3.320540	-2.712613	-1.126885
1	2.515101	-3.415652	-2.562333
1	4.045166	-2.508137	-2.743491
1	1.266463	-0.210031	-4.028109
1	2.799474	-0.991350	-4.504509
1	1.345683	-1.989307	-4.216387
6	6.242934	1.829842	-2.586234

6	7.367933	1.772179	-1.548088
6	6.166650	3.203303	-3.259829
1	6.462157	1.080349	-3.366364
1	7.411714	0.779469	-1.070239
1	8.345660	1.979822	-2.014581
1	7.206361	2.520989	-0.753053
1	5.361775	3.226685	-4.012923
1	5.956637	3.992894	-2.517393
1	7.119596	3.450370	-3.757422
6	2.664676	2.762601	0.819665
6	2.119916	4.088382	0.273834
6	3.711995	3.001073	1.910676
1	1.822896	2.256691	1.319947
1	1.292497	3.921722	-0.435902
1	1.735380	4.716930	1.096617
1	2.916963	4.649330	-0.245866
1	4.128619	2.045221	2.270906
1	4.543865	3.627037	1.546310
1	3.252443	3.526658	2.766436
6	-2.827155	-1.992452	0.647802
6	-3.096518	-1.322250	1.873855
6	-3.949410	-2.814038	0.351929
6	-4.380411	-1.728223	2.330303
1	-2.432192	-0.612912	2.371278
6	-4.906721	-2.653475	1.388375
1	-4.057354	-3.438783	-0.535885
1	-4.880056	-1.381483	3.233789
1	-5.880636	-3.138128	1.439807
26	-4.569492	-0.774873	0.421156
6	-6.309611	-0.216796	-0.654993
6	-6.126290	0.677017	0.435587
6	-5.179855	-0.101529	-1.511171
1	-7.148637	-0.897433	-0.791680
6	-4.886173	1.346269	0.249168
1	-6.801700	0.804515	1.280097
6	-4.299345	0.863518	-0.950316
1	-5.010573	-0.668893	-2.425739
1	-4.447020	2.095995	0.905813
1	-3.335960	1.183467	-1.350438
6	0.950144	-0.315739	2.384255

6	1.661362	0.326013	3.439562
6	0.472712	-1.559121	2.895492
6	1.619213	-0.513792	4.586425
1	2.175734	1.284744	3.376566
6	0.885722	-1.681390	4.248598
1	-0.093736	-2.311032	2.340915
1	2.093957	-0.312027	5.545625
1	0.692756	-2.532860	4.899484
26	2.601962	-1.526329	2.983148
6	4.088431	-1.739349	1.450334
6	4.691482	-1.264838	2.646362
6	3.502502	-3.004946	1.729356
1	4.071186	-1.209637	0.496311
6	4.481790	-2.235879	3.663221
1	5.208270	-0.312989	2.761660
6	3.746325	-3.311924	3.096071
1	2.944443	-3.626149	1.029348
1	4.798257	-2.154210	4.701992
1	3.402076	-4.201181	3.622073
6	0.000457	-3.804101	-0.699850
6	-1.422414	-2.137893	-2.763467
6	-0.301899	-4.301754	-2.094240
6	-0.945111	-3.551818	-3.022962
6	0.169971	-5.717974	-2.306526
1	-0.017429	-6.120459	-3.310746
1	1.254178	-5.781847	-2.101779
1	-0.322874	-6.378954	-1.570405
6	-1.288453	-4.021691	-4.414092
1	-0.846308	-3.339455	-5.162858
1	-0.956196	-5.043697	-4.639238
1	-2.383211	-3.975486	-4.558261
1	1.086921	-3.681824	-0.542980
1	-0.367959	-4.504297	0.069392
1	-0.861262	-1.402289	-3.367726
1	-2.491236	-2.015666	-3.011720

8-C-C

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

6	0.836620	-1.188103	0.201150
6	-0.822006	0.954360	1.149721
6	2.298868	-0.777594	-0.061432
6	2.720678	-0.275431	-1.350903
6	3.393115	-0.959119	0.860605
6	4.078905	-0.151007	-1.683124
6	4.733324	-0.813671	0.462983
6	5.130487	-0.438459	-0.815240
1	4.335570	0.216911	-2.681037
1	5.510717	-1.001075	1.211022
6	-2.250625	0.708271	0.630053
6	-2.726278	1.237008	-0.630618
6	-3.267026	-0.045079	1.335638
6	-4.040565	1.016793	-1.084185
6	-4.571032	-0.193279	0.836352
6	-5.013761	0.319123	-0.376822
1	-4.322482	1.428848	-2.056993
1	-5.292305	-0.745330	1.446494
6	1.794793	0.276738	-2.431689
6	2.124782	-0.228049	-3.847194
6	1.868838	1.805868	-2.412669
1	0.761481	0.003545	-2.200107
1	2.296286	-1.315217	-3.876337
1	1.293555	0.006087	-4.533360
1	3.025489	0.266174	-4.252416
1	1.559884	2.209088	-1.434418
1	2.898163	2.151376	-2.622143
1	1.209329	2.224568	-3.192500
6	6.595102	-0.311838	-1.233207
6	7.348736	-1.649977	-1.183059
6	7.377131	0.731653	-0.420561
1	6.600010	0.025961	-2.284872
1	6.866668	-2.418126	-1.808182
1	8.384204	-1.514819	-1.545042
1	7.409411	-2.033365	-0.149231
1	6.913447	1.729685	-0.470655
1	7.453252	0.438942	0.641448
1	8.407625	0.815324	-0.811276
6	3.265496	-1.290877	2.338979

6	3.907771	-0.203443	3.214336
6	3.858853	-2.666309	2.665830
1	2.210898	-1.293104	2.607764
1	3.539705	0.799343	2.938263
1	3.662844	-0.380776	4.275796
1	5.008200	-0.193222	3.124581
1	3.397440	-3.458101	2.051047
1	4.945551	-2.686245	2.469225
1	3.708930	-2.912898	3.730754
6	-3.114860	-0.709263	2.695348
6	-3.631971	-2.155052	2.730577
6	-3.784957	0.131979	3.788343
1	-2.058610	-0.792519	2.920908
1	-3.284158	-2.720386	1.848731
1	-3.255419	-2.660527	3.636897
1	-4.733517	-2.216532	2.758645
1	-3.401392	1.166757	3.789653
1	-4.876947	0.182640	3.625579
1	-3.610963	-0.310071	4.784916
6	-6.450126	0.120106	-0.862765
6	-6.544953	-0.704209	-2.155119
6	-7.227271	1.433019	-1.046380
1	-6.971395	-0.453618	-0.075606
1	-6.066624	-1.691044	-2.049212
1	-7.605413	-0.866741	-2.420972
1	-6.070790	-0.177737	-3.001888
1	-7.256074	2.030841	-0.121533
1	-6.787968	2.054021	-1.846674
1	-8.269968	1.211976	-1.339544
6	-1.915641	2.058634	-1.629844
6	-2.631763	3.384701	-1.938363
6	-1.697508	1.275992	-2.931694
1	-0.931103	2.289155	-1.201331
1	-2.822622	3.964702	-1.019875
1	-2.036895	4.001784	-2.628643
1	-3.603054	3.214521	-2.432439
1	-1.210026	0.306980	-2.740358
1	-2.658094	1.070850	-3.437349
1	-1.072046	1.857893	-3.631623
6	-0.259551	2.399780	1.092524

6	1.112134	2.757118	1.328818
6	-1.027794	3.515967	1.565208
6	1.167778	3.980744	2.054612
1	1.977349	2.137912	1.082863
6	-0.163513	4.459266	2.192170
1	-2.115862	3.588471	1.534504
1	2.069283	4.493031	2.393452
1	-0.464520	5.395768	2.663452
26	0.397757	4.457392	0.171103
6	0.320329	6.529405	-0.432916
6	1.657117	6.065796	-0.531928
6	-0.482548	5.748433	-1.301933
1	-0.029413	7.337534	0.209241
6	1.683915	4.995938	-1.462683
1	2.509863	6.457372	0.022435
6	0.360751	4.796493	-1.939417
1	-1.555228	5.861283	-1.436355
1	2.565023	4.422594	-1.743992
1	0.054389	4.035877	-2.653478
6	0.186581	-1.842504	-1.010340
6	-1.205101	-1.907836	-1.365719
6	0.882823	-2.570271	-2.030474
6	-1.331003	-2.559726	-2.626896
1	-2.040113	-1.494326	-0.798770
6	-0.035479	-2.972574	-3.038105
1	1.954121	-2.765393	-2.041873
1	-2.261997	-2.752205	-3.160712
1	0.203103	-3.545335	-3.934470
26	-0.570177	-3.972170	-1.270531
6	-0.241489	-5.350700	0.340871
6	-1.639673	-5.160346	0.166744
6	0.280572	-5.901290	-0.859786
1	0.331052	-5.106075	1.233454
6	-1.980400	-5.598041	-1.140676
1	-2.332708	-4.748815	0.898915
6	-0.795169	-6.055624	-1.773504
1	1.322107	-6.154096	-1.052085
1	-2.974202	-5.583748	-1.587072
1	-0.724788	-6.450947	-2.786542
6	-0.410358	0.658960	2.636665

6	0.408866	-2.083381	1.391006
1	0.522636	1.217443	2.806156
1	-1.145498	1.225165	3.248020
1	1.099483	-2.951980	1.330274
1	-0.566663	-2.514567	1.100493
6	0.244707	-1.792944	2.875177
6	-0.144486	-0.626444	3.401620
6	-0.250938	-0.375279	4.894116
1	0.363885	0.502293	5.169780
1	-1.287301	-0.136739	5.196813
1	0.095350	-1.211060	5.516976
6	0.412763	-3.052052	3.701659
1	0.142045	-2.925928	4.758754
1	-0.240506	-3.851915	3.303389
1	1.447291	-3.438136	3.664249

8-Si-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	0.363968	-1.133410	0.251581
14	-0.362625	0.986082	1.050008
6	2.243286	-1.323419	-0.156208
6	2.706545	-1.014654	-1.464486
6	3.194453	-1.830662	0.766687
6	4.026303	-1.306674	-1.829633
6	4.504232	-2.104993	0.357468
6	4.942249	-1.869915	-0.943999
1	4.363930	-1.068900	-2.843264
1	5.209652	-2.511551	1.090648
6	-2.198347	1.326967	0.529533
6	-2.478352	1.940154	-0.723906
6	-3.313611	0.901045	1.299861
6	-3.801616	2.096815	-1.154385
6	-4.619473	1.111270	0.841109
6	-4.894943	1.701805	-0.386459
1	-3.987649	2.556234	-2.130383
1	-5.459227	0.797187	1.469137
6	1.877089	-0.255908	-2.494722

6	1.963560	-0.833085	-3.912933
6	2.305343	1.213349	-2.498868
1	0.819443	-0.280326	-2.199742
1	1.804450	-1.922673	-3.923956
1	1.192418	-0.370291	-4.552333
1	2.943345	-0.623330	-4.376038
1	2.131284	1.686217	-1.516935
1	3.380532	1.301582	-2.738718
1	1.739534	1.773555	-3.263216
6	6.363967	-2.184331	-1.371950
6	6.659697	-3.685626	-1.282486
6	7.391395	-1.380214	-0.567652
1	6.457275	-1.885284	-2.430621
1	5.945177	-4.269537	-1.885204
1	7.679177	-3.902198	-1.645818
1	6.591169	-4.037236	-0.238110
1	7.195658	-0.297780	-0.637940
1	7.364954	-1.661572	0.499581
1	8.411838	-1.573733	-0.940947
6	2.889498	-2.066509	2.238190
6	3.784369	-1.209640	3.142531
6	2.995821	-3.548286	2.614102
1	1.863379	-1.740210	2.437750
1	3.725897	-0.144275	2.862641
1	3.463567	-1.307183	4.194295
1	4.842625	-1.518579	3.081999
1	2.313724	-4.166853	2.006000
1	4.021207	-3.924905	2.450536
1	2.750036	-3.698579	3.679431
6	-3.197048	0.233769	2.659743
6	-4.037126	-1.042591	2.780779
6	-3.540907	1.223578	3.779078
1	-2.162707	-0.084231	2.797416
1	-3.867838	-1.707520	1.916417
1	-3.756282	-1.587776	3.698816
1	-5.118606	-0.830090	2.839177
1	-2.885846	2.110820	3.742877
1	-4.584272	1.573643	3.680820
1	-3.434437	0.748492	4.769913
6	-6.321937	1.909565	-0.858719

6	-6.613645	1.124807	-2.141721
6	-6.648193	3.395988	-1.041488
1	-6.983502	1.516900	-0.066801
1	-6.408852	0.050121	-2.005902
1	-7.670868	1.242673	-2.436140
1	-5.988514	1.487978	-2.976038
1	-6.467005	3.961234	-0.112684
1	-6.027083	3.842499	-1.837588
1	-7.706435	3.527024	-1.326617
6	-1.413362	2.464322	-1.685134
6	-1.662557	3.945729	-1.998694
6	-1.365847	1.638314	-2.976304
1	-0.422583	2.401505	-1.205366
1	-1.635207	4.552393	-1.077496
1	-0.902916	4.333473	-2.696054
1	-2.645407	4.096597	-2.476128
1	-1.148687	0.576627	-2.769770
1	-2.332064	1.683920	-3.509825
1	-0.589407	2.029502	-3.657605
6	0.715487	2.554784	1.045959
6	2.119644	2.523800	1.328341
6	0.235009	3.798193	1.568964
6	2.480351	3.699635	2.038367
1	2.797244	1.709173	1.062441
6	1.310833	4.494617	2.182757
1	-0.800279	4.141256	1.523416
1	3.483249	3.968812	2.368839
1	1.258538	5.479830	2.645446
26	1.771839	4.262622	0.130322
6	2.189014	6.230158	-0.581703
6	3.351657	5.424677	-0.705549
6	1.166655	5.653758	-1.380065
1	2.088070	7.117812	0.041489
6	3.049593	4.348039	-1.579975
1	4.297938	5.584274	-0.190256
6	1.698038	4.488288	-1.996474
1	0.152532	6.033297	-1.482607
1	3.727270	3.543761	-1.859889
1	1.164384	3.809739	-2.658523
6	-0.607192	-1.881368	-1.197910

6	-1.957577	-1.584108	-1.566388
6	-0.103356	-2.771587	-2.196503
6	-2.258834	-2.248872	-2.785871
1	-2.643857	-0.942626	-1.009102
6	-1.107406	-2.983749	-3.178569
1	0.895061	-3.211712	-2.199435
1	-3.215338	-2.226762	-3.307049
1	-1.026313	-3.631789	-4.050817
26	-1.809439	-3.710991	-1.317508
6	-1.684136	-5.079896	0.336418
6	-2.983493	-4.504892	0.291767
6	-1.468684	-5.777876	-0.880932
1	-0.976212	-4.998548	1.158703
6	-3.572430	-4.852673	-0.954075
1	-3.443957	-3.898514	1.070741
6	-2.636510	-5.639094	-1.678253
1	-0.560511	-6.309459	-1.161557
1	-4.556852	-4.546396	-1.305391
1	-2.778300	-6.039075	-2.681593
6	-0.014084	0.648288	2.926214
6	-0.322524	-2.187819	1.702673
1	1.061430	0.905738	3.006312
1	-0.511574	1.473603	3.473464
1	0.139334	-3.184378	1.564573
1	-1.377251	-2.348502	1.393411
6	-0.320637	-1.867215	3.183366
6	-0.214610	-0.632899	3.712584
6	-0.238876	-0.352059	5.198379
1	0.628563	0.276947	5.468021
1	-1.139869	0.233161	5.460623
1	-0.214287	-1.246793	5.833951
6	-0.526959	-3.120350	4.004786
1	-0.700768	-2.941088	5.073884
1	-1.398176	-3.678162	3.613081
1	0.344956	-3.793498	3.906332

8-Ge-Ge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

32	0.475963	-1.123705	0.223352
32	-0.468066	1.010739	0.989779
6	2.429910	-1.177896	-0.197985
6	2.862182	-0.862187	-1.512247
6	3.406529	-1.585671	0.743918
6	4.204121	-1.051678	-1.866083
6	4.736316	-1.761574	0.343452
6	5.157640	-1.519652	-0.963522
1	4.526415	-0.811803	-2.884041
1	5.469760	-2.094447	1.086099
6	-2.388890	1.207579	0.448642
6	-2.707650	1.778680	-0.811831
6	-3.456507	0.705736	1.234998
6	-4.039955	1.825937	-1.241282
6	-4.775748	0.805248	0.775185
6	-5.096168	1.354174	-0.462350
1	-4.263082	2.255008	-2.223425
1	-5.588406	0.434744	1.408063
6	1.964428	-0.207566	-2.558311
6	2.105583	-0.809434	-3.962071
6	2.242715	1.299534	-2.595682
1	0.913107	-0.333529	-2.264627
1	2.028393	-1.908119	-3.944629
1	1.305489	-0.423436	-4.616657
1	3.069705	-0.539077	-4.426459
1	2.028197	1.775547	-1.621982
1	3.302279	1.489270	-2.846331
1	1.619084	1.784843	-3.366861
6	6.601204	-1.732074	-1.383293
6	7.010096	-3.205216	-1.266120
6	7.563147	-0.836325	-0.594296
1	6.674045	-1.447098	-2.447318
1	6.343977	-3.852214	-1.859600
1	8.043997	-3.350414	-1.623744
1	6.965035	-3.542891	-0.216055
1	7.286336	0.226407	-0.687132
1	7.555777	-1.096597	0.478396
1	8.596086	-0.959394	-0.962596
6	3.103491	-1.812631	2.218950

6	3.920936	-0.870124	3.112230
6	3.318830	-3.273904	2.629157
1	2.051214	-1.563087	2.403523
1	3.784753	0.181475	2.807985
1	3.597488	-0.968896	4.163038
1	5.000017	-1.099498	3.067909
1	2.688258	-3.955620	2.033321
1	4.370434	-3.575601	2.478219
1	3.079263	-3.418118	3.696713
6	-3.269211	0.073936	2.605824
6	-4.002749	-1.263626	2.759869
6	-3.681747	1.052426	3.713044
1	-2.207905	-0.154176	2.738175
1	-3.780351	-1.935089	1.913006
1	-3.679581	-1.760747	3.690891
1	-5.097500	-1.136233	2.815086
1	-3.101771	1.989383	3.656063
1	-4.750968	1.314571	3.620272
1	-3.527672	0.604533	4.710287
6	-6.536047	1.433360	-0.937051
6	-6.762572	0.592389	-2.198157
6	-6.983790	2.882750	-1.158630
1	-7.163591	1.008885	-0.134084
1	-6.471753	-0.457995	-2.033340
1	-7.825474	0.615970	-2.494242
1	-6.168199	0.981362	-3.043070
1	-6.851578	3.485065	-0.245163
1	-6.400740	3.358400	-1.966239
1	-8.048580	2.918594	-1.446546
6	-1.672702	2.360136	-1.773531
6	-2.019668	3.811199	-2.133184
6	-1.541626	1.503991	-3.039682
1	-0.686413	2.384665	-1.279995
1	-2.070642	4.441158	-1.229032
1	-1.263646	4.236703	-2.813081
1	-2.992814	3.877261	-2.648556
1	-1.243579	0.469053	-2.798926
1	-2.501352	1.457601	-3.584831
1	-0.789472	1.935864	-3.723568
6	0.529944	2.711325	0.983094

6	1.929817	2.779851	1.275031
6	-0.040504	3.930148	1.468559
6	2.204696	3.999973	1.950552
1	2.662727	2.005792	1.036549
6	0.982155	4.716831	2.066095
1	-1.095919	4.200687	1.407088
1	3.184163	4.346853	2.277963
1	0.859099	5.708521	2.499933
26	1.466057	4.449911	0.027319
6	1.741706	6.414461	-0.740370
6	2.959677	5.689572	-0.840233
6	0.763334	5.742045	-1.520840
1	1.577387	7.311207	-0.144615
6	2.735898	4.567384	-1.682034
1	3.891358	5.931906	-0.331046
6	1.377650	4.598605	-2.102497
1	-0.275732	6.043819	-1.633936
1	3.469757	3.805847	-1.938710
1	0.894695	3.864471	-2.744634
6	-0.473888	-2.012806	-1.251808
6	-1.840210	-1.814866	-1.623682
6	0.093644	-2.887882	-2.227699
6	-2.095236	-2.531097	-2.826001
1	-2.566860	-1.206323	-1.080186
6	-0.895049	-3.194521	-3.202262
1	1.120288	-3.257160	-2.221402
1	-3.050451	-2.587983	-3.346265
1	-0.769257	-3.856132	-4.058468
26	-1.542817	-3.916840	-1.323811
6	-1.382245	-5.191060	0.397850
6	-2.726099	-4.749287	0.252637
6	-1.026966	-5.915325	-0.771137
1	-0.737388	-5.002590	1.253291
6	-3.203340	-5.207071	-1.005969
1	-3.289560	-4.158822	0.973519
6	-2.153506	-5.927249	-1.638282
1	-0.057385	-6.367434	-0.973957
1	-4.189968	-5.016607	-1.425429
1	-2.195418	-6.381921	-2.626920
6	-0.078321	0.717725	2.939531

6	-0.156344	-2.214786	1.768764
1	0.970766	1.067570	3.010060
1	-0.649816	1.499768	3.475642
1	0.387389	-3.173626	1.676800
1	-1.192860	-2.466982	1.462195
6	-0.177027	-1.825567	3.234405
6	-0.175521	-0.571316	3.732746
6	-0.222765	-0.263312	5.214852
1	0.590328	0.440388	5.469226
1	-1.168427	0.253338	5.464277
1	-0.126449	-1.136979	5.872069
6	-0.269933	-3.065086	4.099959
1	-0.457137	-2.868644	5.163226
1	-1.087380	-3.711987	3.731045
1	0.659081	-3.659452	4.019031

8-Sn-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.346689	-1.183747	0.200783
50	-0.417171	1.307226	0.956359
6	2.370427	-1.529486	-0.449757
6	2.749846	-1.065617	-1.732643
6	3.312025	-2.213476	0.350701
6	4.050640	-1.314598	-2.193294
6	4.580589	-2.461857	-0.165988
6	4.974527	-2.021046	-1.425605
1	4.354738	-0.945357	-3.178024
1	5.293617	-3.021941	0.444146
6	-2.370879	1.763570	0.120660
6	-2.500610	2.330554	-1.168443
6	-3.535174	1.322783	0.794362
6	-3.774946	2.517687	-1.714815
6	-4.784721	1.528124	0.204553
6	-4.932651	2.145171	-1.031502
1	-3.865320	2.976801	-2.704556
1	-5.682539	1.197729	0.735112
6	1.835564	-0.228541	-2.632548

6	1.743036	-0.753512	-4.070360
6	2.289672	1.237833	-2.626460
1	0.807357	-0.255040	-2.233261
1	1.413151	-1.804513	-4.096995
1	1.012837	-0.153569	-4.641101
1	2.712024	-0.679018	-4.593246
1	2.203964	1.686760	-1.621753
1	3.344971	1.314807	-2.944671
1	1.683683	1.841919	-3.324533
6	6.383472	-2.321883	-1.889361
6	6.580209	-3.836157	-2.035665
6	7.405082	-1.718036	-0.916768
1	6.525265	-1.854475	-2.878729
1	5.850993	-4.261155	-2.744524
1	7.596540	-4.073532	-2.390868
1	6.433726	-4.340459	-1.064505
1	7.246514	-0.633203	-0.801898
1	7.307436	-2.174401	0.083507
1	8.436832	-1.888943	-1.264934
6	3.052538	-2.745831	1.756997
6	4.091116	-2.246582	2.770491
6	2.984117	-4.280187	1.733233
1	2.087709	-2.365304	2.112705
1	4.058339	-1.147089	2.851767
1	3.882588	-2.671053	3.767555
1	5.118579	-2.536897	2.493972
1	2.175470	-4.634273	1.069662
1	3.930470	-4.704539	1.352764
1	2.812687	-4.691755	2.743075
6	-3.549056	0.587899	2.129440
6	-3.926140	-0.889571	1.958678
6	-4.433974	1.284367	3.168668
1	-2.539074	0.589249	2.535754
1	-3.196645	-1.411172	1.315386
1	-3.932056	-1.400413	2.938936
1	-4.923893	-1.009998	1.498889
1	-4.111206	2.328962	3.317335
1	-5.495545	1.296571	2.869453
1	-4.366828	0.761872	4.137354
6	-6.314243	2.410856	-1.588300

6	-6.540604	1.669206	-2.907943
6	-6.563347	3.917744	-1.716274
1	-7.034841	2.015209	-0.851917
1	-6.365695	0.588314	-2.778620
1	-7.572597	1.814661	-3.268190
1	-5.850703	2.031243	-3.689180
1	-6.404923	4.420464	-0.747720
1	-5.872155	4.371532	-2.447282
1	-7.595264	4.120368	-2.048267
6	-1.317992	2.770461	-2.028251
6	-1.370605	4.284893	-2.276786
6	-1.262730	2.003003	-3.357804
1	-0.377121	2.547097	-1.487126
1	-1.273537	4.842401	-1.330269
1	-0.569333	4.613190	-2.958629
1	-2.330497	4.567656	-2.739274
1	-1.193280	0.912975	-3.196196
1	-2.163605	2.198064	-3.964103
1	-0.391157	2.325374	-3.953792
6	1.299404	2.543494	1.229514
6	2.645338	2.059100	1.129756
6	1.321915	3.614687	2.176871
6	3.476637	2.848681	1.971138
1	2.988069	1.232168	0.503396
6	2.655396	3.809464	2.623195
1	0.452386	4.188499	2.499091
1	4.555473	2.748162	2.078228
1	2.990679	4.572994	3.322831
26	2.519738	4.079929	0.513191
6	2.899294	6.090304	0.011425
6	3.905876	5.262941	-0.562921
6	1.640989	5.687293	-0.519900
1	3.057367	6.863917	0.760454
6	3.270887	4.349161	-1.447775
1	4.970144	5.294905	-0.339075
6	1.874588	4.609996	-1.420313
1	0.669097	6.094936	-0.244842
1	3.756282	3.559820	-2.017976
1	1.119976	4.039055	-1.953095
6	-0.968756	-1.993785	-1.274665

6	-2.356210	-1.688753	-1.429655
6	-0.640559	-2.952171	-2.279580
6	-2.872200	-2.454067	-2.509699
1	-2.930137	-0.980923	-0.829273
6	-1.808661	-3.234993	-3.040141
1	0.343547	-3.401737	-2.419244
1	-3.904697	-2.452165	-2.855280
1	-1.882439	-3.942537	-3.863970
26	-2.140743	-3.785123	-1.013657
6	-1.877065	-4.838591	0.870999
6	-3.233916	-4.445295	0.716479
6	-1.529711	-5.680314	-0.215551
1	-1.219342	-4.557843	1.687500
6	-3.734335	-5.067700	-0.460603
1	-3.789999	-3.786218	1.382718
6	-2.680642	-5.830881	-1.036851
1	-0.547611	-6.118542	-0.386077
1	-4.739574	-4.955028	-0.862122
1	-2.733153	-6.404918	-1.959577
6	-0.454078	0.962423	3.106870
6	-0.313287	-2.166126	2.017119
1	0.595669	1.175606	3.379285
1	-1.036525	1.809663	3.513048
1	0.285932	-3.083358	2.126020
1	-1.286948	-2.527853	1.641001
6	-0.636633	-1.595413	3.381286
6	-0.890832	-0.322126	3.767347
6	-1.692735	-0.118317	5.044173
1	-2.034598	0.924936	5.124600
1	-2.593274	-0.760499	5.043503
1	-1.128360	-0.355398	5.963034
6	-0.933333	-2.711089	4.368709
1	-0.598244	-2.454773	5.386951
1	-2.013688	-2.945649	4.421007
1	-0.412786	-3.635424	4.071014

8-Pb-Pb

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

82	0.451184	-1.156434	0.169094
82	-0.530001	1.303506	0.860790
6	2.516927	-1.378017	-0.508645
6	2.843547	-0.890381	-1.791360
6	3.484929	-1.985408	0.312318
6	4.160484	-1.048269	-2.243774
6	4.766939	-2.143157	-0.200718
6	5.125793	-1.681284	-1.463199
1	4.441578	-0.665223	-3.229877
1	5.516511	-2.645999	0.414744
6	-2.536436	1.596298	0.007945
6	-2.682612	2.130744	-1.286181
6	-3.641282	1.062162	0.700877
6	-3.967531	2.213181	-1.828905
6	-4.900352	1.165127	0.109930
6	-5.088530	1.760892	-1.131414
1	-4.094268	2.654284	-2.822582
1	-5.770300	0.771779	0.643345
6	1.866155	-0.127301	-2.694097
6	1.795484	-0.676895	-4.123928
6	2.222741	1.365974	-2.711171
1	0.844965	-0.212609	-2.287489
1	1.493580	-1.736204	-4.135172
1	1.050563	-0.107153	-4.706545
1	2.763507	-0.583953	-4.644757
1	2.131912	1.817879	-1.708476
1	3.261997	1.510202	-3.056662
1	1.561232	1.922381	-3.398683
6	6.552890	-1.886997	-1.913515
6	6.845802	-3.387326	-2.038492
6	7.515026	-1.201962	-0.934747
1	6.669774	-1.421215	-2.906450
1	6.144919	-3.865639	-2.742206
1	7.875540	-3.567403	-2.386904
1	6.724482	-3.886278	-1.061087
1	7.274286	-0.130787	-0.833304
1	7.434264	-1.653114	0.069266
1	8.561402	-1.300147	-1.265229
6	3.254392	-2.523372	1.723059

6	4.246330	-1.936066	2.736829
6	3.303570	-4.059070	1.713711
1	2.261254	-2.216513	2.071366
1	4.122451	-0.843118	2.815013
1	4.073049	-2.372656	3.735403
1	5.294388	-2.140774	2.461991
1	2.514124	-4.480875	1.066847
1	4.273297	-4.413321	1.321730
1	3.179674	-4.473309	2.729450
6	-3.579394	0.340108	2.043155
6	-3.834234	-1.166235	1.894154
6	-4.505868	0.977354	3.084496
1	-2.568585	0.424111	2.438894
1	-3.081876	-1.630035	1.233528
1	-3.762389	-1.664773	2.878253
1	-4.832212	-1.378593	1.470227
1	-4.233268	2.033428	3.250789
1	-5.563351	0.945122	2.774358
1	-4.424022	0.445920	4.046765
6	-6.484322	1.922639	-1.683610
6	-6.651566	1.152822	-2.994912
6	-6.832805	3.408896	-1.816421
1	-7.171939	1.482457	-0.941349
1	-6.392452	0.090676	-2.850647
1	-7.690167	1.213763	-3.358633
1	-5.987090	1.556468	-3.777759
1	-6.702711	3.922343	-0.848996
1	-6.173113	3.905331	-2.548723
1	-7.876354	3.543897	-2.144725
6	-1.524327	2.641107	-2.141605
6	-1.674497	4.146950	-2.398731
6	-1.400848	1.868019	-3.463266
1	-0.575199	2.484910	-1.593585
1	-1.617655	4.713463	-1.454222
1	-0.891616	4.523660	-3.076998
1	-2.648341	4.363784	-2.866931
1	-1.249306	0.788344	-3.289565
1	-2.306635	1.987974	-4.081476
1	-0.549125	2.249827	-4.053184
6	1.152096	2.645908	1.158344

6	2.521117	2.248894	1.059851
6	1.084904	3.714009	2.098879
6	3.290559	3.105916	1.895167
1	2.914372	1.439576	0.439660
6	2.400715	4.008847	2.541388
1	0.167949	4.212570	2.414632
1	4.373276	3.084588	2.003742
1	2.674698	4.798202	3.238188
26	2.236503	4.245650	0.425479
6	2.454390	6.265663	-0.103860
6	3.514913	5.508720	-0.680504
6	1.224333	5.763009	-0.617155
1	2.560115	7.055414	0.637209
6	2.940665	4.539223	-1.547598
1	4.575826	5.619359	-0.467127
6	1.529201	4.695754	-1.507816
1	0.226052	6.096985	-0.336513
1	3.475528	3.780251	-2.114685
1	0.814656	4.063048	-2.026052
6	-0.832834	-2.097369	-1.330436
6	-2.234917	-1.895680	-1.488578
6	-0.422480	-3.042239	-2.311452
6	-2.685599	-2.718651	-2.556474
1	-2.857195	-1.218428	-0.900678
6	-1.563347	-3.426235	-3.069367
1	0.595685	-3.413922	-2.434960
1	-3.713203	-2.799113	-2.906186
1	-1.576863	-4.150011	-3.881786
26	-1.857583	-3.958221	-1.030670
6	-1.498719	-4.953392	0.871930
6	-2.881423	-4.658405	0.725997
6	-1.103459	-5.787005	-0.204168
1	-0.854256	-4.616233	1.677545
6	-3.348613	-5.335164	-0.435207
1	-3.474323	-4.026443	1.387040
6	-2.248906	-6.032972	-1.010216
1	-0.093183	-6.154828	-0.376905
1	-4.362746	-5.298721	-0.827988
1	-2.268451	-6.624364	-1.923004
6	-0.521016	0.963613	3.075929

6	-0.159184	-2.191738	2.031956
1	0.518184	1.246412	3.315040
1	-1.161141	1.775093	3.462932
1	0.519934	-3.048040	2.150070
1	-1.099537	-2.617886	1.644386
6	-0.521402	-1.601516	3.369923
6	-0.879056	-0.343077	3.726410
6	-1.739046	-0.187032	4.970010
1	-2.183800	0.819603	5.001987
1	-2.569651	-0.915987	4.957488
1	-1.183644	-0.337123	5.911688
6	-0.731365	-2.717767	4.376685
1	-0.433313	-2.412057	5.391997
1	-1.785573	-3.051253	4.414343
1	-0.122696	-3.593152	4.098182

TS1-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.488739	-1.228877	0.489450
6	-0.419901	0.515200	0.083218
6	-1.189022	-0.787584	0.616099
6	0.633752	1.705060	0.492959
6	0.638022	2.550047	1.652408
6	1.536973	2.211268	-0.525106
6	1.515533	3.642140	1.811885
6	2.377883	3.326472	-0.314658
6	2.417560	4.078980	0.856899
1	1.467195	4.200232	2.752350
1	3.037848	3.632115	-1.132291
6	-1.727952	-1.103387	1.920551
6	-1.579296	-1.812540	-0.353158
6	-2.744542	-2.059727	2.122320
6	-2.595118	-2.748671	-0.081175
6	-3.266417	-2.873482	1.130229
1	-3.135193	-2.172969	3.138097
1	-2.871523	-3.452047	-0.872758
6	-0.271079	2.409208	2.853989

6	-1.040726	3.685385	3.221181
6	0.556568	1.929681	4.058691
1	-1.028160	1.677624	2.578937
1	-1.568711	4.105935	2.349112
1	-1.786710	3.450396	4.001095
1	-0.383771	4.472843	3.627104
1	1.196947	1.071907	3.793783
1	1.228092	2.739665	4.394097
1	-0.079707	1.648071	4.914585
6	3.305910	5.305824	1.104891
6	2.822382	6.580154	0.390732
6	4.792459	5.097313	0.785233
1	3.241465	5.513992	2.188095
1	1.785412	6.837430	0.657927
1	3.465792	7.434094	0.674525
1	2.881561	6.473797	-0.706168
1	5.217802	4.239205	1.328976
1	4.959343	4.944278	-0.295070
1	5.364327	5.998087	1.075108
6	1.716909	1.651822	-1.937848
6	3.080094	0.966314	-2.057677
6	1.593263	2.740513	-3.025550
1	0.948208	0.890892	-2.112919
1	3.171701	0.163614	-1.308644
1	3.220896	0.536113	-3.066711
1	3.900144	1.687297	-1.882760
1	0.704300	3.376171	-2.879843
1	2.475635	3.405498	-3.036949
1	1.536547	2.283800	-4.029359
6	-0.914753	-2.128556	-1.701981
6	-1.831494	-1.848256	-2.896024
6	-0.499621	-3.619962	-1.783436
1	-0.012676	-1.505537	-1.792558
1	-2.162738	-0.802421	-2.908860
1	-1.314545	-2.081486	-3.843874
1	-2.732653	-2.487751	-2.846775
1	0.055136	-3.968684	-0.896419
1	-1.381262	-4.275565	-1.893844
1	0.129016	-3.795281	-2.673712
6	-4.410910	-3.865259	1.347873

6	-5.681411	-3.207287	1.905838
6	-4.038278	-5.059682	2.242713
1	-4.666948	-4.277379	0.355275
1	-6.031112	-2.376852	1.271527
1	-6.494587	-3.952914	1.970657
1	-5.514772	-2.818056	2.925855
1	-3.178377	-5.624315	1.848350
1	-3.795522	-4.731717	3.268886
1	-4.895169	-5.754906	2.315558
6	-1.299275	-0.495593	3.242876
6	-0.850839	-1.543120	4.274422
6	-2.440448	0.352426	3.829924
1	-0.410542	0.098521	3.041865
1	-0.043871	-2.178577	3.874294
1	-0.472076	-1.026977	5.174776
1	-1.675281	-2.200560	4.599500
1	-2.882275	1.023110	3.073559
1	-3.253108	-0.304064	4.186851
1	-2.103918	0.959325	4.686801
6	2.034058	-2.358085	-0.200944
6	2.395975	-2.601452	-1.589758
6	2.484370	-3.559667	0.527037
6	3.001249	-3.860827	-1.695984
1	2.231616	-1.893385	-2.399526
6	3.041677	-4.460492	-0.392813
1	2.389862	-3.722391	1.600274
1	3.410035	-4.305302	-2.604715
1	3.483668	-5.432839	-0.163978
26	4.169754	-2.629005	-0.383212
6	6.197703	-3.102139	0.089393
6	6.131278	-2.525077	-1.205323
6	5.693447	-2.152714	1.021441
1	6.556694	-4.104265	0.322334
6	5.587155	-1.217472	-1.078601
1	6.419149	-3.011089	-2.137059
6	5.317437	-0.987722	0.298378
1	5.596161	-2.301871	2.095385
1	5.376737	-0.529150	-1.895516
1	4.847105	-0.098263	0.717563
6	-1.371929	1.357308	-0.813562

6	-2.171265	2.391527	-0.203630
6	-1.415802	1.636851	-2.216938
6	-2.604337	3.315158	-1.192864
1	-2.369328	2.483765	0.864658
6	-2.143903	2.841077	-2.447927
1	-0.943458	1.052330	-3.003723
1	-3.229834	4.194063	-1.028140
1	-2.347009	3.293104	-3.419512
26	-3.490768	1.457857	-1.617240
6	-4.716910	-0.284969	-1.469615
6	-5.301028	0.769608	-0.716275
6	-4.659894	0.129875	-2.829121
1	-4.338611	-1.221522	-1.063308
6	-5.602094	1.833553	-1.609505
1	-5.465016	0.774364	0.359987
6	-5.204694	1.437463	-2.913496
1	-4.257395	-0.442990	-3.662727
1	-6.043599	2.794232	-1.345727
1	-5.287328	2.039349	-3.818502

TS1-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	1.048230	-1.418221	0.789561
14	-0.020124	0.556361	-0.147008
6	-1.376075	-1.249649	0.791350
6	1.113054	2.110244	0.502695
6	1.139094	2.816432	1.726549
6	2.058130	2.530899	-0.480720
6	2.100356	3.814218	1.971587
6	2.996253	3.534688	-0.199518
6	3.056861	4.188690	1.031345
1	2.104634	4.322214	2.943194
1	3.713180	3.820742	-0.977019
6	-2.089244	-1.211764	2.033185
6	-1.947674	-2.088651	-0.217200
6	-3.294320	-1.907628	2.209908
6	-3.150283	-2.778295	0.012582

6	-3.858494	-2.702262	1.209593
1	-3.804043	-1.847011	3.178629
1	-3.552154	-3.419975	-0.779376
6	0.153171	2.538368	2.844685
6	-0.591653	3.796608	3.305910
6	0.852237	1.851542	4.023243
1	-0.602970	1.850104	2.431801
1	-1.082604	4.304506	2.458698
1	-1.362435	3.533465	4.050893
1	0.090995	4.522567	3.780055
1	1.385025	0.943089	3.694053
1	1.595366	2.533276	4.474597
1	0.129603	1.572497	4.810007
6	4.081129	5.283184	1.314886
6	3.765823	6.569871	0.538213
6	5.523226	4.841330	1.033961
1	4.011822	5.521572	2.391261
1	2.755769	6.944306	0.771143
1	4.493970	7.362657	0.786712
1	3.820284	6.393280	-0.550499
1	5.783218	3.924379	1.587183
1	5.680367	4.648278	-0.041702
1	6.231797	5.635053	1.330083
6	2.132508	1.926287	-1.880165
6	3.317988	0.963776	-1.989389
6	2.165344	2.989230	-2.986684
1	1.217003	1.336827	-2.062850
1	3.235273	0.152745	-1.243629
1	3.364203	0.508610	-2.994688
1	4.267834	1.499016	-1.808633
1	1.334453	3.705849	-2.873957
1	3.110965	3.558412	-2.981357
1	2.081131	2.509738	-3.976999
6	-1.300574	-2.367099	-1.568524
6	-2.123906	-1.788339	-2.721412
6	-1.059262	-3.871031	-1.769419
1	-0.319304	-1.874404	-1.585178
1	-2.242358	-0.697906	-2.611428
1	-1.628581	-1.997411	-3.685601
1	-3.133508	-2.237425	-2.756208

1	-0.524779	-4.313412	-0.912337
1	-2.011758	-4.414582	-1.900413
1	-0.447920	-4.041029	-2.671398
6	-5.135837	-3.508030	1.417214
6	-6.294829	-2.685467	1.991861
6	-4.879512	-4.745409	2.291419
1	-5.450072	-3.869746	0.422303
1	-6.506699	-1.796501	1.375516
1	-7.210910	-3.300729	2.032131
1	-6.080928	-2.351067	3.021834
1	-4.088997	-5.382731	1.863425
1	-4.568399	-4.450049	3.308752
1	-5.798995	-5.350695	2.382018
6	-1.575718	-0.472468	3.255542
6	-1.254184	-1.443079	4.398932
6	-2.560131	0.606030	3.726832
1	-0.629510	0.004177	2.965127
1	-0.549077	-2.222477	4.066237
1	-0.798300	-0.900056	5.244979
1	-2.166220	-1.942665	4.771139
1	-2.816284	1.311256	2.917005
1	-3.503344	0.151503	4.079436
1	-2.139032	1.180954	4.569948
6	1.733390	-2.944922	-0.282993
6	2.111973	-3.011389	-1.667245
6	2.161344	-4.209804	0.278392
6	2.713092	-4.266285	-1.951257
1	1.972404	-2.209804	-2.392407
6	2.742562	-5.013823	-0.742334
1	2.090243	-4.524335	1.321291
1	3.122677	-4.586588	-2.910697
1	3.183654	-6.006493	-0.623389
26	3.903757	-3.254732	-0.511247
6	5.909541	-3.819221	0.026272
6	5.918479	-3.181402	-1.241998
6	5.401326	-2.896728	0.979163
1	6.230483	-4.841231	0.227262
6	5.417898	-1.861969	-1.074916
1	6.241380	-3.631347	-2.180493
6	5.098065	-1.684412	0.299409

1	5.262026	-3.090731	2.041404
1	5.283287	-1.126748	-1.866934
1	4.678140	-0.786549	0.751375
6	-1.319088	1.697274	-1.099659
6	-1.969093	2.779228	-0.409602
6	-1.391518	2.048152	-2.494420
6	-2.387859	3.766271	-1.340205
1	-2.115421	2.848547	0.669061
6	-2.029070	3.313321	-2.637245
1	-1.016839	1.458966	-3.332461
1	-2.926043	4.686694	-1.108337
1	-2.243500	3.831351	-3.573688
26	-3.416470	1.967330	-1.770181
6	-4.682970	0.281728	-1.485745
6	-5.209876	1.389730	-0.768244
6	-4.664611	0.624933	-2.866750
1	-4.313268	-0.643933	-1.044947
6	-5.514531	2.415613	-1.703416
1	-5.334246	1.453115	0.311624
6	-5.178603	1.942275	-2.998824
1	-4.300227	0.002734	-3.682579
1	-5.922971	3.398972	-1.471538
1	-5.286030	2.499921	-3.929110

TS1-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.140265	-1.406531	0.823474
32	-0.089642	0.578574	-0.181339
6	-1.406515	-1.300241	0.776399
6	0.998389	2.230851	0.505750
6	0.997281	2.905242	1.742869
6	1.917525	2.690644	-0.478419
6	1.920205	3.933912	1.999857
6	2.817374	3.723566	-0.186148
6	2.854166	4.356657	1.056837
1	1.912446	4.426343	2.979362
1	3.520409	4.048981	-0.960611

6	-2.108340	-1.300187	2.016219
6	-1.926878	-2.150361	-0.243731
6	-3.280322	-2.049860	2.188354
6	-3.099795	-2.890327	-0.024460
6	-3.806369	-2.854550	1.175569
1	-3.790776	-2.022988	3.158005
1	-3.476290	-3.539337	-0.822862
6	0.023642	2.557885	2.853177
6	-0.778096	3.772404	3.334347
6	0.748684	1.879120	4.020499
1	-0.700398	1.843161	2.426395
1	-1.293715	4.267766	2.494404
1	-1.534412	3.464071	4.076745
1	-0.127240	4.522157	3.816042
1	1.315208	0.996398	3.677558
1	1.465639	2.580721	4.483413
1	0.037290	1.559150	4.801964
6	3.831057	5.487830	1.349734
6	3.418546	6.780065	0.631379
6	5.280786	5.129583	1.002689
1	3.786514	5.681899	2.435981
1	2.398892	7.088299	0.913958
1	4.111395	7.603423	0.880044
1	3.439239	6.639344	-0.463661
1	5.599137	4.198836	1.499640
1	5.410474	4.997155	-0.085627
1	5.961969	5.939816	1.316454
6	2.004869	2.100249	-1.884945
6	3.229155	1.190004	-2.018096
6	1.976262	3.172095	-2.981935
1	1.115703	1.473873	-2.071351
1	3.189689	0.367194	-1.281677
1	3.283155	0.747690	-3.028843
1	4.157751	1.762046	-1.841332
1	1.109527	3.842318	-2.856053
1	2.891428	3.788505	-2.977187
1	1.908064	2.696601	-3.975509
6	-1.261762	-2.378234	-1.598246
6	-2.102832	-1.811801	-2.746110
6	-0.959559	-3.866443	-1.828476

1	-0.297784	-1.850352	-1.603001
1	-2.266180	-0.728467	-2.621909
1	-1.599100	-1.986642	-3.712987
1	-3.093870	-2.299709	-2.790601
1	-0.403587	-4.301588	-0.981605
1	-1.888821	-4.446513	-1.967633
1	-0.344378	-3.994187	-2.735018
6	-5.044723	-3.716473	1.375632
6	-6.232326	-2.946759	1.962581
6	-4.725960	-4.948834	2.234882
1	-5.345747	-4.079797	0.377336
1	-6.478608	-2.060343	1.355195
1	-7.123898	-3.596565	2.000511
1	-6.025521	-2.612997	2.994154
1	-3.908165	-5.542158	1.794644
1	-4.420431	-4.648132	3.252378
1	-5.614504	-5.598189	2.325409
6	-1.610860	-0.542777	3.234317
6	-1.242937	-1.501740	4.372892
6	-2.627969	0.500724	3.711576
1	-0.685295	-0.029747	2.935120
1	-0.510341	-2.252573	4.032967
1	-0.802771	-0.944897	5.218221
1	-2.132500	-2.038356	4.747630
1	-2.904101	1.201246	2.904225
1	-3.556305	0.013421	4.059284
1	-2.225865	1.084710	4.557747
6	1.858492	-2.918186	-0.343852
6	2.210160	-2.946650	-1.733170
6	2.356757	-4.156003	0.203166
6	2.874035	-4.165879	-2.034314
1	2.014937	-2.146275	-2.447235
6	2.965524	-4.918336	-0.831576
1	2.312760	-4.470977	1.247380
1	3.282034	-4.458525	-3.002410
1	3.458090	-5.886558	-0.723249
26	4.022480	-3.090472	-0.603978
6	6.058955	-3.529703	-0.095606
6	6.012156	-2.882942	-1.359199
6	5.510095	-2.645684	0.871375

1	6.437593	-4.534008	0.092602
6	5.436078	-1.597173	-1.174702
1	6.343783	-3.306627	-2.306629
6	5.125938	-1.448711	0.205232
1	5.397322	-2.853887	1.934127
1	5.247034	-0.864334	-1.957794
1	4.669171	-0.575761	0.670924
6	-1.470574	1.720994	-1.142892
6	-2.143283	2.769782	-0.431176
6	-1.561106	2.076340	-2.530296
6	-2.608132	3.747163	-1.350119
1	-2.275297	2.821795	0.650382
6	-2.246924	3.317705	-2.654746
1	-1.171663	1.502459	-3.372131
1	-3.175004	4.645871	-1.104325
1	-2.488271	3.833603	-3.585104
26	-3.565675	1.906608	-1.778567
6	-4.746366	0.159738	-1.484981
6	-5.313456	1.239170	-0.754832
6	-4.759902	0.510848	-2.864106
1	-4.332878	-0.752030	-1.053751
6	-5.674861	2.255906	-1.679893
1	-5.425916	1.290593	0.327066
6	-5.333772	1.805108	-2.982570
1	-4.376951	-0.090846	-3.686779
1	-6.119156	3.220441	-1.435439
1	-5.472847	2.364208	-3.907554

TS1-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	1.326312	-1.454946	0.980384
50	-0.196069	0.570905	-0.225889
6	-1.428118	-1.400846	0.750567
6	0.840486	2.413968	0.523348
6	0.822053	3.025765	1.787128
6	1.714594	2.934806	-0.466412
6	1.690237	4.093595	2.064138

6	2.562037	4.002650	-0.155977
6	2.576146	4.592690	1.110204
1	1.677915	4.553629	3.058613
1	3.235057	4.389846	-0.928019
6	-2.108112	-1.470917	1.995515
6	-1.883980	-2.261905	-0.290208
6	-3.223365	-2.302319	2.159485
6	-3.007933	-3.074921	-0.085520
6	-3.701971	-3.107924	1.123083
1	-3.724927	-2.335765	3.132591
1	-3.350934	-3.725637	-0.896917
6	-0.116807	2.558955	2.887627
6	-1.011446	3.689028	3.409237
6	0.654330	1.890141	4.032026
1	-0.785372	1.804366	2.435269
1	-1.579453	4.154630	2.586316
1	-1.727914	3.303986	4.155469
1	-0.415182	4.480145	3.895163
1	1.275250	1.055896	3.662161
1	1.326283	2.619061	4.518720
1	-0.032961	1.498021	4.802218
6	3.485524	5.770905	1.415219
6	2.972372	7.044306	0.728678
6	4.946066	5.502156	1.034568
1	3.447192	5.937210	2.505803
1	1.938820	7.272121	1.035983
1	3.609762	7.910093	0.978042
1	2.977841	6.920804	-0.368393
1	5.319220	4.574963	1.499839
1	5.061830	5.403372	-0.058898
1	5.589604	6.337606	1.359452
6	1.804993	2.369876	-1.887421
6	3.063571	1.513524	-2.067411
6	1.699396	3.448952	-2.971638
1	0.941776	1.706846	-2.074085
1	3.073174	0.672652	-1.351774
1	3.112114	1.094573	-3.088622
1	3.972577	2.116794	-1.897693
1	0.796294	4.063980	-2.825293
1	2.578125	4.115333	-2.971968

1	1.642554	2.978628	-3.968558
6	-1.202110	-2.410025	-1.652501
6	-2.068184	-1.857009	-2.791828
6	-0.810053	-3.869073	-1.930959
1	-0.265070	-1.833049	-1.639276
1	-2.291773	-0.786351	-2.646819
1	-1.553657	-1.981504	-3.760826
1	-3.030990	-2.395999	-2.853024
1	-0.220019	-4.292769	-1.102128
1	-1.701034	-4.502135	-2.084263
1	-0.193943	-3.929177	-2.843878
6	-4.878629	-4.051071	1.309421
6	-6.102525	-3.369352	1.929511
6	-4.462421	-5.280242	2.131062
1	-5.167107	-4.405713	0.304746
1	-6.405434	-2.483384	1.347756
1	-6.954086	-4.070080	1.960052
1	-5.901539	-3.048694	2.966018
1	-3.612982	-5.802485	1.661819
1	-4.158093	-4.983639	3.149773
1	-5.301206	-5.991907	2.219204
6	-1.629913	-0.702472	3.217996
6	-1.166598	-1.657789	4.325820
6	-2.694990	0.267217	3.742538
1	-0.748322	-0.117827	2.910044
1	-0.392922	-2.350430	3.952912
1	-0.742684	-1.091980	5.173292
1	-2.007140	-2.263508	4.707192
1	-3.016056	0.977660	2.960906
1	-3.590529	-0.280891	4.084145
1	-2.311529	0.844631	4.601602
6	2.088303	-2.928647	-0.425125
6	2.370696	-2.888583	-1.827909
6	2.741278	-4.100934	0.080797
6	3.154401	-4.022859	-2.175487
1	2.056179	-2.103385	-2.516841
6	3.387788	-4.774225	-0.989490
1	2.764109	-4.415258	1.125887
1	3.544709	-4.258765	-3.164668
1	3.982052	-5.683804	-0.911963

26	4.221704	-2.826802	-0.776843
6	6.298363	-3.024685	-0.348246
6	6.129656	-2.380998	-1.605439
6	5.693641	-2.209938	0.647608
1	6.782238	-3.985931	-0.182969
6	5.422437	-1.167010	-1.387202
1	6.463421	-2.761648	-2.569474
6	5.154130	-1.058756	0.006083
1	5.645933	-2.431547	1.712413
1	5.125617	-0.453289	-2.153526
1	4.640225	-0.232737	0.497976
6	-1.742029	1.757678	-1.183608
6	-2.454581	2.729573	-0.408560
6	-1.853513	2.172484	-2.547584
6	-2.988529	3.717928	-1.277605
1	-2.572884	2.717666	0.676020
6	-2.616652	3.372864	-2.605791
1	-1.431442	1.655647	-3.410086
1	-3.602514	4.568131	-0.983173
1	-2.894338	3.914856	-3.508883
26	-3.813981	1.826877	-1.773277
6	-4.835802	-0.024243	-1.510123
6	-5.483043	0.988748	-0.750487
6	-4.883861	0.359128	-2.881138
1	-4.352215	-0.912520	-1.103104
6	-5.929633	1.997793	-1.648811
1	-5.589600	1.002812	0.332983
6	-5.560269	1.607755	-2.965780
1	-4.454016	-0.189744	-3.717157
1	-6.438784	2.920757	-1.375362
1	-5.738738	2.180512	-3.874718

TS1-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	1.591393	-1.271846	0.945597
82	-0.348224	0.528021	-0.225177
6	-1.515940	-1.396728	0.720786

6	0.491994	2.531789	0.565797
6	0.413670	3.150543	1.821686
6	1.306008	3.117472	-0.435369
6	1.178786	4.296270	2.085254
6	2.048867	4.262254	-0.137781
6	2.011200	4.862062	1.121725
1	1.125079	4.765922	3.074230
1	2.676749	4.704082	-0.918722
6	-2.130515	-1.564977	1.981413
6	-1.839093	-2.319109	-0.309052
6	-3.109778	-2.548589	2.168565
6	-2.830276	-3.283590	-0.084163
6	-3.495999	-3.402817	1.133282
1	-3.572982	-2.662777	3.155369
1	-3.090677	-3.980491	-0.888006
6	-0.479104	2.609080	2.925619
6	-1.443759	3.665055	3.473028
6	0.351982	1.980844	4.049468
1	-1.098409	1.818569	2.468592
1	-2.046628	4.103831	2.660137
1	-2.129537	3.216571	4.212847
1	-0.903539	4.486855	3.973251
1	1.016113	1.188937	3.659788
1	0.989666	2.745678	4.527726
1	-0.293148	1.539228	4.829799
6	2.805637	6.122305	1.404891
6	2.162220	7.330032	0.712673
6	4.277498	5.986259	1.004117
1	2.765050	6.294254	2.494568
1	1.112929	7.453556	1.026895
1	2.710700	8.258302	0.948504
1	2.170913	7.195101	-0.383330
1	4.740473	5.102482	1.473246
1	4.383914	5.883401	-0.089856
1	4.846125	6.881344	1.308326
6	1.438405	2.571206	-1.861302
6	2.788927	1.881016	-2.076514
6	1.169094	3.635595	-2.930043
1	0.665377	1.810400	-2.042166
1	2.911970	1.032628	-1.378934

1	2.869650	1.487126	-3.105926
1	3.623232	2.584452	-1.908043
1	0.195444	4.122294	-2.752195
1	1.952286	4.411973	-2.945783
1	1.143951	3.166699	-3.929345
6	-1.154928	-2.380550	-1.679258
6	-2.072862	-1.924363	-2.819247
6	-0.603610	-3.783972	-1.960476
1	-0.282109	-1.709943	-1.675164
1	-2.398803	-0.879694	-2.685301
1	-1.550260	-2.008534	-3.788906
1	-2.978785	-2.555874	-2.870997
1	0.012402	-4.144452	-1.120511
1	-1.417140	-4.508405	-2.135907
1	0.033382	-3.767717	-2.861015
6	-4.553298	-4.473522	1.323939
6	-5.838834	-3.918063	1.941405
6	-4.004591	-5.647716	2.143870
1	-4.802339	-4.856908	0.319128
1	-6.223017	-3.066340	1.355812
1	-6.618545	-4.697690	1.973985
1	-5.668358	-3.573461	2.975955
1	-3.105200	-6.074097	1.669755
1	-3.728835	-5.318696	3.161161
1	-4.760681	-6.446549	2.235614
6	-1.712253	-0.741873	3.188450
6	-1.121847	-1.640629	4.280026
6	-2.851427	0.122951	3.736095
1	-0.902830	-0.073564	2.852176
1	-0.292214	-2.247808	3.877388
1	-0.734748	-1.036976	5.118861
1	-1.881402	-2.334900	4.679788
1	-3.247908	0.804243	2.962955
1	-3.687089	-0.506264	4.090297
1	-2.506804	0.732155	4.590355
6	2.330856	-2.749024	-0.573415
6	2.571131	-2.633642	-1.977908
6	3.112368	-3.860423	-0.120422
6	3.463540	-3.664655	-2.378217
1	2.159664	-1.864502	-2.633945

6	3.802238	-4.424476	-1.224630
1	3.191465	-4.205725	0.912671
1	3.852372	-3.829735	-3.382630
1	4.488238	-5.270409	-1.190179
26	4.417919	-2.398775	-0.949903
6	6.499893	-2.341869	-0.500712
6	6.263725	-1.711339	-1.753109
6	5.791613	-1.619267	0.495664
1	7.097321	-3.237841	-0.338268
6	5.409897	-0.597934	-1.531948
1	6.648423	-2.039192	-2.717854
6	5.120366	-0.536795	-0.140772
1	5.766971	-1.854066	1.558999
1	5.030098	0.081336	-2.293617
1	4.519979	0.228324	0.353947
6	-1.959633	1.630537	-1.297237
6	-2.725118	2.572438	-0.545048
6	-2.122871	1.969570	-2.671403
6	-3.352515	3.476063	-1.442262
1	-2.814530	2.595508	0.542845
6	-2.980264	3.102336	-2.762014
1	-1.675213	1.448426	-3.519013
1	-4.024601	4.288246	-1.167699
1	-3.315539	3.581999	-3.680741
26	-4.037340	1.503703	-1.835834
6	-4.894591	-0.426743	-1.509234
6	-5.584657	0.539005	-0.729172
6	-5.035621	-0.065227	-2.878341
1	-4.329348	-1.271630	-1.114899
6	-6.152168	1.497206	-1.612635
1	-5.639433	0.554808	0.358444
6	-5.813540	1.122685	-2.941354
1	-4.603925	-0.589523	-3.729767
1	-6.718467	2.381207	-1.322248
1	-6.076680	1.669346	-3.846004

TS2-C

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

6	-1.902387	1.244022	3.018047
6	-0.198322	0.814258	0.303893
6	-0.796663	2.786069	0.921597
6	-2.164646	2.862997	1.216684
6	-2.715042	2.038460	2.268611
1	-2.323872	0.548645	3.750757
1	-0.816100	1.343065	2.987746
6	-4.218275	1.978487	2.444605
1	-4.720221	1.610507	1.530556
1	-4.489077	1.305677	3.273713
1	-4.650879	2.971445	2.664235
6	-3.113816	3.718785	0.411289
1	-3.971812	3.155030	-0.003373
1	-3.566078	4.501626	1.053108
1	-2.606077	4.234426	-0.418920
1	-0.086324	2.717362	1.751240
1	-0.451990	3.443639	0.112590
6	1.304880	0.506439	0.217134
6	2.194631	1.234532	-0.623786
6	1.913394	-0.558913	0.960535
6	3.559934	0.911316	-0.713049
6	3.281283	-0.853348	0.823207
6	4.145439	-0.139717	-0.009977
1	4.197392	1.499471	-1.383882
1	3.692651	-1.695668	1.392301
6	1.720699	2.403815	-1.466987
6	1.890918	2.120930	-2.961364
6	2.424389	3.703082	-1.054399
1	0.645251	2.529381	-1.286465
1	1.350449	1.201882	-3.242752
1	1.490640	2.957756	-3.557828
1	2.954152	1.988428	-3.227018
1	2.321644	3.885171	0.028976
1	3.504128	3.659329	-1.282701
1	2.002184	4.565996	-1.596911
6	5.629703	-0.481716	-0.160688
6	5.868386	-1.861227	-0.793999
6	6.409388	-0.383192	1.158900
1	6.061526	0.267640	-0.848020

1	5.383214	-1.948091	-1.779358
1	6.951214	-2.036467	-0.930701
1	5.482884	-2.669363	-0.148005
1	6.303535	0.610954	1.621498
1	6.065293	-1.139883	1.885576
1	7.484935	-0.564703	0.980871
6	1.139911	-1.456028	1.917553
6	1.522101	-1.148729	3.371698
6	1.355599	-2.949848	1.626072
1	0.071099	-1.229167	1.786897
1	1.338707	-0.090251	3.617346
1	0.943651	-1.777808	4.070634
1	2.594892	-1.353063	3.544094
1	1.224084	-3.179548	0.555188
1	2.370983	-3.279112	1.911616
1	0.645448	-3.562318	2.208084
6	-0.944528	0.445431	-0.903774
6	-2.292412	0.823332	-1.329028
6	-0.496864	-0.502329	-1.900074
6	-2.599573	0.157537	-2.538251
1	-2.966916	1.520801	-0.837666
6	-1.495698	-0.682590	-2.877747
1	0.463157	-1.013160	-1.858589
1	-3.530831	0.228449	-3.104555
1	-1.445445	-1.355808	-3.733660
26	-2.312419	-1.276818	-0.996569
6	-2.558115	-2.252788	0.867569
6	-3.826235	-1.816194	0.399695
6	-2.031872	-3.174493	-0.080008
1	-2.058201	-1.894270	1.766221
6	-4.085914	-2.469186	-0.836335
1	-4.473467	-1.089504	0.888048
6	-2.979198	-3.307155	-1.132174
1	-1.065103	-3.671933	-0.026899
1	-4.973561	-2.342220	-1.455793
1	-2.870841	-3.929317	-2.020099

TS2-Si

Atomic

Coordinates (Angstroms)

Number	X	Y	Z
6	-2.031932	1.944853	2.939898
14	-0.343477	0.850233	0.449359
6	-1.055913	3.322735	0.607511
6	-2.404857	3.225796	0.879556
6	-2.890387	2.526571	2.058956
1	-2.414984	1.337505	3.767178
1	-0.958656	2.133063	2.936740
6	-4.379707	2.308024	2.211229
1	-4.793211	1.711716	1.378839
1	-4.600059	1.774896	3.148351
1	-4.930757	3.263218	2.228630
6	-3.412351	3.714169	-0.131761
1	-4.161872	2.947038	-0.394770
1	-3.979143	4.571651	0.277570
1	-2.917818	4.050649	-1.056403
1	-0.316279	3.312253	1.411662
1	-0.731513	3.811050	-0.319494
6	1.527668	0.449960	0.143245
6	2.321650	1.106540	-0.821396
6	2.153658	-0.475750	1.012666
6	3.694944	0.833707	-0.898178
6	3.524623	-0.723748	0.910462
6	4.318259	-0.075651	-0.042057
1	4.305927	1.345725	-1.649814
1	3.988767	-1.446957	1.589547
6	1.728025	2.125279	-1.788264
6	1.840227	1.657050	-3.244237
6	2.358364	3.512808	-1.606086
1	0.650152	2.219977	-1.566256
1	1.321020	0.695723	-3.388788
1	1.391865	2.399067	-3.926820
1	2.896902	1.525172	-3.535381
1	2.267134	3.859959	-0.563218
1	3.432068	3.496203	-1.861459
1	1.870445	4.252393	-2.263962
6	5.806020	-0.365332	-0.149285
6	6.064602	-1.818321	-0.569325
6	6.549280	-0.034059	1.151068

1	6.208664	0.289554	-0.941269
1	5.567062	-2.050040	-1.524802
1	7.145901	-2.004179	-0.686054
1	5.681171	-2.520987	0.190434
1	6.381516	1.013073	1.450083
1	6.209359	-0.681312	1.977655
1	7.634414	-0.190979	1.027982
6	1.354346	-1.209978	2.084703
6	1.636526	-0.623827	3.473886
6	1.576697	-2.726712	2.060861
1	0.279393	-1.047654	1.875476
1	1.376618	0.448559	3.507580
1	1.054427	-1.148561	4.251146
1	2.708663	-0.720712	3.722187
1	1.443005	-3.131194	1.042639
1	2.594303	-2.991737	2.398984
1	0.861431	-3.229177	2.735164
6	-1.101694	0.153574	-1.134060
6	-2.439272	0.399217	-1.599475
6	-0.591258	-0.921695	-1.937864
6	-2.730456	-0.491221	-2.664197
1	-3.124940	1.136888	-1.184063
6	-1.586450	-1.318120	-2.866941
1	0.394756	-1.372927	-1.822618
1	-3.669812	-0.556692	-3.211317
1	-1.505180	-2.125739	-3.593002
26	-2.327274	-1.587656	-0.879375
6	-2.457869	-2.182188	1.169027
6	-3.757091	-1.891149	0.668246
6	-1.916319	-3.248634	0.396958
1	-1.963372	-1.657302	1.985319
6	-4.021563	-2.780639	-0.410205
1	-4.419705	-1.108634	1.033376
6	-2.884497	-3.619109	-0.577972
1	-0.929434	-3.691047	0.519115
1	-4.924371	-2.798501	-1.018261
1	-2.765699	-4.390098	-1.336998

TS2-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

6	-1.936652	1.883001	2.798773
32	-0.331467	0.918663	0.420468
6	-1.097945	3.397842	0.523346
6	-2.441177	3.230693	0.820742
6	-2.858906	2.457487	1.966075
1	-2.258922	1.196823	3.589786
1	-0.900690	2.215987	2.852235
6	-4.323924	2.114302	2.122708
1	-4.709343	1.542257	1.259323
1	-4.488647	1.511981	3.029430
1	-4.943579	3.023640	2.208072
6	-3.491487	3.695817	-0.157828
1	-4.173143	2.885402	-0.471185
1	-4.126815	4.473646	0.304489
1	-3.033166	4.131253	-1.058840
1	-0.346621	3.431208	1.316008
1	-0.818840	3.919717	-0.400276
6	1.607168	0.421901	0.111484
6	2.411148	1.057380	-0.853714
6	2.202835	-0.515790	0.983792
6	3.778627	0.754128	-0.927607
6	3.569209	-0.792533	0.889075
6	4.379100	-0.162705	-0.062722
1	4.402552	1.246660	-1.681731
1	4.016715	-1.522133	1.572608
6	1.828853	2.071216	-1.832326
6	1.903193	1.563016	-3.277241
6	2.492903	3.447221	-1.694478
1	0.756111	2.200750	-1.595035
1	1.370725	0.604089	-3.383713
1	1.448677	2.291001	-3.970507
1	2.952232	1.410986	-3.585303
1	2.406592	3.830398	-0.663997
1	3.566285	3.395205	-1.944945
1	2.025356	4.176477	-2.378014
6	5.862287	-0.478722	-0.158645
6	6.100503	-1.943138	-0.549423

6	6.604336	-0.133315	1.138718
1	6.278530	0.154266	-0.961338
1	5.590733	-2.189712	-1.494672
1	7.178414	-2.143499	-0.672690
1	5.717496	-2.625081	0.229197
1	6.462335	0.925450	1.408707
1	6.239493	-0.748788	1.978847
1	7.685880	-0.322356	1.029721
6	1.375051	-1.223618	2.051282
6	1.640543	-0.625660	3.438848
6	1.573210	-2.743421	2.051423
1	0.306174	-1.051818	1.818497
1	1.411233	0.453669	3.453937
1	1.027020	-1.123458	4.209580
1	2.703476	-0.749239	3.711956
1	1.445989	-3.159196	1.037314
1	2.582010	-3.018161	2.406205
1	0.842321	-3.225759	2.723498
6	-1.130606	0.076275	-1.175322
6	-2.460478	0.294390	-1.666852
6	-0.594703	-1.017476	-1.931879
6	-2.726805	-0.635012	-2.706370
1	-3.159944	1.039108	-1.287634
6	-1.571079	-1.454121	-2.865298
1	0.394982	-1.452402	-1.787671
1	-3.657184	-0.728846	-3.264555
1	-1.469346	-2.282366	-3.565132
26	-2.337841	-1.671043	-0.884784
6	-2.455933	-2.229466	1.174798
6	-3.758255	-1.941445	0.679193
6	-1.925441	-3.311696	0.417192
1	-1.954188	-1.697935	1.982484
6	-4.034636	-2.847690	-0.381784
1	-4.415893	-1.151315	1.036436
6	-2.902514	-3.694013	-0.543949
1	-0.939767	-3.756827	0.539331
1	-4.942125	-2.871907	-0.982520
1	-2.792864	-4.478383	-1.290553

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-2.575109	1.842092	2.614744
50	-0.419515	0.905472	0.761356
6	-1.035338	3.409346	0.802387
6	-2.415811	3.260261	0.632683
6	-3.188560	2.475350	1.554070
1	-3.143388	1.140526	3.235041
1	-1.635115	2.189838	3.041899
6	-4.651483	2.214874	1.271571
1	-4.841203	1.874743	0.240404
1	-5.050878	1.456012	1.960888
1	-5.244152	3.134873	1.415754
6	-3.075590	3.747811	-0.633206
1	-3.408817	2.912655	-1.276636
1	-3.972621	4.345638	-0.391220
1	-2.394248	4.379826	-1.221729
1	-0.609154	3.471834	1.806948
1	-0.475374	3.961814	0.037766
6	1.688222	0.392127	0.190662
6	2.372384	1.075622	-0.834708
6	2.399138	-0.553212	0.960636
6	3.731817	0.815341	-1.062881
6	3.756204	-0.788500	0.713526
6	4.444279	-0.109485	-0.297545
1	4.259902	1.349954	-1.860562
1	4.293504	-1.522138	1.325280
6	1.679147	2.118591	-1.705421
6	1.720345	1.749597	-3.193149
6	2.258685	3.519936	-1.470918
1	0.610795	2.149315	-1.420408
1	1.242475	0.772101	-3.369678
1	1.189636	2.506918	-3.795300
1	2.760502	1.696003	-3.559095
1	2.226332	3.792858	-0.402288
1	3.313044	3.566058	-1.795852
1	1.696480	4.278152	-2.043498
6	5.918558	-0.372836	-0.555731

6	6.173243	-1.833620	-0.947874
6	6.783266	0.027799	0.646531
1	6.216402	0.260203	-1.409606
1	5.561564	-2.124313	-1.817411
1	7.235716	-1.988976	-1.202208
1	5.924502	-2.514285	-0.115273
1	6.640508	1.090165	0.902511
1	6.521891	-0.572421	1.535257
1	7.852623	-0.137675	0.430079
6	1.723663	-1.333621	2.084115
6	2.220071	-0.877112	3.461060
6	1.869664	-2.849262	1.912932
1	0.637685	-1.119653	2.043127
1	2.046503	0.202404	3.605053
1	1.705504	-1.424341	4.269439
1	3.304066	-1.059425	3.560297
1	1.548858	-3.162975	0.905812
1	2.918191	-3.166142	2.047245
1	1.260052	-3.386542	2.659890
6	-1.377340	0.065720	-1.007206
6	-2.748116	0.114345	-1.418344
6	-0.726318	-0.847764	-1.900968
6	-2.930186	-0.735812	-2.543968
1	-3.540944	0.673926	-0.922801
6	-1.674551	-1.336444	-2.840916
1	0.323818	-1.138483	-1.847096
1	-3.867804	-0.921212	-3.066145
1	-1.485400	-2.061602	-3.631322
26	-2.285336	-1.877522	-0.871967
6	-2.079124	-2.730010	1.078925
6	-3.453974	-2.482422	0.804173
6	-1.593018	-3.647284	0.104711
1	-1.502686	-2.290928	1.892897
6	-3.818177	-3.251501	-0.336256
1	-4.104843	-1.806878	1.357117
6	-2.668192	-3.970562	-0.768102
1	-0.574330	-4.022946	0.029760
1	-4.797317	-3.267988	-0.812201
1	-2.614554	-4.631135	-1.631994

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-2.068397	-1.519351	-2.377270
82	-0.364626	-1.101686	-0.417965
6	-1.465502	-3.466573	-0.432979
6	-2.790668	-2.994123	-0.570947
6	-3.091758	-2.018755	-1.544064
1	-2.297655	-0.668945	-3.030043
1	-1.313733	-2.197822	-2.785746
6	-4.443314	-1.343355	-1.531942
1	-4.637150	-0.807249	-0.584109
1	-4.531909	-0.620009	-2.356497
1	-5.251806	-2.085243	-1.652491
6	-3.832365	-3.378154	0.453067
1	-4.276947	-2.504507	0.961060
1	-4.665076	-3.921131	-0.030015
1	-3.407352	-4.041775	1.221590
1	-0.865954	-3.673234	-1.324788
1	-1.232967	-4.121020	0.415213
6	1.821326	-0.359707	-0.085213
6	2.556110	-0.852049	1.006508
6	2.448680	0.487760	-1.017258
6	3.906044	-0.496129	1.146209
6	3.798703	0.820149	-0.853747
6	4.546873	0.333372	0.224208
1	4.483223	-0.878013	1.995993
1	4.283771	1.475619	-1.585784
6	1.936057	-1.786376	2.040574
6	2.038163	-1.230152	3.465038
6	2.538222	-3.194618	1.951216
1	0.854694	-1.876546	1.822377
1	1.592146	-0.223873	3.528419
1	1.507579	-1.887786	4.174866
1	3.091142	-1.163664	3.790457
1	2.411749	-3.618327	0.940481
1	3.619416	-3.169293	2.171419
1	2.059336	-3.873907	2.677306

6	6.013130	0.696026	0.388395
6	6.207048	2.206352	0.571783
6	6.859905	0.174205	-0.779217
1	6.368887	0.199056	1.307522
1	5.624987	2.580052	1.429588
1	7.270757	2.444044	0.743051
1	5.878701	2.757814	-0.326001
1	6.743426	-0.915045	-0.899044
1	6.560362	0.652897	-1.727512
1	7.928640	0.393323	-0.613943
6	1.696019	1.031572	-2.226827
6	2.111125	0.298431	-3.510550
6	1.844156	2.549388	-2.387463
1	0.616551	0.837763	-2.063452
1	1.946693	-0.789442	-3.420255
1	1.542407	0.666942	-4.381652
1	3.185780	0.458643	-3.710248
1	1.602360	3.073280	-1.446535
1	2.876325	2.823051	-2.672050
1	1.171352	2.921824	-3.179307
6	-1.333561	0.130487	1.212291
6	-2.678907	0.130168	1.695224
6	-0.647175	1.163053	1.927789
6	-2.815477	1.137095	2.692201
1	-3.482379	-0.517413	1.344761
6	-1.553922	1.778959	2.835353
1	0.395045	1.449624	1.778311
1	-3.726913	1.389137	3.232665
1	-1.331707	2.611345	3.501804
26	-2.260686	2.030289	0.843007
6	-2.207407	2.554118	-1.229362
6	-3.559836	2.451190	-0.797280
6	-1.576771	3.573861	-0.462578
1	-1.738646	1.953359	-2.008134
6	-3.764664	3.409563	0.233939
1	-4.302748	1.752855	-1.177781
6	-2.539721	4.102445	0.440543
1	-0.535657	3.880720	-0.538053
1	-4.689201	3.568648	0.786157
1	-2.363056	4.881865	1.179518

TS3-C-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.756879	1.129947	-0.118278
6	-1.093997	1.176069	-1.516183
6	-1.432060	2.046876	0.756409
6	-1.974614	2.160538	-1.977341
6	-2.305109	2.988376	0.205129
6	-2.579290	3.090798	-1.150104
1	-2.193192	2.210858	-3.047544
1	-2.772486	3.705279	0.884754
6	1.599342	0.143625	-0.628000
6	2.247257	1.432442	-0.757284
6	2.252186	-0.927753	-1.311739
6	3.485861	1.544269	-1.405168
6	3.470732	-0.718400	-1.985465
6	4.133726	0.493145	-2.038786
1	3.942089	2.534678	-1.471212
1	3.935176	-1.570974	-2.488531
6	-0.580030	0.277716	-2.670900
6	0.452073	0.976536	-3.573695
6	-1.689760	-0.191317	-3.645633
1	-0.106522	-0.620281	-2.256585
1	1.377018	1.252304	-3.050992
1	0.715790	0.308435	-4.412213
1	0.009153	1.889934	-4.010684
1	-2.607860	-0.568476	-3.171908
1	-1.998575	0.615458	-4.329481
1	-1.282530	-1.006116	-4.271449
6	-3.389415	4.236333	-1.708239
6	-2.507940	5.491030	-1.680641
6	-4.716057	4.459682	-0.980658
1	-3.615169	3.994837	-2.761278
1	-1.559171	5.304244	-2.211118
1	-3.012683	6.353277	-2.146942
1	-2.258071	5.752629	-0.636687
1	-5.339723	3.550418	-0.998528

1	-4.554685	4.745121	0.073784
1	-5.280408	5.276930	-1.460388
6	-1.267359	2.283409	2.278126
6	-2.598649	2.345419	3.059001
6	-0.535698	3.610391	2.552017
1	-0.673043	1.487620	2.732670
1	-3.271568	1.500121	2.849559
1	-2.371951	2.344966	4.140333
1	-3.160211	3.270390	2.850268
1	0.392384	3.719270	1.972900
1	-1.186472	4.464440	2.295052
1	-0.282091	3.689959	3.623534
6	1.759713	-2.359944	-1.519847
6	2.571950	-3.392894	-0.733699
6	1.740030	-2.733434	-3.014362
1	0.744885	-2.438545	-1.151865
1	3.659847	-3.281249	-0.897989
1	2.357706	-3.297437	0.342520
1	2.279518	-4.410612	-1.047295
1	1.290531	-1.937517	-3.634564
1	2.753478	-2.925830	-3.409186
1	1.156330	-3.658897	-3.162173
6	5.400678	0.679162	-2.854348
6	6.526371	1.413857	-2.118927
6	5.056595	1.394634	-4.167903
1	5.772572	-0.329200	-3.107934
1	6.798651	0.908040	-1.177713
1	7.426850	1.455764	-2.757023
1	6.245663	2.455268	-1.882618
1	4.262603	0.855781	-4.710737
1	4.691189	2.416763	-3.962734
1	5.941387	1.471510	-4.823304
6	1.717422	2.844961	-0.412699
6	1.272067	3.595588	-1.681572
6	2.757839	3.749079	0.283349
1	0.841491	2.775476	0.234559
1	0.377509	3.155432	-2.137957
1	1.044809	4.646815	-1.431760
1	2.081045	3.595042	-2.435024
1	3.362795	3.225261	1.041537

1	3.456343	4.191530	-0.447341
1	2.241278	4.597562	0.765409
6	-1.815237	-1.508131	1.164043
6	-2.364505	-0.777045	2.268714
6	-2.671102	-2.699363	1.075723
6	-3.439150	-1.480315	2.858653
1	-1.925425	0.131796	2.640911
6	-3.629160	-2.673711	2.110983
1	-2.669590	-3.474982	0.316179
1	-4.020907	-1.154175	3.719392
1	-4.421268	-3.409341	2.262643
26	-3.976435	-1.039759	0.827614
6	-5.964738	-1.281195	-0.014699
6	-5.899899	-0.071853	0.724627
6	-5.000025	-1.213412	-1.055008
1	-6.645548	-2.110881	0.173114
6	-4.897149	0.749207	0.142787
1	-6.510884	0.177642	1.590786
6	-4.344527	0.041628	-0.959995
1	-4.795073	-1.996150	-1.785896
1	-4.572479	1.724121	0.499835
1	-3.522400	0.384265	-1.580285
6	0.923898	0.142895	1.760164
6	1.576255	1.273171	2.341319
6	0.878196	-0.857885	2.783576
6	1.814866	1.015119	3.716373
1	1.819426	2.203844	1.851274
6	1.394728	-0.311235	3.988209
1	0.511020	-1.874282	2.662455
1	2.293944	1.699999	4.414251
1	1.495387	-0.843559	4.932374
26	2.971797	-0.313982	2.572193
6	4.567028	-0.788185	1.209111
6	4.967262	0.283283	2.047540
6	4.290278	-1.912586	2.031023
1	4.464994	-0.740602	0.129414
6	4.941926	-0.179047	3.391033
1	5.234535	1.286497	1.715745
6	4.523276	-1.536041	3.380268
1	3.943497	-2.884647	1.688708

1	5.181895	0.409638	4.275698
1	4.377052	-2.166232	4.256085
6	-1.482176	-2.478334	-1.525138
6	-0.328433	-4.465128	0.292901
6	-0.662747	-4.729019	-0.984771
6	-1.400509	-3.766753	-1.857038
6	-2.047688	-4.196690	-3.148858
1	-1.264404	-4.406586	-3.900338
1	-2.685691	-5.088349	-3.051438
1	-2.657271	-3.363312	-3.540017
6	-0.298157	-6.075550	-1.545544
1	0.308372	-5.980712	-2.462888
1	0.289480	-6.627052	-0.793872
1	-1.196088	-6.669211	-1.785723
6	0.276472	0.039520	0.330550
6	-0.472149	-1.298652	0.567819
1	-0.516168	-3.515411	0.794302
1	0.205503	-5.219450	0.880799
1	-0.849731	-2.151150	-0.662664
1	-2.106210	-1.729712	-2.001499

TS3-Si-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.883847	1.398655	-0.244430
6	-1.146894	1.490709	-1.642548
6	-1.499472	2.336648	0.630106
6	-1.952498	2.528909	-2.120236
6	-2.290795	3.349651	0.092443
6	-2.516653	3.475392	-1.274237
1	-2.140807	2.614056	-3.194879
1	-2.730822	4.083507	0.774480
6	1.923234	0.218573	-0.803726
6	2.614348	1.462997	-0.804364
6	2.467223	-0.853620	-1.552934
6	3.850578	1.563178	-1.439594
6	3.706105	-0.697089	-2.182058
6	4.421466	0.489831	-2.119760

1	4.369283	2.525826	-1.434969
1	4.138497	-1.537104	-2.733609
6	-0.604971	0.533833	-2.720038
6	0.544318	1.132030	-3.551816
6	-1.679476	0.108806	-3.740364
1	-0.237225	-0.384942	-2.232057
1	1.449474	1.342776	-2.969393
1	0.818072	0.429764	-4.358880
1	0.207068	2.071748	-4.024603
1	-2.650698	-0.145054	-3.288604
1	-1.858788	0.910155	-4.476262
1	-1.317230	-0.769092	-4.303872
6	-3.261767	4.671450	-1.811066
6	-2.332901	5.886702	-1.697622
6	-4.597523	4.884674	-1.096972
1	-3.465553	4.485730	-2.879526
1	-1.376515	5.681604	-2.208300
1	-2.783344	6.792301	-2.136101
1	-2.102212	6.086916	-0.636081
1	-5.221449	3.976924	-1.159078
1	-4.445542	5.117054	-0.028779
1	-5.153785	5.724424	-1.544493
6	-1.312420	2.407416	2.148841
6	-2.635859	2.436278	2.930289
6	-0.487277	3.641457	2.547763
1	-0.757042	1.524241	2.484497
1	-3.313003	1.617977	2.637556
1	-2.424684	2.344356	4.010988
1	-3.172376	3.389748	2.784516
1	0.459353	3.709576	1.989378
1	-1.056558	4.567035	2.350609
1	-0.248231	3.610550	3.625333
6	1.809599	-2.215740	-1.755832
6	2.444213	-3.290578	-0.869114
6	1.790462	-2.660034	-3.222135
1	0.750542	-2.146785	-1.475150
1	3.536871	-3.340095	-1.029830
1	2.257214	-3.075401	0.196765
1	2.008590	-4.282373	-1.090045
1	1.345882	-1.883226	-3.868522

1	2.796658	-2.894175	-3.608396
1	1.182802	-3.577269	-3.312287
6	5.713725	0.655125	-2.878261
6	6.812344	1.274229	-2.014006
6	5.420145	1.476317	-4.139060
1	6.043047	-0.351473	-3.189010
1	6.966980	0.680993	-1.096540
1	7.765501	1.321729	-2.565716
1	6.547657	2.301834	-1.710710
1	4.612406	1.000141	-4.720888
1	5.073658	2.487062	-3.859755
1	6.310646	1.574151	-4.781378
6	2.038390	2.778979	-0.273529
6	1.493925	3.639590	-1.428032
6	3.043599	3.625618	0.516365
1	1.191860	2.559412	0.391220
1	0.606374	3.195434	-1.898742
1	1.212792	4.642443	-1.060154
1	2.268975	3.766035	-2.206522
1	3.597762	3.034483	1.263135
1	3.776054	4.105937	-0.154328
1	2.508353	4.440028	1.036431
6	-2.233823	-1.882135	1.372412
6	-2.558430	-0.908039	2.362329
6	-3.317261	-2.830484	1.393372
6	-3.789387	-1.250511	2.980390
1	-1.940117	-0.047704	2.609276
6	-4.255943	-2.449912	2.379319
1	-3.455723	-3.669497	0.711029
1	-4.294578	-0.686804	3.762636
1	-5.190083	-2.968297	2.588200
26	-4.150442	-0.956085	0.882283
6	-6.012921	-1.025757	-0.153132
6	-5.932875	0.179454	0.595187
6	-4.956883	-1.024474	-1.103880
1	-6.736290	-1.826224	-0.004949
6	-4.829642	0.928239	0.105498
1	-6.584942	0.465626	1.418554
6	-4.227515	0.182604	-0.942180
1	-4.737589	-1.819127	-1.817299

1	-4.484147	1.894812	0.467482
1	-3.346937	0.489417	-1.498176
6	1.049950	0.173723	2.097895
6	1.716124	1.240223	2.780274
6	0.908002	-0.878193	3.061948
6	1.948291	0.861932	4.127197
1	2.001696	2.193733	2.345426
6	1.456996	-0.459136	4.300755
1	0.467999	-1.863998	2.889184
1	2.456610	1.462510	4.879933
1	1.517349	-1.058332	5.207867
26	2.997645	-0.446525	2.823585
6	4.439553	-0.951138	1.304822
6	4.951846	0.076837	2.138787
6	4.182057	-2.088624	2.116699
1	4.261244	-0.868443	0.233924
6	5.014708	-0.425194	3.468509
1	5.224724	1.080224	1.812020
6	4.539146	-1.764490	3.454073
1	3.777804	-3.040089	1.775292
1	5.328240	0.132947	4.349890
1	4.433381	-2.416511	4.320187
6	-1.957316	-2.658106	-1.711819
6	-1.074912	-4.986389	-0.081013
6	-1.053406	-4.972173	-1.433946
6	-1.602225	-3.867905	-2.230881
6	-1.728806	-4.048660	-3.724958
1	-0.761279	-4.195050	-4.232259
1	-2.347310	-4.939811	-3.933636
1	-2.231175	-3.179380	-4.177215
6	-0.359089	-6.101701	-2.153366
1	0.338037	-5.763045	-2.938220
1	0.203516	-6.707709	-1.425941
1	-1.103556	-6.764746	-2.630220
14	0.370955	0.057675	0.315896
14	-0.562192	-2.148966	0.453381
1	-1.705492	-4.340683	0.521256
1	-0.494413	-5.727192	0.481216
1	-2.297408	-2.492454	-0.688114
1	-2.241382	-1.847086	-2.387393

TS3-Ge-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.929709	1.468999	-0.222799
6	-1.180956	1.563302	-1.617273
6	-1.517689	2.381502	0.689630
6	-1.990070	2.603950	-2.069081
6	-2.313290	3.395469	0.171729
6	-2.545567	3.525993	-1.193724
1	-2.186399	2.711204	-3.139463
1	-2.743929	4.123964	0.864380
6	1.920240	0.310835	-0.855206
6	2.586440	1.561569	-0.837912
6	2.450057	-0.776327	-1.584299
6	3.822561	1.661013	-1.462780
6	3.686707	-0.613676	-2.204534
6	4.385246	0.581014	-2.138038
1	4.339181	2.623527	-1.457734
1	4.125388	-1.451052	-2.753317
6	-0.629321	0.624754	-2.712032
6	0.511939	1.240505	-3.544502
6	-1.697980	0.215135	-3.744545
1	-0.254809	-0.304131	-2.248382
1	1.427714	1.438774	-2.975697
1	0.771434	0.554535	-4.370152
1	0.167202	2.188396	-3.993728
1	-2.665546	-0.066798	-3.304838
1	-1.885342	1.034498	-4.457270
1	-1.321813	-0.643013	-4.329554
6	-3.283117	4.727098	-1.708766
6	-2.327601	5.918680	-1.584043
6	-4.607560	4.925674	-0.974795
1	-3.494188	4.550992	-2.776865
1	-1.378323	5.690062	-2.098947
1	-2.753668	6.840362	-2.010149
1	-2.085348	6.094991	-0.520768
1	-5.223166	4.012357	-1.044450

1	-4.440073	5.135120	0.095553
1	-5.174282	5.768581	-1.399508
6	-1.295046	2.434979	2.208889
6	-2.599387	2.448955	3.022843
6	-0.474490	3.673306	2.608540
1	-0.723920	1.556062	2.530041
1	-3.273164	1.619722	2.755048
1	-2.360059	2.368299	4.098859
1	-3.151003	3.394473	2.883638
1	0.468960	3.754384	2.046792
1	-1.053362	4.595189	2.423311
1	-0.228121	3.638121	3.684846
6	1.793433	-2.139437	-1.816980
6	2.436029	-3.253761	-0.984634
6	1.751862	-2.523954	-3.299043
1	0.733902	-2.094265	-1.536697
1	3.532967	-3.264810	-1.113143
1	2.215249	-3.122816	0.088408
1	2.035462	-4.239572	-1.285548
1	1.298369	-1.717540	-3.900655
1	2.752034	-2.742775	-3.707566
1	1.136698	-3.433463	-3.416349
6	5.653918	0.753580	-2.918634
6	6.753718	1.393106	-2.076208
6	5.300087	1.559416	-4.172183
1	5.984257	-0.252758	-3.226931
1	6.923469	0.806814	-1.156540
1	7.697286	1.447970	-2.641025
1	6.476550	2.417598	-1.774674
1	4.476233	1.064540	-4.715198
1	4.942440	2.563746	-3.883443
1	6.161721	1.668138	-4.848967
6	1.992052	2.876511	-0.314280
6	1.459758	3.731542	-1.480049
6	2.989125	3.732115	0.476478
1	1.137939	2.666249	0.345481
1	0.555034	3.306844	-1.935594
1	1.212969	4.749768	-1.130687
1	2.232533	3.818964	-2.265655
1	3.547851	3.146466	1.223914

1	3.717247	4.214748	-0.196888
1	2.448993	4.544862	0.994331
6	-2.188581	-1.814970	1.287762
6	-2.522266	-0.872964	2.298816
6	-3.255594	-2.767575	1.252809
6	-3.748718	-1.260596	2.900659
1	-1.919893	-0.006346	2.566421
6	-4.196033	-2.443885	2.253298
1	-3.370753	-3.560629	0.514390
1	-4.257393	-0.740530	3.709177
1	-5.110594	-3.000133	2.440683
26	-4.120635	-0.892026	0.812131
6	-6.007283	-0.959010	-0.181377
6	-5.917197	0.234060	0.585179
6	-4.976719	-0.933259	-1.158667
1	-6.720945	-1.767167	-0.028903
6	-4.833435	1.000312	0.080102
1	-6.549476	0.500319	1.430222
6	-4.254428	0.276947	-0.995706
1	-4.768429	-1.712953	-1.891705
1	-4.486022	1.962675	0.450647
1	-3.396845	0.600939	-1.574685
6	1.073158	0.226294	2.093550
6	1.739726	1.288666	2.762154
6	0.936646	-0.837927	3.033824
6	1.986734	0.895974	4.101123
1	2.010148	2.239570	2.311353
6	1.499241	-0.428465	4.268077
1	0.489845	-1.817945	2.843691
1	2.498294	1.494407	4.850977
1	1.566107	-1.039051	5.165441
26	3.017030	-0.399915	2.764835
6	4.477382	-0.834116	1.230716
6	4.983932	0.137391	2.131696
6	4.189555	-2.012142	1.969854
1	4.330875	-0.691785	0.161777
6	5.013090	-0.439668	3.431677
1	5.274993	1.153464	1.866158
6	4.521262	-1.770132	3.330811
1	3.783606	-2.936743	1.563756

1	5.303028	0.068533	4.349878
1	4.375825	-2.466139	4.155315
6	-1.924717	-2.492717	-1.795873
6	-0.927032	-4.691126	-0.086757
6	-0.977937	-4.770449	-1.447476
6	-1.592385	-3.730082	-2.265573
6	-1.798740	-3.965149	-3.744169
1	-0.855768	-4.085092	-4.303515
1	-2.397477	-4.880093	-3.895567
1	-2.355193	-3.122541	-4.185377
6	-0.286985	-5.932057	-2.111382
1	0.379375	-5.655972	-2.946876
1	0.302874	-6.474255	-1.355339
1	-1.044519	-6.638148	-2.498945
32	0.371182	0.128910	0.292538
32	-0.459432	-2.121744	0.389450
1	-1.651183	-4.155693	0.511589
1	-0.265500	-5.349360	0.488227
1	-2.197562	-2.243052	-0.768982
1	-2.256628	-1.723700	-2.494115

TS3-Sn-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.950520	1.704995	0.252938
6	1.172697	1.872670	1.639522
6	1.492272	2.598435	-0.695460
6	1.942417	2.959870	2.053028
6	2.242908	3.669081	-0.225606
6	2.471149	3.860648	1.135040
1	2.131908	3.120190	3.118639
1	2.651570	4.380437	-0.949429
6	-2.086778	0.418167	0.919526
6	-2.775908	1.643540	0.798905
6	-2.591093	-0.627657	1.713646
6	-4.017377	1.760617	1.412086
6	-3.837337	-0.463298	2.312283
6	-4.558764	0.712202	2.156090

1	-4.559061	2.707069	1.339692
1	-4.262160	-1.270297	2.916202
6	0.621001	0.947120	2.739448
6	-0.573007	1.539160	3.511172
6	1.672338	0.580643	3.800032
1	0.292385	-0.002443	2.278291
1	-1.468103	1.687648	2.896205
1	-0.847312	0.861669	4.339457
1	-0.286015	2.510559	3.950524
1	2.652942	0.315815	3.376509
1	1.823756	1.419316	4.499336
1	1.305159	-0.275931	4.392381
6	3.191098	5.098718	1.590094
6	2.226201	6.274035	1.397851
6	4.517323	5.270021	0.849735
1	3.401309	4.984460	2.666821
1	1.276272	6.064951	1.919711
1	2.641458	7.221297	1.776379
1	1.988191	6.392747	0.325775
1	5.139164	4.365559	0.965965
1	4.351044	5.422490	-0.230359
1	5.079166	6.137287	1.230186
6	1.263694	2.526785	-2.207775
6	2.564575	2.517249	-3.023075
6	0.383871	3.687461	-2.698807
1	0.728261	1.598340	-2.447722
1	3.258848	1.730535	-2.686446
1	2.330713	2.342568	-4.088922
1	3.086202	3.487797	-2.957470
1	-0.567491	3.753896	-2.146519
1	0.910029	4.650742	-2.576397
1	0.147953	3.562406	-3.770677
6	-1.871943	-1.947703	1.981313
6	-2.437615	-3.091044	1.131585
6	-1.842246	-2.333833	3.461679
1	-0.810460	-1.821363	1.726863
1	-3.527893	-3.185059	1.280248
1	-2.262937	-2.917034	0.055200
1	-1.958875	-4.052618	1.396502
1	-1.418549	-1.516291	4.069988

1	-2.842087	-2.581187	3.854129
1	-1.203932	-3.225955	3.586754
6	-5.836599	0.912441	2.917213
6	-6.933740	1.485715	2.024461
6	-5.496815	1.791855	4.125143
1	-6.159013	-0.077775	3.281680
1	-7.070381	0.847211	1.134415
1	-7.891179	1.552642	2.563772
1	-6.669512	2.496978	1.671953
1	-4.671746	1.333379	4.697765
1	-5.141822	2.779472	3.781121
1	-6.359745	1.935035	4.793945
6	-2.181152	2.901113	0.155722
6	-1.628487	3.856409	1.229860
6	-3.165198	3.675404	-0.724864
1	-1.331369	2.614757	-0.484580
1	-0.728641	3.459956	1.720773
1	-1.360623	4.829739	0.781693
1	-2.394030	4.035468	2.006801
1	-3.670150	3.023549	-1.456016
1	-3.934129	4.179241	-0.115136
1	-2.623839	4.466664	-1.273732
6	2.399868	-1.872358	-1.296252
6	2.636732	-0.877404	-2.287050
6	3.545730	-2.719592	-1.290618
6	3.896748	-1.126628	-2.895069
1	1.957573	-0.061003	-2.539714
6	4.457737	-2.276313	-2.276412
1	3.720918	-3.538662	-0.591379
1	4.355718	-0.536244	-3.685774
1	5.424142	-2.730892	-2.479969
26	4.218260	-0.763390	-0.803351
6	6.064309	-0.668077	0.247474
6	5.916643	0.495389	-0.556103
6	5.005122	-0.685516	1.194461
1	6.829840	-1.434216	0.135317
6	4.767687	1.197879	-0.104517
1	6.551676	0.779855	-1.393311
6	4.205827	0.466505	0.975071
1	4.827368	-1.455253	1.945522

1	4.369025	2.127343	-0.507723
1	3.312227	0.754125	1.520726
6	-1.095671	0.161663	-2.264544
6	-1.773102	1.155657	-3.016724
6	-0.943997	-0.975774	-3.109095
6	-2.026952	0.642494	-4.314518
1	-2.054458	2.138399	-2.641622
6	-1.519037	-0.683254	-4.370721
1	-0.476270	-1.927268	-2.837740
1	-2.548087	1.165521	-5.112440
1	-1.572326	-1.366186	-5.215247
26	-3.024092	-0.554278	-2.855579
6	-4.428939	-0.946061	-1.250858
6	-4.966182	-0.001033	-2.163434
6	-4.166902	-2.145669	-1.965380
1	-4.249958	-0.773084	-0.189773
6	-5.041375	-0.616801	-3.444132
1	-5.244896	1.023474	-1.917351
6	-4.545617	-1.944222	-3.321009
1	-3.753419	-3.061719	-1.545807
1	-5.360393	-0.135121	-4.367020
1	-4.431633	-2.666462	-4.127937
6	2.108260	-2.400444	1.974240
6	1.279443	-4.806853	0.569799
6	1.193034	-4.705948	1.936557
6	1.713002	-3.544255	2.626711
6	1.749286	-3.537489	4.134604
1	0.753252	-3.614368	4.601192
1	2.341854	-4.403665	4.478664
1	2.240428	-2.624376	4.504859
6	0.380062	-5.724676	2.690420
1	-0.324311	-5.288158	3.419543
1	-0.198715	-6.333468	1.977606
1	1.047763	-6.411157	3.241682
50	-0.371749	0.143261	-0.284735
50	0.579989	-2.400515	-0.259988
1	2.107842	-4.374165	0.008436
1	0.698860	-5.556484	0.022035
1	2.529540	-2.381706	0.964943
1	2.372496	-1.511137	2.554241

TS3-Pb-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.786344	1.930331	0.341651
6	1.009719	2.087923	1.726974
6	1.255182	2.886641	-0.579923
6	1.686369	3.231254	2.165129
6	1.918757	4.010296	-0.090778
6	2.136209	4.200976	1.272240
1	1.864669	3.380454	3.235183
1	2.265804	4.766089	-0.802855
6	-2.252230	0.366992	0.970580
6	-3.021329	1.542676	0.876044
6	-2.679516	-0.712321	1.763901
6	-4.261483	1.574997	1.512102
6	-3.930360	-0.641182	2.377273
6	-4.735452	0.484936	2.243814
1	-4.865413	2.485378	1.456265
1	-4.294058	-1.482007	2.976229
6	0.553171	1.087163	2.798196
6	-0.684119	1.552795	3.584019
6	1.648016	0.768625	3.828860
1	0.296388	0.135850	2.298518
1	-1.578627	1.660075	2.958204
1	-0.917349	0.820724	4.377745
1	-0.477888	2.524043	4.067679
1	2.636361	0.593115	3.375019
1	1.752988	1.594536	4.552489
1	1.360828	-0.130256	4.402208
6	2.765517	5.484948	1.753575
6	1.733061	6.607109	1.591550
6	4.075462	5.782949	1.021030
1	2.987999	5.366593	2.827848
1	0.799682	6.343083	2.117371
1	2.103447	7.567725	1.985570
1	1.482997	6.738524	0.523766
1	4.774091	4.933963	1.112612

1	3.898328	5.956746	-0.054319
1	4.561250	6.684346	1.428823
6	1.029649	2.812603	-2.087900
6	2.325266	2.906173	-2.903718
6	0.052750	3.900713	-2.555628
1	0.568679	1.844074	-2.325834
1	3.066861	2.158037	-2.579932
1	2.104032	2.735255	-3.972382
1	2.783779	3.907074	-2.817985
1	-0.889794	3.878878	-1.983789
1	0.497816	4.903676	-2.428320
1	-0.190122	3.766273	-3.624321
6	-1.849660	-1.972557	1.984927
6	-2.266434	-3.101801	1.036117
6	-1.832630	-2.458102	3.435685
1	-0.803780	-1.713523	1.770344
1	-3.338612	-3.336380	1.164767
1	-2.117834	-2.813800	-0.021312
1	-1.683690	-4.021797	1.232929
1	-1.509310	-1.651093	4.115324
1	-2.815770	-2.825205	3.772957
1	-1.118831	-3.295553	3.528500
6	-6.039154	0.578485	2.992373
6	-7.172722	1.072524	2.094734
6	-5.807465	1.467668	4.218844
1	-6.291080	-0.437623	3.342072
1	-7.256026	0.436168	1.197067
1	-8.136664	1.057368	2.628229
1	-6.989672	2.106538	1.756359
1	-4.968288	1.071454	4.816224
1	-5.527474	2.486451	3.897782
1	-6.701390	1.531185	4.860192
6	-2.513593	2.826580	0.217857
6	-1.996610	3.817824	1.275086
6	-3.551080	3.526015	-0.662167
1	-1.658676	2.574703	-0.430708
1	-1.089270	3.453097	1.777703
1	-1.748925	4.787548	0.807714
1	-2.770675	3.991995	2.044817
1	-3.997102	2.835941	-1.397029

1	-4.361438	3.965807	-0.056128
1	-3.070413	4.357209	-1.208207
6	2.631614	-1.635511	-1.415535
6	2.708949	-0.557433	-2.343540
6	3.874166	-2.329914	-1.496401
6	3.974005	-0.597280	-2.991349
1	1.927780	0.182645	-2.529468
6	4.696739	-1.702549	-2.466301
1	4.166221	-3.183546	-0.881007
1	4.335430	0.103755	-3.742522
1	5.711253	-1.999118	-2.725772
26	4.298710	-0.330912	-0.893197
6	6.106838	-0.071510	0.198048
6	5.859370	1.085303	-0.589879
6	5.036912	-0.209686	1.122319
1	6.947474	-0.755257	0.090112
6	4.637153	1.661265	-0.151946
1	6.478991	1.447001	-1.408746
6	4.127584	0.858885	0.902978
1	4.929359	-1.002907	1.861237
1	4.158162	2.555901	-0.546494
1	3.198407	1.049621	1.434068
6	-1.199277	0.254889	-2.370204
6	-1.941489	1.212247	-3.112095
6	-0.984767	-0.865591	-3.222015
6	-2.177751	0.688198	-4.412194
1	-2.285633	2.176323	-2.739405
6	-1.588440	-0.602498	-4.479481
1	-0.449675	-1.779398	-2.951218
1	-2.738912	1.177935	-5.205673
1	-1.608805	-1.278609	-5.332149
26	-3.085277	-0.576708	-2.955845
6	-4.407165	-1.084398	-1.316669
6	-5.037314	-0.162871	-2.193581
6	-4.094598	-2.252862	-2.061885
1	-4.201575	-0.916454	-0.259190
6	-5.121043	-0.763114	-3.480561
1	-5.374357	0.836788	-1.921056
6	-4.536348	-2.056398	-3.398699
1	-3.604890	-3.145701	-1.675597

1	-5.514167	-0.294221	-4.381093
1	-4.412907	-2.759394	-4.220935
6	2.467128	-2.297494	1.957989
6	1.736739	-4.709077	0.596071
6	1.631561	-4.618113	1.982675
6	2.058253	-3.443536	2.657899
6	1.915988	-3.345351	4.157066
1	0.866145	-3.349822	4.500572
1	2.419470	-4.207727	4.629183
1	2.396689	-2.428823	4.530328
6	0.834741	-5.662578	2.724094
1	0.117360	-5.225633	3.438873
1	0.268795	-6.282301	2.010680
1	1.498226	-6.336964	3.294054
82	-0.447957	0.186915	-0.303885
82	0.953850	-2.280156	-0.057373
1	2.597636	-4.288435	0.065287
1	1.229879	-5.518797	0.060029
1	3.128774	-2.357713	1.082667
1	2.597486	-1.365557	2.520532

TS4-C-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.219189	1.833344	1.943121
6	-1.518812	1.032098	0.128482
6	1.541117	-0.730736	0.560933
6	0.334164	-0.125822	3.653180
6	-0.897972	0.334953	3.983925
6	-1.621368	1.351724	3.225789
1	-1.746729	2.756093	1.659972
1	-0.147192	1.904808	1.742633
6	-2.825275	1.947616	3.922057
1	-3.563477	1.196863	4.261215
1	-2.504757	2.484460	4.837497
1	-3.355057	2.674750	3.287427
6	-1.564574	-0.282356	5.203068
1	-0.897461	-1.031434	5.658180

1	-1.815464	0.459571	5.979897
1	-2.502758	-0.796519	4.927565
1	0.830763	-0.899077	4.248768
1	0.872839	0.251623	2.786905
6	-2.569372	0.160898	-0.432965
6	-2.425575	-0.419374	-1.766868
6	-3.768717	-0.236689	0.263512
6	-3.474761	-1.158641	-2.324506
6	-4.786052	-0.941363	-0.383313
6	-4.693127	-1.404676	-1.690709
1	-3.335035	-1.573652	-3.327134
1	-5.701910	-1.139515	0.181495
6	2.890891	-0.203775	0.337530
6	3.697231	-0.766864	-0.705330
6	3.392005	1.025086	0.911370
6	4.928791	-0.205615	-1.053976
6	4.654921	1.502408	0.547760
6	5.464357	0.913975	-0.420124
1	5.497172	-0.676030	-1.862661
1	5.026565	2.401725	1.048081
6	-1.155273	-0.431648	-2.633452
6	-1.405221	0.144097	-4.039326
6	-0.612521	-1.867131	-2.781274
1	-0.364870	0.157788	-2.150623
1	-1.864619	1.142128	-3.997590
1	-0.456384	0.224256	-4.597046
1	-2.072523	-0.510859	-4.626863
1	-0.352855	-2.307169	-1.803653
1	-1.350543	-2.526834	-3.272679
1	0.293118	-1.866545	-3.412898
6	-5.840692	-2.134942	-2.371977
6	-7.074395	-1.231237	-2.525336
6	-6.234581	-3.434049	-1.653094
1	-5.499252	-2.407200	-3.385981
1	-6.837099	-0.313553	-3.086553
1	-7.880013	-1.764479	-3.059589
1	-7.469424	-0.932985	-1.538475
1	-5.384267	-4.130112	-1.573003
1	-6.604314	-3.229303	-0.633416
1	-7.045554	-3.943654	-2.202331

6	-4.092064	0.142427	1.692598
6	-4.400120	-1.082816	2.564315
6	-5.224374	1.174706	1.734683
1	-3.197924	0.592436	2.113042
1	-3.561891	-1.800638	2.543543
1	-4.561465	-0.777144	3.612621
1	-5.310173	-1.613880	2.236413
1	-4.945551	2.074713	1.158803
1	-6.152708	0.771313	1.294473
1	-5.443618	1.481271	2.771273
6	2.690108	1.849830	1.987133
6	2.705341	3.368640	1.733541
6	3.296645	1.570782	3.372058
1	1.635063	1.555866	1.994455
1	2.295485	3.628247	0.743037
1	2.089089	3.874377	2.499580
1	3.719368	3.799169	1.808229
1	3.308584	0.493827	3.604386
1	4.341364	1.932526	3.397903
1	2.735429	2.091915	4.166866
6	6.838069	1.473995	-0.756421
6	6.940317	1.962700	-2.207793
6	7.956349	0.467194	-0.452241
1	6.996161	2.350143	-0.102839
1	6.184854	2.734399	-2.426837
1	7.938285	2.394256	-2.399734
1	6.794024	1.131427	-2.918812
1	7.934590	0.151209	0.602993
1	7.855481	-0.435328	-1.079566
1	8.945469	0.911228	-0.659982
6	3.223504	-1.933937	-1.559428
6	4.176688	-3.124309	-1.418991
6	3.072610	-1.510348	-3.028608
1	2.229052	-2.248006	-1.209301
1	4.247117	-3.442559	-0.365224
1	3.843764	-3.981558	-2.027695
1	5.191683	-2.852118	-1.754595
1	2.387657	-0.650489	-3.122722
1	4.043624	-1.214670	-3.461627
1	2.674922	-2.340431	-3.638888

6	1.163991	-1.983562	1.157873
6	-0.226945	-2.396756	1.354070
6	1.946079	-2.920367	1.964835
6	-0.274399	-3.461995	2.266563
1	-1.088143	-1.922197	0.879370
6	1.074943	-3.777761	2.657303
1	3.031372	-2.906931	2.053642
1	-1.165096	-3.993672	2.605532
1	1.361475	-4.574238	3.345318
26	0.802704	-4.160972	0.578996
6	1.146186	-6.276106	0.377689
6	-0.203328	-5.997532	0.043160
6	1.983296	-5.561189	-0.522843
1	1.480211	-6.918364	1.192154
6	-0.209897	-5.107399	-1.065705
1	-1.080873	-6.394681	0.552985
6	1.142051	-4.840776	-1.417394
1	3.070162	-5.565354	-0.512785
1	-1.095321	-4.703571	-1.553182
1	1.466723	-4.177053	-2.217355
6	-1.044482	2.055724	-0.833685
6	0.323425	2.455124	-1.119511
6	-1.852022	2.681052	-1.844929
6	0.327023	3.218862	-2.316748
1	1.215717	2.136680	-0.577597
6	-1.024727	3.383086	-2.749658
1	-2.937553	2.602340	-1.886076
1	1.198081	3.654034	-2.808188
1	-1.362794	3.967553	-3.605744
26	-0.772459	4.290241	-0.862522
6	-0.823973	5.393763	0.969819
6	0.280247	5.840944	0.195359
6	-2.012409	5.636435	0.221856
1	-0.764922	4.929310	1.952437
6	-0.222013	6.359055	-1.029492
1	1.329000	5.794751	0.483130
6	-1.637164	6.236372	-1.012185
1	-3.028568	5.391306	0.524864
1	0.376521	6.772351	-1.841020
1	-2.308722	6.527398	-1.818926

TS4-Si-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.047700	-2.149226	3.450636
14	0.493590	-1.074008	-0.001712
14	-0.541098	0.862626	1.030512
6	-0.387441	0.922223	3.050461
6	-0.347895	0.058672	4.303943
6	-0.564076	-1.307357	4.466009
1	-1.201717	-3.211086	3.679183
1	-1.508135	-1.751250	2.545732
6	-0.263642	-1.933318	5.831128
1	0.682004	-1.565425	6.265766
1	-1.054483	-1.709237	6.575064
1	-0.189973	-3.031619	5.763488
6	0.112774	0.846944	5.517838
1	0.002210	1.932701	5.366738
1	-0.456343	0.578750	6.426599
1	1.181430	0.661605	5.756419
1	0.563035	1.486569	3.129601
1	-1.137057	1.720250	3.244056
6	2.413043	-1.133661	-0.397618
6	2.955096	-0.842442	-1.684520
6	3.324680	-1.550303	0.609948
6	4.326428	-1.028339	-1.927403
6	4.684499	-1.727352	0.316650
6	5.214983	-1.486429	-0.952038
1	4.728717	-0.792482	-2.919084
1	5.354749	-2.073483	1.111305
6	-2.378209	1.084863	0.293231
6	-2.620686	1.526282	-1.051245
6	-3.534986	0.747626	1.054897
6	-3.931369	1.587119	-1.554334
6	-4.823640	0.859709	0.508287
6	-5.059577	1.263325	-0.800380
1	-4.080595	1.908756	-2.590180
1	-5.686424	0.608937	1.133571

6	2.139110	-0.217606	-2.812571
6	2.336513	-0.890958	-4.176612
6	2.456263	1.281797	-2.908084
1	1.072206	-0.309123	-2.556270
1	2.140125	-1.974129	-4.129798
1	1.643544	-0.451922	-4.914840
1	3.359822	-0.745139	-4.565113
1	2.262139	1.789870	-1.947418
1	3.517379	1.442236	-3.174960
1	1.837200	1.760227	-3.688253
6	6.692700	-1.711077	-1.258606
6	7.087046	-3.189433	-1.128666
6	7.615941	-0.843461	-0.391883
1	6.855484	-1.417171	-2.310510
1	6.472163	-3.831366	-1.779561
1	8.146272	-3.331275	-1.407111
1	6.965274	-3.540580	-0.089197
1	7.387930	0.228679	-0.503403
1	7.521320	-1.103851	0.676586
1	8.670682	-1.001773	-0.678426
6	2.876420	-1.846064	2.033621
6	3.663916	-1.039771	3.070526
6	2.938839	-3.348125	2.328648
1	1.816229	-1.546913	2.126682
1	3.614581	0.040965	2.854858
1	3.245854	-1.210815	4.077226
1	4.728141	-1.333183	3.095963
1	2.327677	-3.916487	1.606587
1	3.977212	-3.720411	2.264153
1	2.559174	-3.558760	3.342976
6	-3.503291	0.263856	2.498600
6	-4.241085	-1.067219	2.683542
6	-4.049887	1.335762	3.450423
1	-2.465452	0.075540	2.783851
1	-3.872849	-1.819899	1.966009
1	-4.070437	-1.454775	3.701955
1	-5.329796	-0.963110	2.537252
1	-3.522873	2.296091	3.316387
1	-5.123852	1.518926	3.267654
1	-3.932154	1.016394	4.500198

6	-6.475606	1.329209	-1.361314
6	-6.677118	0.373795	-2.545097
6	-6.900848	2.751733	-1.751125
1	-7.150731	0.997413	-0.553052
1	-6.411180	-0.661425	-2.276570
1	-7.732292	0.384072	-2.870453
1	-6.058863	0.673771	-3.409003
1	-6.811780	3.449115	-0.902790
1	-6.285237	3.140085	-2.580984
1	-7.952916	2.754272	-2.087434
6	-1.549764	1.966968	-2.058253
6	-1.845924	3.381567	-2.586545
6	-1.454181	1.010878	-3.259610
1	-0.567683	1.995059	-1.553445
1	-1.926224	4.116801	-1.768640
1	-1.056021	3.709948	-3.283101
1	-2.791285	3.402408	-3.156344
1	-1.160884	-0.006828	-2.965174
1	-2.427127	0.938280	-3.779187
1	-0.716817	1.388050	-3.990292
6	0.524679	2.483784	0.985775
6	1.950778	2.478690	1.158338
6	0.064629	3.690464	1.614793
6	2.341820	3.626440	1.902594
1	2.628579	1.701753	0.798103
6	1.169260	4.379700	2.186447
1	-0.974335	4.019392	1.671271
1	3.361950	3.911793	2.160672
1	1.135134	5.341992	2.698380
26	1.460785	4.282928	0.097563
6	1.572044	6.316115	-0.551555
6	2.841380	5.698512	-0.710701
6	0.635693	5.614630	-1.357941
1	1.353038	7.162934	0.097892
6	2.692967	4.613406	-1.615145
1	3.761770	5.989900	-0.205851
6	1.330423	4.561031	-2.015607
1	-0.425353	5.842046	-1.440894
1	3.479697	3.929910	-1.929783
1	0.898650	3.824762	-2.688118

6	-0.459608	-2.009432	-1.360113
6	-1.855765	-1.931267	-1.705705
6	0.116159	-2.962337	-2.276994
6	-2.110621	-2.778703	-2.817477
1	-2.600334	-1.305777	-1.212980
6	-0.889936	-3.419927	-3.170003
1	1.154107	-3.297564	-2.279122
1	-3.077133	-2.940776	-3.295493
1	-0.765300	-4.165454	-3.956666
26	-1.427854	-3.938670	-1.180940
6	-1.373460	-4.645098	0.815240
6	-2.723280	-4.574202	0.371613
6	-0.682631	-5.560266	-0.025358
1	-0.923498	-4.051141	1.610183
6	-2.865269	-5.444851	-0.744608
1	-3.503658	-3.936805	0.784528
6	-1.604634	-6.054713	-0.989300
1	0.373460	-5.816398	0.041941
1	-3.773048	-5.596577	-1.327439
1	-1.381919	-6.760579	-1.787968

TS4-Ge-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.017348	-2.064925	3.422345
32	0.506355	-1.124287	0.032076
32	-0.566691	0.892929	0.987557
6	-0.405772	1.017890	3.044042
6	-0.362746	0.155980	4.290912
6	-0.559247	-1.209777	4.446643
1	-1.165842	-3.125735	3.661120
1	-1.504393	-1.679520	2.526329
6	-0.274415	-1.822229	5.820282
1	0.668443	-1.449929	6.257729
1	-1.072359	-1.580839	6.552104
1	-0.206294	-2.922071	5.770632
6	0.087558	0.960592	5.496299
1	-0.037051	2.042259	5.326668

1	-0.472186	0.697591	6.411391
1	1.161401	0.792889	5.724006
1	0.549429	1.576086	3.095709
1	-1.153743	1.816595	3.230483
6	2.470561	-1.119608	-0.408560
6	2.992323	-0.833919	-1.700262
6	3.379151	-1.500490	0.608813
6	4.365866	-1.000219	-1.941199
6	4.739562	-1.659136	0.318150
6	5.258838	-1.430685	-0.957519
1	4.764365	-0.774768	-2.936603
1	5.415345	-1.981595	1.117532
6	-2.437507	1.078908	0.220996
6	-2.661319	1.479124	-1.132548
6	-3.579577	0.742124	0.995082
6	-3.968148	1.513269	-1.642159
6	-4.865004	0.825840	0.441568
6	-5.092080	1.197058	-0.878454
1	-4.116459	1.806955	-2.686166
1	-5.728262	0.581146	1.068086
6	2.156923	-0.239414	-2.831650
6	2.361330	-0.926749	-4.187834
6	2.444623	1.264777	-2.950482
1	1.092703	-0.348895	-2.569526
1	2.181146	-2.011920	-4.126732
1	1.661000	-0.507589	-4.930660
1	3.381845	-0.770249	-4.579325
1	2.238904	1.785446	-1.999147
1	3.502922	1.441061	-3.218110
1	1.818794	1.718898	-3.739820
6	6.736377	-1.643027	-1.260406
6	7.140455	-3.115523	-1.102657
6	7.643048	-0.748871	-0.404489
1	6.896575	-1.365349	-2.316898
1	6.530236	-3.771993	-1.743487
1	8.201154	-3.256523	-1.374409
1	7.015003	-3.448112	-0.057567
1	7.396172	0.317164	-0.533177
1	7.546140	-0.994216	0.667253
1	8.701109	-0.894251	-0.683922

6	2.923317	-1.775335	2.034221
6	3.684120	-0.932979	3.060936
6	2.999256	-3.270404	2.356656
1	1.858584	-1.491184	2.116344
1	3.609365	0.141679	2.822977
1	3.260587	-1.093553	4.067108
1	4.754443	-1.200334	3.099011
1	2.398392	-3.856092	1.639367
1	4.041454	-3.632954	2.305367
1	2.612094	-3.467613	3.370820
6	-3.528234	0.293581	2.449719
6	-4.252829	-1.038616	2.673909
6	-4.072116	1.384636	3.380604
1	-2.485328	0.121017	2.730528
1	-3.880314	-1.807763	1.976201
1	-4.075789	-1.396854	3.701971
1	-5.342658	-0.947172	2.528165
1	-3.546102	2.341960	3.222784
1	-5.146788	1.561808	3.197108
1	-3.949070	1.088862	4.436712
6	-6.502440	1.240628	-1.446521
6	-6.683303	0.258084	-2.610059
6	-6.924886	2.654587	-1.866165
1	-7.179850	0.921951	-0.635216
1	-6.406891	-0.767073	-2.314539
1	-7.734740	0.248905	-2.945880
1	-6.058144	0.545354	-3.473238
1	-6.837009	3.366705	-1.029876
1	-6.301689	3.025598	-2.698289
1	-7.974625	2.653084	-2.208239
6	-1.576412	1.905102	-2.130365
6	-1.864533	3.316540	-2.668628
6	-1.465800	0.939028	-3.322266
1	-0.599425	1.936069	-1.615438
1	-1.923727	4.058186	-1.855181
1	-1.082094	3.630751	-3.379720
1	-2.818878	3.339900	-3.222058
1	-1.175088	-0.076079	-3.016462
1	-2.431311	0.862419	-3.854090
1	-0.718623	1.310472	-4.045873

6	0.516880	2.558685	0.908647
6	1.938836	2.554863	1.086263
6	0.043881	3.764342	1.522966
6	2.321974	3.716503	1.812043
1	2.616140	1.773268	0.735370
6	1.144787	4.467644	2.083754
1	-0.999235	4.081476	1.573576
1	3.340123	4.009392	2.066644
1	1.103145	5.435254	2.583656
26	1.432492	4.328991	-0.006322
6	1.520584	6.340245	-0.704220
6	2.796085	5.730709	-0.849708
6	0.590577	5.610938	-1.493637
1	1.291583	7.196191	-0.070653
6	2.657130	4.623051	-1.728575
1	3.712879	6.039090	-0.349034
6	1.294789	4.548758	-2.126695
1	-0.473254	5.824184	-1.580142
1	3.448967	3.938718	-2.027780
1	0.869181	3.793601	-2.781958
6	-0.446618	-2.070667	-1.392024
6	-1.837835	-2.001749	-1.740328
6	0.147083	-3.028403	-2.283939
6	-2.079387	-2.872312	-2.837334
1	-2.585642	-1.371870	-1.257456
6	-0.851771	-3.510641	-3.171736
1	1.189892	-3.348160	-2.271089
1	-3.041956	-3.049673	-3.316323
1	-0.715077	-4.267426	-3.944377
26	-1.393819	-3.989236	-1.170039
6	-1.329616	-4.644126	0.846662
6	-2.680772	-4.584715	0.405648
6	-0.640222	-5.577500	0.025330
1	-0.878761	-4.032728	1.627961
6	-2.825750	-5.481386	-0.689787
1	-3.459242	-3.937842	0.807400
6	-1.564585	-6.095429	-0.924519
1	0.416677	-5.829428	0.095980
1	-3.734887	-5.645254	-1.266739
1	-1.342033	-6.817454	-1.708318

TS4-Sn-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.176087	-2.233173	3.033830
50	0.472784	-1.531700	0.401283
50	-0.575478	1.026280	0.527057
6	-0.426249	0.635940	3.558804
6	0.577918	-0.141677	4.098950
6	0.653747	-1.569833	3.921117
1	-0.087938	-3.320069	2.935663
1	-1.144543	-1.825838	2.735065
6	1.720308	-2.370387	4.634114
1	2.714829	-1.894334	4.617175
1	1.454834	-2.520553	5.698630
1	1.814477	-3.370888	4.181523
6	1.676985	0.531314	4.892669
1	1.467734	1.602435	5.035537
1	1.774740	0.065566	5.889570
1	2.658542	0.435760	4.394536
1	-0.437420	1.713006	3.754109
1	-1.376638	0.182097	3.285269
6	2.429826	-1.196954	-0.592463
6	2.562717	-0.829240	-1.954843
6	3.596771	-1.496126	0.147858
6	3.835615	-0.835093	-2.544147
6	4.845698	-1.495523	-0.484718
6	4.986410	-1.183337	-1.837857
1	3.937341	-0.553336	-3.597413
1	5.736372	-1.758220	0.095240
6	-2.713437	1.455974	0.227632
6	-3.034893	2.327061	-0.840680
6	-3.763841	0.760286	0.870058
6	-4.372923	2.520390	-1.203123
6	-5.089534	0.994188	0.485546
6	-5.420122	1.872937	-0.544439
1	-4.604935	3.189743	-2.037895
1	-5.897585	0.470298	1.005870

6	1.409575	-0.334064	-2.826250
6	1.291375	-1.075240	-4.164665
6	1.548777	1.178570	-3.058393
1	0.466319	-0.496772	-2.285130
1	1.228400	-2.164335	-4.014272
1	0.377631	-0.754515	-4.694466
1	2.149423	-0.864966	-4.826799
1	1.541135	1.729667	-2.099933
1	2.497010	1.412561	-3.574690
1	0.723442	1.554555	-3.687452
6	6.344804	-1.219230	-2.515367
6	6.933003	-2.636279	-2.506142
6	7.317265	-0.212733	-1.888022
1	6.191532	-0.927307	-3.568785
1	6.237483	-3.356079	-2.967561
1	7.885615	-2.668185	-3.061686
1	7.131730	-2.973335	-1.474034
1	6.916447	0.812708	-1.944540
1	7.496305	-0.446999	-0.824396
1	8.290817	-0.234017	-2.406894
6	3.567541	-1.853333	1.632978
6	4.504198	-0.960746	2.456466
6	3.880981	-3.340268	1.843192
1	2.548136	-1.672141	2.019248
1	4.237377	0.102759	2.339686
1	4.438483	-1.215887	3.527588
1	5.557414	-1.082025	2.154272
1	3.149100	-3.976363	1.315465
1	4.881999	-3.587276	1.449654
1	3.860709	-3.602448	2.914246
6	-3.532183	-0.222957	2.008176
6	-4.248399	-1.566892	1.828352
6	-3.906723	0.411812	3.355768
1	-2.455735	-0.454617	2.015983
1	-3.996229	-2.030286	0.859905
1	-3.943142	-2.261947	2.630802
1	-5.344832	-1.458417	1.888028
1	-3.368593	1.359852	3.519951
1	-4.988641	0.631125	3.379661
1	-3.675805	-0.268314	4.193758

6	-6.865920	2.098620	-0.947336
6	-7.131161	1.607175	-2.376350
6	-7.272191	3.567923	-0.780257
1	-7.490772	1.497140	-0.264785
1	-6.863943	0.543657	-2.485072
1	-8.195860	1.726193	-2.638727
1	-6.536216	2.181228	-3.107204
1	-7.103554	3.909715	0.253634
1	-6.685208	4.218246	-1.451030
1	-8.338903	3.707684	-1.023050
6	-1.978591	3.040042	-1.681512
6	-2.152196	4.562556	-1.656661
6	-1.972017	2.504148	-3.120814
1	-0.977376	2.839969	-1.253938
1	-2.078764	4.949926	-0.626940
1	-1.376346	5.050375	-2.270063
1	-3.133327	4.857829	-2.065069
1	-1.789332	1.415762	-3.140971
1	-2.941323	2.692440	-3.613810
1	-1.189152	3.000645	-3.719877
6	0.639750	2.650871	1.193372
6	2.044346	2.447652	1.383873
6	0.307938	3.883860	1.831095
6	2.561550	3.529943	2.145563
1	2.619849	1.605454	0.993853
6	1.485780	4.421629	2.421199
1	-0.684041	4.334312	1.862807
1	3.603085	3.674038	2.428621
1	1.560377	5.366004	2.957775
26	1.777225	4.277785	0.322336
6	2.340690	6.210648	-0.347356
6	3.374725	5.283030	-0.654277
6	1.164464	5.803044	-1.036077
1	2.424734	7.063034	0.324702
6	2.839480	4.300511	-1.532674
1	4.388730	5.302855	-0.258676
6	1.473366	4.622479	-1.770239
1	0.196849	6.298092	-0.988108
1	3.373722	3.441465	-1.934931
1	0.788850	4.054538	-2.399107

6	-0.705068	-2.439512	-1.170110
6	-2.079578	-2.256582	-1.511864
6	-0.188829	-3.433094	-2.056910
6	-2.399479	-3.117512	-2.601432
1	-2.772528	-1.566709	-1.026906
6	-1.226196	-3.846414	-2.940225
1	0.831664	-3.819102	-2.047065
1	-3.375229	-3.218078	-3.073718
1	-1.143338	-4.608207	-3.713553
26	-1.774274	-4.292603	-0.941625
6	-1.946157	-4.946532	1.092488
6	-3.217798	-5.020779	0.458789
6	-1.051205	-5.798453	0.385841
1	-1.700177	-4.337186	1.960123
6	-3.110180	-5.918746	-0.638988
1	-4.111225	-4.475396	0.756053
6	-1.771511	-6.400082	-0.684447
1	0.004044	-5.949174	0.608893
1	-3.906131	-6.170358	-1.337593
1	-1.363273	-7.083637	-1.426805

TS4-Pb-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.278172	-2.121682	2.818627
82	0.435286	-1.719591	0.404224
82	-0.503129	1.021240	0.723069
6	-0.464809	0.776311	3.322084
6	0.543588	-0.063912	3.894960
6	0.580843	-1.458899	3.735981
1	-0.279387	-3.216646	2.836257
1	-1.263226	-1.698764	2.590733
6	1.557949	-2.322078	4.507779
1	2.569502	-1.891292	4.584237
1	1.203189	-2.493107	5.543400
1	1.650935	-3.315824	4.039052
6	1.626118	0.574391	4.739432
1	1.486560	1.661996	4.824071

1	1.615670	0.145240	5.758948
1	2.634035	0.384618	4.327994
1	-0.430792	1.824003	3.644797
1	-1.474295	0.357932	3.359061
6	2.422692	-1.280956	-0.643048
6	2.544386	-0.906024	-1.999377
6	3.570057	-1.615804	0.103248
6	3.816260	-0.962513	-2.592624
6	4.813890	-1.660913	-0.535107
6	4.954400	-1.361092	-1.892038
1	3.924630	-0.682919	-3.645778
1	5.697688	-1.952441	0.041141
6	-2.653559	1.625325	0.179286
6	-2.894192	2.480046	-0.920776
6	-3.753588	0.993550	0.800196
6	-4.214960	2.738899	-1.315644
6	-5.056449	1.288461	0.381116
6	-5.313014	2.170072	-0.667162
1	-4.391694	3.404127	-2.167434
1	-5.903354	0.817417	0.890499
6	1.404218	-0.355991	-2.857241
6	1.228889	-1.104959	-4.186306
6	1.626042	1.142926	-3.120501
1	0.461778	-0.456603	-2.297048
1	1.085763	-2.184478	-4.027219
1	0.343310	-0.722860	-4.722707
1	2.101107	-0.965505	-4.848400
1	1.666352	1.714698	-2.176214
1	2.574502	1.311800	-3.661188
1	0.811472	1.549983	-3.743470
6	6.305757	-1.463784	-2.576396
6	6.809240	-2.913730	-2.585435
6	7.335820	-0.523619	-1.938130
1	6.166755	-1.149727	-3.625262
1	6.088811	-3.580166	-3.086870
1	7.776597	-2.990364	-3.110018
1	6.951804	-3.286339	-1.556356
1	6.975731	0.517953	-1.940956
1	7.535104	-0.808647	-0.890834
1	8.292694	-0.562702	-2.485231

6	3.517948	-1.961122	1.589142
6	4.508369	-1.129018	2.411747
6	3.719524	-3.465922	1.806296
1	2.517378	-1.698469	1.975118
1	4.331990	-0.051401	2.260625
1	4.392638	-1.349066	3.486310
1	5.554335	-1.346186	2.140896
1	2.934363	-4.047202	1.291084
1	4.693083	-3.789315	1.400324
1	3.692104	-3.720773	2.878737
6	-3.597784	0.013727	1.954888
6	-4.359346	-1.303178	1.766001
6	-3.971464	0.680670	3.286124
1	-2.535795	-0.263917	1.997262
1	-4.070818	-1.797328	0.823172
1	-4.127219	-1.991708	2.598354
1	-5.451612	-1.152802	1.758837
1	-3.401767	1.611940	3.438700
1	-5.044603	0.938535	3.292349
1	-3.775047	0.009116	4.139916
6	-6.737029	2.482878	-1.090636
6	-7.019629	2.006003	-2.521108
6	-7.055684	3.974556	-0.927823
1	-7.405189	1.922657	-0.413775
1	-6.815532	0.928151	-2.625780
1	-8.073246	2.187614	-2.792717
1	-6.385578	2.541587	-3.248166
1	-6.873120	4.306488	0.106944
1	-6.425929	4.587823	-1.594695
1	-8.110713	4.178379	-1.177075
6	-1.787721	3.120401	-1.759490
6	-1.872465	4.652204	-1.739293
6	-1.822202	2.597713	-3.204830
1	-0.805570	2.848672	-1.331595
1	-1.745069	5.042531	-0.716317
1	-1.092310	5.094983	-2.381007
1	-2.848144	4.999818	-2.119303
1	-1.722946	1.499312	-3.238243
1	-2.771804	2.865308	-3.699766
1	-1.003995	3.040078	-3.799619

6	0.849053	2.734243	1.083457
6	2.241523	2.472506	1.272234
6	0.569177	3.981941	1.713332
6	2.809779	3.543532	2.017446
1	2.777968	1.601669	0.889204
6	1.772237	4.480384	2.290330
1	-0.406129	4.467806	1.747294
1	3.858295	3.649252	2.291249
1	1.887143	5.427175	2.815248
26	2.038738	4.297914	0.193507
6	2.666676	6.197367	-0.501393
6	3.663167	5.226617	-0.802896
6	1.471570	5.826557	-1.179055
1	2.785067	7.050748	0.164134
6	3.084772	4.255182	-1.667150
1	4.677823	5.208826	-0.409137
6	1.730395	4.626384	-1.900864
1	0.522452	6.356130	-1.129941
1	3.582735	3.370522	-2.060146
1	1.017772	4.076335	-2.514283
6	-0.885542	-2.367371	-1.270051
6	-2.244092	-2.078817	-1.592115
6	-0.440002	-3.379688	-2.171875
6	-2.628594	-2.903706	-2.690170
1	-2.882091	-1.349654	-1.089766
6	-1.511224	-3.707323	-3.050771
1	0.551422	-3.836098	-2.173295
1	-3.611528	-2.929374	-3.157325
1	-1.486085	-4.459989	-3.836799
26	-2.061591	-4.137225	-1.047435
6	-2.255465	-4.779139	0.989375
6	-3.531750	-4.791580	0.359987
6	-1.404615	-5.673250	0.279655
1	-1.980763	-4.188377	1.861424
6	-3.471156	-5.694001	-0.737722
1	-4.396240	-4.203891	0.661938
6	-2.156861	-6.239406	-0.788023
1	-0.357341	-5.876187	0.500085
1	-4.279637	-5.904964	-1.434939
1	-1.782512	-6.939475	-1.532604
