

Supplementary Materials

Theoretical Investigations of Phosphino Disilenes and its Derivatives with an E=E (E = C, Si, Ge, Sn, and Pb) Double Bond

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(All at the B3LYP/LANL2DZ level of theory)

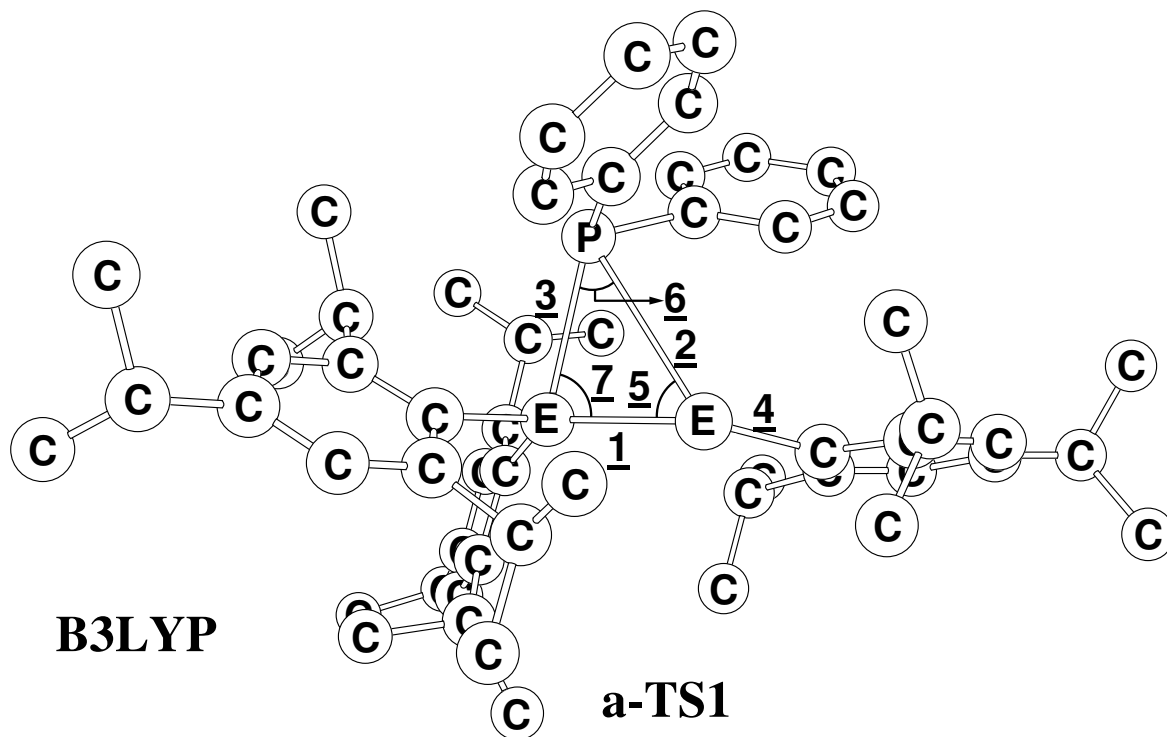
Figure Captions

Figure A: B3LYP/LANL2DZ optimized geometries (in Å and deg) of the transition states (**a-TS1**). Hydrogens are omitted for clarity.

Figure B: B3LYP/LANL2DZ optimized geometries (in Å and deg) of the intermediates (**a-Int-E-E**). Hydrogens are omitted for clarity.

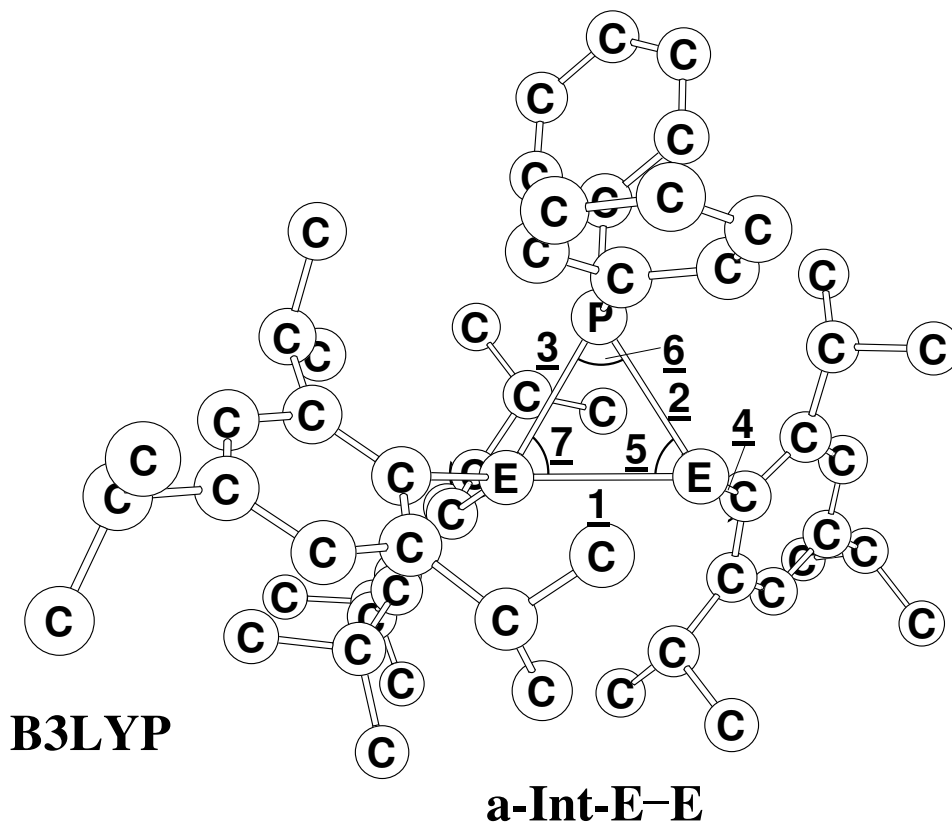
Figure C: B3LYP/LANL2DZ optimized geometries (in Å and deg) of the transition states (**a-TS2**). Hydrogens are omitted for clarity.

Figure D: B3LYP/LANL2DZ optimized geometries (in Å and deg) of the transition states (**a-Pro-E-E**). Hydrogens are omitted for clarity.

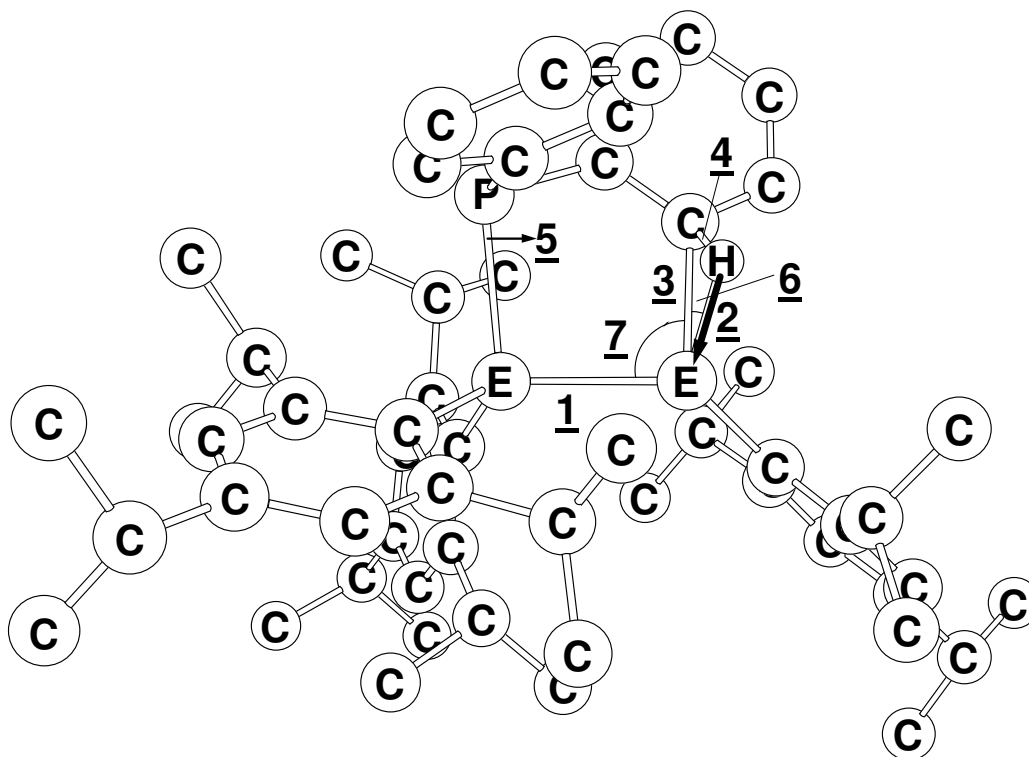


E	C	Si	Ge	Sn	Pb
<u>1</u>	1.425	2.333	2.526	2.767	2.889
<u>2</u>	2.847	2.742	3.358	3.414	3.712
<u>3</u>	2.624	2.994	2.728	2.911	2.936
<u>4</u>	1.937	1.952	2.027	2.174	2.247
<u>5</u>	66.39°	71.81°	52.99°	54.99°	50.97°
<u>6</u>	29.84°	47.74°	47.67°	51.14°	49.85°
<u>7</u>	83.77°	60.45°	79.34°	73.86°	79.18°

Fig. A



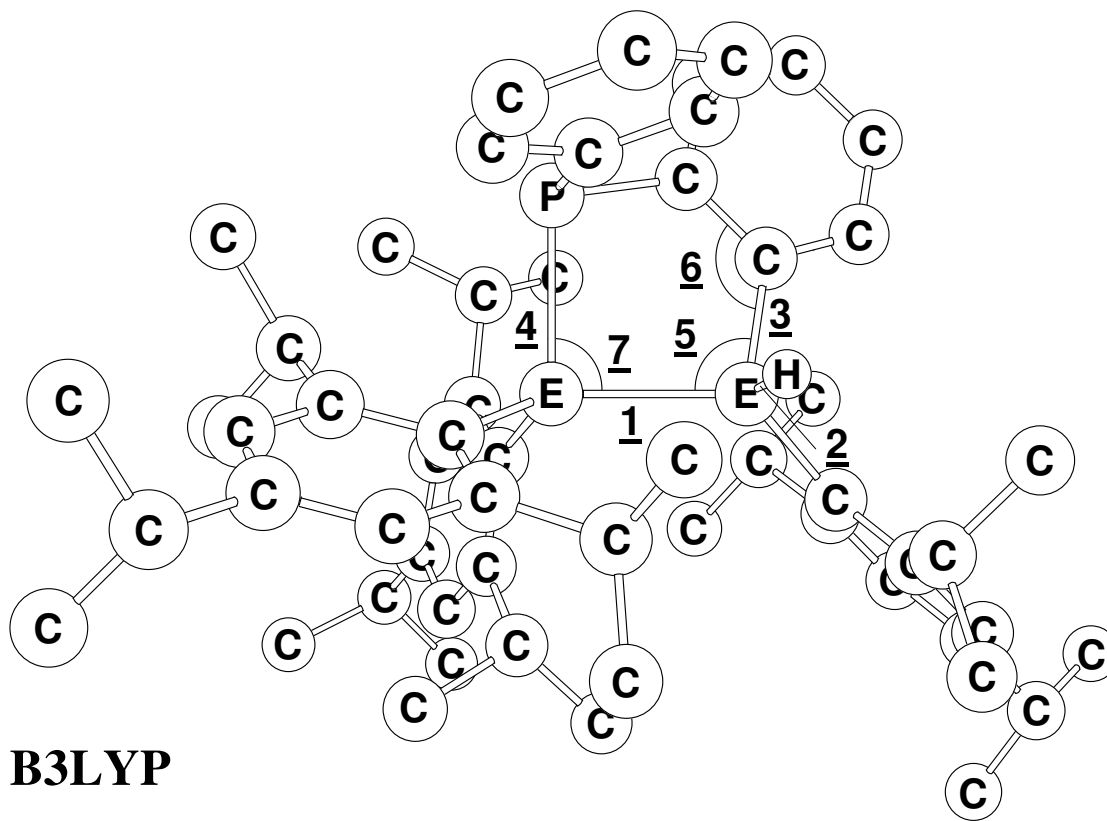
E	C	Si	Ge	Sn	Pb
<u>1</u>	1.416	2.552	2.708	2.758	3.180
<u>2</u>	2.040	2.540	2.654	2.654	2.896
<u>3</u>	2.713	2.498	2.641	2.911	2.928
<u>4</u>	1.518	1.956	2.050	2.174	2.280
<u>5</u>	101.9°	58.75°	58.37°	58.37°	57.39°
<u>6</u>	30.72°	60.86°	62.79°	62.79°	66.19°
<u>7</u>	47.38°	60.39°	58.84°	58.84°	56.42°



B3LYP

a-TS2

E	C	Si	Ge	Sn	Pb
<u>1</u>	1.555	2.382	2.498	2.764	2.805
<u>2</u>	1.328	1.628	1.650	1.781	1.797
<u>3</u>	2.394	2.399	2.343	2.416	2.473
<u>4</u>	1.285	1.275	1.360	1.466	1.638
<u>5</u>	2.111	2.429	2.493	2.653	2.685
<u>6</u>	23.21°	29.76°	34.64°	37.15°	41.42°
<u>7</u>	101.5°	91.31°	89.99°	87.27°	84.82°



B3LYP

a-Pro-E-E

E	C	Si	Ge	Sn	Pb
<u>1</u>	1.691	2.411	2.527	2.830	2.893
<u>2</u>	1.094	1.478	1.543	1.720	1.758
<u>3</u>	1.552	1.911	1.987	2.162	2.222
<u>4</u>	2.054	2.421	2.491	2.652	2.705
<u>5</u>	108.5°	98.87°	97.29°	93.56°	92.39°
<u>6</u>	116.4°	119.7°	120.4°	122.3°	123.2°
<u>7</u>	97.99°	89.85°	88.98°	86.31°	86.21°

Rea-C=C-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.620733	0.434945	0.076743
6	-0.477570	-0.413587	0.004454
6	0.536973	2.001581	0.058172
6	0.612930	4.929232	0.047587
6	-0.171522	2.790966	-0.930695
6	1.273467	2.764676	1.040081
6	1.299658	4.174718	1.000844
6	-0.114693	4.200755	-0.897833
1	1.876046	4.701979	1.755933
1	-0.664956	4.746301	-1.658554
6	-1.935671	-0.004148	0.015413
6	-4.743419	0.638143	0.231126
6	-2.484741	0.563084	1.218731
6	-2.836005	-0.259476	-1.083293
6	-4.198421	0.086406	-0.936165
6	-3.861546	0.858725	1.295953
1	-4.854855	-0.078331	-1.788509
1	-4.259669	1.272378	2.218779
6	2.072684	-0.142070	0.090705
6	4.830502	-1.034075	-0.088825
6	2.693485	-0.896005	1.167734
6	2.885674	0.126595	-1.062343
6	4.227059	-0.311061	-1.121569
6	4.033905	-1.310840	1.032238
1	4.814128	-0.079908	-2.007573
1	4.472460	-1.878415	1.848278
6	2.091323	2.172498	2.193052
1	1.839320	1.120275	2.275596
6	3.613911	2.303199	1.910755
1	3.891422	1.840046	0.959592
1	4.200166	1.825978	2.706902
1	3.900840	3.362814	1.870846
6	1.773522	2.829583	3.564998
1	0.697737	2.867552	3.758461
1	2.162850	3.853387	3.626568
1	2.248767	2.261207	4.375680
6	-1.029662	2.270044	-2.095225
1	-1.049505	1.187850	-2.054120
6	-2.490030	2.790527	-1.977873
1	-3.134099	2.285136	-2.708714
1	-2.539232	3.867182	-2.186846
1	-2.903095	2.619171	-0.980492
6	-0.485890	2.680537	-3.493122
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1	0.527308	2.313801	-3.675074
1	-0.471969	3.771291	-3.613248
6	0.656312	6.456097	0.051515
1	1.289065	6.765217	0.897225
6	1.301456	7.017801	-1.242084
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1	2.312157	6.615776	-1.386474
1	1.369769	8.113204	-1.194957
6	-0.750571	7.070209	0.275156
1	-1.430977	6.810516	-0.546913
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6	2.133310	-2.894019	2.690594
1	3.143006	-3.201923	2.993763
1	1.872776	-3.421048	1.771438
1	1.441320	-3.210596	3.482905

6	2.764519	-0.758626	3.774439
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1	2.771424	0.329581	3.810820
6	2.395270	0.898397	-2.296226
1	1.326527	1.071938	-2.188894
6	2.586917	0.109160	-3.618918
1	2.174347	0.683783	-4.459689
1	2.074156	-0.858820	-3.590183
1	3.646533	-0.073122	-3.838056
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1	4.185118	2.154134	-2.513056
1	2.923968	2.879172	-1.494494
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6	-1.163906	-0.953890	-3.109624
1	-1.061984	-1.849636	-3.732866
1	-0.366693	-0.988552	-2.370584
1	-0.984550	-0.088007	-3.755764
6	-3.253035	-2.311609	-2.532510
1	-3.166482	-2.731212	-3.544976
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1	-2.946304	2.419178	3.326969
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1	-6.889045	-1.010079	0.926191
1	-7.032132	-0.688562	-0.813793
1	-8.192230	0.036245	0.316385
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1	-6.494007	1.752031	-1.710575
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1	6.833397	-1.213813	1.923739
6	6.389152	-3.048566	-0.175744
1	5.794562	-3.492379	-0.984163
1	6.025643	-3.464354	0.773337
1	7.433845	-3.363682	-0.302440
15	-0.122921	-2.314246	0.324712
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6	0.919752	-5.009059	-3.420637
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6	1.385077	-3.115474	-1.950334
6	1.746950	-3.936218	-3.032633
6	-0.265512	-5.255447	-2.703629
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1	2.054790	-2.319418	-1.641672
1	2.679111	-3.745740	-3.560334
1	-0.907893	-6.089280	-2.979508
1	1.201086	-5.647033	-4.255414
6	-1.620652	-3.207420	1.088731
6	-3.515744	-4.822989	2.484439
6	-3.000717	-2.908704	1.045791

6	-1.214118	-4.339621	1.845409
6	-2.144543	-5.144044	2.525452
6	-3.933779	-3.704253	1.742429
1	-3.369297	-2.065606	0.479964
1	-0.158287	-4.592650	1.904325
1	-1.797343	-6.005508	3.091741
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1	-4.240128	-5.431019	3.022348

Rea-Si=Si-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-1.031984	0.184567	-0.179638
14	1.038782	-0.448843	0.238617
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6	-2.879781	4.632211	-0.105876
6	-1.296949	2.987974	0.839878
6	-2.659373	2.392433	-1.111351
6	-3.236644	3.678675	-1.070023
6	-1.900058	4.262923	0.829570
1	-3.981470	3.945306	-1.817208
1	-1.590207	4.987391	1.578708
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6	4.694669	2.605378	-0.341396
6	2.824524	1.286380	-1.256516
6	3.441349	1.041151	1.119178
6	4.472003	1.981253	0.899061
6	3.864541	2.230928	-1.404990
1	5.121236	2.230780	1.736497
1	4.033081	2.678434	-2.382399
6	-2.456772	-1.103896	-0.016025
6	-4.772895	-2.791592	0.234848
6	-2.789877	-2.053311	-1.041848
6	-3.285949	-1.053902	1.150859
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6	-3.936446	-2.860581	-0.892458
1	-5.041424	-1.834275	2.140215
1	-4.178130	-3.567737	-1.682444
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1	-2.525095	0.553877	-2.208275
6	-4.611745	1.068068	-2.072875
1	-4.773228	0.555665	-1.117797
1	-4.928202	0.393000	-2.878779
1	-5.261408	1.952801	-2.101491
6	-2.880356	2.101027	-3.641592
1	-1.830065	2.389043	-3.768903
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1	-3.139931	1.385266	-4.433531
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1	1.793648	3.480764	2.392251
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6	-4.381705	6.217948	1.200762
1	-3.749626	6.186916	2.098153
1	-5.144943	5.435941	1.301051
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1	-1.919067	7.032837	-1.170532
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1	-1.073282	-1.637731	-2.278306
6	-1.487289	-3.749892	-2.435586
1	-2.337149	-4.430618	-2.576560
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6	-2.750082	-1.918263	-3.616555
1	-3.634710	-2.559047	-3.726969
1	-2.111993	-2.077391	-4.496552
1	-3.088365	-0.879192	-3.627356
6	-2.990308	-0.136929	2.345708
1	-2.071515	0.423210	2.132214
6	-2.713833	-0.955478	3.634008
1	-2.435486	-0.286242	4.459511
1	-1.894636	-1.669221	3.478754
1	-3.598611	-1.524391	3.946856
6	-4.121185	0.897864	2.576169
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1	-4.256073	1.534979	1.694193
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1	1.421909	-0.321211	2.882084
1	1.698114	1.339320	3.441491
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1	4.367056	-1.293278	3.561123
1	5.153794	-0.899288	2.016869
1	3.575130	-1.722988	2.044979
6	2.041301	0.933726	-2.530166
1	1.350982	0.115169	-2.295137
6	1.183727	2.127772	-3.022374
1	0.456921	2.437577	-2.262078
1	0.633180	1.851070	-3.932149
1	1.813261	2.995292	-3.261802
6	2.971121	0.424511	-3.662688
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1	3.653462	1.209535	-4.014159
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6	5.804244	3.638981	-0.532719
1	5.776909	3.960928	-1.584498
6	7.207777	3.034287	-0.267804
1	7.392914	2.166876	-0.913990
1	7.306826	2.704656	0.774846
1	7.991242	3.779842	-0.459710
6	5.572739	4.897003	0.344989
1	5.601423	4.644894	1.413336
1	4.596787	5.351979	0.133916
1	6.351720	5.647942	0.155538
6	-6.014068	-3.674237	0.368246
1	-6.495702	-3.424610	1.325611
6	-7.043250	-3.393020	-0.757346
1	-7.334931	-2.335215	-0.771943
1	-7.948412	-3.998174	-0.612339
1	-6.628456	-3.641047	-1.743370
6	-5.644939	-5.180220	0.412615
1	-4.939364	-5.390900	1.225985
1	-5.177335	-5.500645	-0.527711
1	-6.543131	-5.793362	0.567503
15	1.232093	-2.754395	-0.173929
6	1.800151	-3.551179	1.449100
6	2.386060	-4.944905	3.853772
6	2.860727	-4.482861	1.500601
6	1.029136	-3.337024	2.615645
6	1.321150	-4.022585	3.807586

6	3.150961	-5.172526	2.694676
1	3.461452	-4.674436	0.616011
1	0.196275	-2.636480	2.591319
1	0.717309	-3.841321	4.694234
1	3.972553	-5.885516	2.714886
1	2.611447	-5.478073	4.774545
6	2.744667	-2.939239	-1.304878
6	4.885400	-3.354023	-3.123467
6	4.037549	-2.444289	-1.020722
6	2.539621	-3.638206	-2.517278
6	3.600511	-3.845407	-3.421042
6	5.099411	-2.652251	-1.920698
1	4.220422	-1.895948	-0.103646
1	1.551967	-4.027762	-2.748776
1	3.423394	-4.389677	-4.345945
1	6.087158	-2.262958	-1.684767
1	5.707313	-3.513782	-3.817784

Rea-Ge=Ge-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.062454	0.202125	0.376343
32	-1.138801	-0.394673	-0.479541
6	1.951149	2.015144	0.223538
6	3.380048	4.512326	0.147683
6	1.607884	3.029988	-0.726493
6	2.987168	2.304563	1.167348
6	3.682379	3.530304	1.103074
6	2.329847	4.242155	-0.746171
1	4.474294	3.727486	1.823292
1	2.057681	4.996562	-1.480767
6	-2.695893	0.853080	-0.168248
6	-4.809957	2.772089	0.186408
6	-2.957226	1.432282	1.113211
6	-3.550292	1.214965	-1.270446
6	-4.578655	2.158361	-1.059418
6	-3.991692	2.386177	1.255487
1	-5.215961	2.419061	-1.902750
1	-4.167424	2.831163	2.232995
6	2.468627	-1.212257	0.063945
6	4.650916	-3.040641	-0.298282
6	2.750078	-2.218741	1.046125
6	3.265978	-1.174549	-1.121526
6	4.336467	-2.082333	-1.274673
6	3.836799	-3.095672	0.846836
1	4.938571	-2.042987	-2.180786
1	4.045991	-3.845813	1.605983
6	3.371798	1.346948	2.300848
1	2.725496	0.461186	2.240271
6	4.834420	0.851252	2.174086
1	4.991630	0.333894	1.220694
1	5.079257	0.152730	2.985020
1	5.540862	1.689689	2.229711
6	3.112412	1.983266	3.692295
1	2.069748	2.311853	3.787890
1	3.756211	2.856528	3.856561
1	3.321401	1.259413	4.491740
6	0.456678	2.904964	-1.731487
1	0.046411	1.889715	-1.671015
6	-0.687232	3.890470	-1.369352
1	-1.528365	3.784482	-2.065370
1	-0.336427	4.929973	-1.415235
1	-1.065826	3.704554	-0.357456
6	0.920569	3.120048	-3.196258
1	0.089212	2.941976	-3.889630

1	1.737756	2.438302	-3.460848
1	1.273876	4.145976	-3.360727
6	4.160449	5.825983	0.099977
1	4.906805	5.795083	0.907907
6	4.930499	5.984618	-1.237308
1	4.238261	6.036850	-2.088027
1	5.607026	5.137465	-1.406863
1	5.527109	6.906929	-1.232042
6	3.247559	7.052617	0.358513
1	2.487012	7.154411	-0.426966
1	3.839878	7.977551	0.372997
1	2.726639	6.962460	1.320067
6	1.923945	-2.421812	2.329600
1	1.054464	-1.749352	2.293226
6	1.377989	-3.871718	2.431960
1	2.193606	-4.593918	2.569279
1	0.811526	-4.144504	1.537722
1	0.707098	-3.960224	3.297824
6	2.729541	-2.098167	3.617732
1	3.596262	-2.765487	3.713112
1	2.096748	-2.243647	4.503840
1	3.099428	-1.069011	3.630218
6	2.995996	-0.204566	-2.279848
1	2.134666	0.421407	-2.015392
6	2.603893	-0.965245	-3.573897
1	2.364284	-0.255028	-4.377017
1	1.724593	-1.600347	-3.406204
1	3.422314	-1.606634	-3.925358
6	4.193110	0.746678	-2.534202
1	3.967163	1.437806	-3.357217
1	5.096252	0.185627	-2.807831
1	4.417568	1.341974	-1.641395
6	-3.496346	0.640396	-2.705372
1	-4.324795	1.129390	-3.237854
6	-2.221514	0.999212	-3.508872
1	-2.336605	0.669340	-4.550620
1	-1.326882	0.510348	-3.104761
1	-2.052593	2.081881	-3.510033
6	-3.789349	-0.878677	-2.780203
1	-3.862545	-1.194780	-3.829558
1	-4.740192	-1.123088	-2.289327
1	-3.000828	-1.483219	-2.319922
6	-2.173069	1.077635	2.384810
1	-1.506649	0.237071	2.156962
6	-1.277980	2.257446	2.846469
1	-0.556796	2.541685	2.070663
1	-0.716558	1.981352	3.749948
1	-1.884244	3.141880	3.083687
6	-3.100005	0.614865	3.538779
1	-3.742784	-0.214623	3.224750
1	-3.744184	1.429319	3.895097
1	-2.495181	0.275550	4.390732
6	-5.919097	3.806773	0.376825
1	-5.896139	4.124412	1.430055
6	-7.321888	3.203845	0.103776
1	-7.509789	2.334432	0.746475
1	-7.415950	2.877205	-0.940321
1	-8.106119	3.949009	0.294319
6	-5.683428	5.068249	-0.494584
1	-5.708917	4.820983	-1.564175
1	-4.707645	5.521114	-0.278096
1	-6.462120	5.819406	-0.304694
6	5.826183	-3.999296	-0.492619
1	6.306196	-3.744014	-1.449306
6	6.892992	-3.835672	0.621066
1	7.259605	-2.802506	0.669600
1	7.749677	-4.497229	0.434105
1	6.479661	-4.092488	1.605445
6	5.354329	-5.473976	-0.588502

1	4.624101	-5.604347	-1.396944
1	4.880082	-5.799257	0.346829
1	6.206702	-6.139263	-0.782282
15	-1.497011	-2.680400	0.416846
6	-1.873589	-3.660333	-1.161853
6	-2.209139	-5.274353	-3.477546
6	-3.027265	-4.459758	-1.322024
6	-0.883850	-3.690924	-2.174798
6	-1.051370	-4.485294	-3.322465
6	-3.192323	-5.259086	-2.470868
1	-3.796431	-4.465915	-0.555319
1	0.021802	-3.096483	-2.065226
1	-0.279073	-4.492030	-4.088718
1	-4.087936	-5.868302	-2.574459
1	-2.338515	-5.891970	-4.363394
6	-3.148522	-2.691560	1.342537
6	-5.523449	-2.840805	2.892523
6	-4.362880	-2.158229	0.854624
6	-3.141523	-3.293255	2.623166
6	-4.318873	-3.370063	3.393127
6	-5.540672	-2.233025	1.621559
1	-4.391426	-1.680106	-0.118160
1	-2.214884	-3.708769	3.012161
1	-4.293812	-3.841434	4.373041
1	-6.464425	-1.813558	1.229680
1	-6.434414	-2.898738	3.484119

Rea-Sn=Sn-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	1.289020	0.279568	0.616483
50	-1.299109	-0.251982	-0.560414
6	2.545575	2.059125	0.273824
6	4.238767	4.360430	-0.019943
6	2.224175	3.090640	-0.661918
6	3.709284	2.222188	1.084936
6	4.533016	3.357005	0.917490
6	3.073292	4.209573	-0.793512
1	5.423114	3.464164	1.535649
1	2.816104	4.980957	-1.516579
6	-2.936604	1.176342	-0.178554
6	-4.980499	3.150479	0.270700
6	-3.191164	1.686980	1.130106
6	-3.749767	1.651285	-1.264223
6	-4.748261	2.616679	-1.012092
6	-4.192063	2.667639	1.324127
1	-5.356922	2.959526	-1.847641
1	-4.365843	3.057313	2.325675
6	2.564193	-1.456811	0.186406
6	4.187455	-3.752909	-0.368250
6	2.775937	-2.459246	1.184322
6	3.169595	-1.627392	-1.093523
6	3.968862	-2.765619	-1.343925
6	3.579160	-3.580636	0.889492
1	4.429044	-2.889389	-2.323229
1	3.730929	-4.336128	1.658029
6	4.113441	1.211728	2.166987
1	3.361323	0.407952	2.196572
6	5.471081	0.536640	1.845745
1	5.427524	0.008156	0.886377
1	5.738472	-0.190414	2.623974
1	6.276154	1.280764	1.791094
6	4.125426	1.852032	3.579844
1	3.155134	2.306461	3.817522

1	4.889184	2.636438	3.653917
1	4.348435	1.094624	4.343493
6	0.965436	3.056075	-1.536838
1	0.457444	2.094249	-1.375689
6	-0.033918	4.170457	-1.127978
1	-0.958169	4.098613	-1.715112
1	0.398589	5.165915	-1.293860
1	-0.300895	4.092797	-0.066882
6	1.293921	3.135596	-3.050485
1	0.378582	3.033354	-3.647058
1	1.989005	2.340207	-3.347416
1	1.755222	4.097208	-3.309844
6	5.157377	5.572151	-0.182997
1	5.976272	5.465393	0.544124
6	5.794142	5.618735	-1.596927
1	5.025363	5.736240	-2.372166
1	6.348218	4.696211	-1.811424
1	6.488552	6.465747	-1.680373
6	4.424600	6.901741	0.133566
1	3.600784	7.077131	-0.570771
1	5.117089	7.751047	0.057679
1	4.003300	6.890244	1.146668
6	2.166798	-2.371728	2.593314
1	1.568546	-1.445654	2.653453
6	1.195970	-3.546061	2.882982
1	1.725760	-4.507876	2.862542
1	0.386202	-3.582014	2.146507
1	0.748023	-3.432396	3.880199
6	3.252725	-2.288644	3.698184
1	3.851807	-3.207968	3.728813
1	2.785200	-2.161733	4.683994
1	3.938581	-1.450668	3.530657
6	2.980968	-0.620141	-2.236422
1	2.336160	0.194925	-1.876120
6	2.260246	-1.256175	-3.452856
1	2.111159	-0.510246	-4.245462
1	1.276524	-1.650565	-3.167270
1	2.847134	-2.082188	-3.874678
6	4.322024	0.032924	-2.659550
1	4.158112	0.767970	-3.459125
1	5.028874	-0.718857	-3.034184
1	4.790492	0.549577	-1.813326
6	-3.645541	1.187080	-2.733326
1	-4.472591	1.688421	-3.256371
6	-2.351986	1.662696	-3.444973
1	-2.402411	1.427858	-4.517182
1	-1.454944	1.172367	-3.044700
1	-2.224430	2.746780	-3.335092
6	-3.882356	-0.330244	-2.940278
1	-3.918042	-0.563944	-4.012870
1	-4.832634	-0.646170	-2.492267
1	-3.086582	-0.955834	-2.511674
6	-2.414829	1.228224	2.371510
1	-1.780722	0.375653	2.086312
6	-1.472487	2.342462	2.896200
1	-0.762891	2.664357	2.123526
1	-0.896444	1.984141	3.760323
1	-2.046413	3.223130	3.213381
6	-3.345282	0.724442	3.504949
1	-4.008199	-0.071740	3.149974
1	-3.968900	1.534587	3.904971
1	-2.745486	0.327338	4.335114
6	-6.061162	4.203311	0.517793
1	-6.022126	4.470884	1.584382
6	-7.479678	3.644361	0.230809
1	-7.681225	2.750628	0.834883
1	-7.588549	3.367694	-0.826311
1	-8.245853	4.396804	0.462168
6	-5.805358	5.498117	-0.296300

1	-5.851670	5.303127	-1.375905
1	-4.815805	5.916224	-0.072650
1	-6.562432	6.258154	-0.060139
6	5.054154	-4.975523	-0.674834
1	5.412930	-4.874867	-1.710249
6	6.301572	-5.043242	0.244108
1	6.904720	-4.130321	0.160634
1	6.933422	-5.900186	-0.026196
1	6.011513	-5.159321	1.296743
6	4.238185	-6.292168	-0.591606
1	3.374000	-6.266070	-1.267189
1	3.861582	-6.460547	0.425966
1	4.864372	-7.152357	-0.864948
15	-1.933627	-2.631263	0.509724
6	-2.229240	-3.607145	-1.091929
6	-2.472912	-5.190393	-3.443858
6	-3.464078	-4.200857	-1.438596
6	-1.114071	-3.829353	-1.939099
6	-1.235432	-4.607327	-3.104015
6	-3.582576	-4.986192	-2.602767
1	-4.331936	-4.063346	-0.800510
1	-0.143198	-3.408896	-1.680940
1	-0.365114	-4.763296	-3.737978
1	-4.542120	-5.437447	-2.847419
1	-2.566990	-5.796616	-4.341925
6	-3.661631	-2.526309	1.279712
6	-6.174291	-2.485279	2.607599
6	-4.769176	-1.856413	0.711544
6	-3.834065	-3.171997	2.527530
6	-5.079113	-3.153997	3.187018
6	-6.014349	-1.835814	1.367733
1	-4.662121	-1.340492	-0.237025
1	-2.993159	-3.694097	2.977964
1	-5.190515	-3.659863	4.143536
1	-6.851234	-1.308842	0.915102
1	-7.136429	-2.468465	3.114800

Rea-Pb=Pb-Singlet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	1.321419	0.271592	0.649490
82	-1.366152	-0.274999	-0.631591
6	2.665530	2.049078	0.247663
6	4.388078	4.309122	-0.090605
6	2.341121	3.074350	-0.690134
6	3.841724	2.189890	1.038329
6	4.684143	3.308019	0.849822
6	3.206817	4.177255	-0.844980
1	5.587339	3.404228	1.450822
1	2.952581	4.948928	-1.569088
6	-2.984513	1.244195	-0.165295
6	-4.935225	3.292227	0.321885
6	-3.179985	1.768129	1.145542
6	-3.792635	1.752085	-1.235269
6	-4.748746	2.754617	-0.967345
6	-4.140393	2.785259	1.360073
1	-5.359137	3.122743	-1.790961
1	-4.277574	3.185196	2.363634
6	2.600059	-1.526578	0.169950
6	4.133676	-3.868268	-0.413076
6	2.791067	-2.534338	1.163359
6	3.168062	-1.713784	-1.121987
6	3.926805	-2.876624	-1.387549
6	3.552373	-3.681105	0.855901
1	4.363369	-3.016982	-2.375626

1	3.692706	-4.443196	1.620289
6	4.232445	1.169503	2.115906
1	3.461224	0.383060	2.148879
6	5.565891	0.456217	1.779087
1	5.491818	-0.073477	0.822151
1	5.822802	-0.276786	2.555395
1	6.390634	1.177038	1.710098
6	4.271986	1.805419	3.529709
1	3.314183	2.281491	3.776874
1	5.053247	2.572772	3.597795
1	4.484423	1.041571	4.290074
6	1.062015	3.044462	-1.538207
1	0.543748	2.091678	-1.349492
6	0.083986	4.177039	-1.127422
1	-0.851394	4.109778	-1.697827
1	0.526697	5.164227	-1.314131
1	-0.166032	4.117326	-0.061016
6	1.356009	3.095655	-3.060228
1	0.425077	3.002968	-3.634578
1	2.030108	2.284243	-3.362050
1	1.828121	4.045359	-3.342942
6	5.323857	5.502814	-0.280206
1	6.154141	5.387880	0.432494
6	5.933591	5.524724	-1.706350
1	5.151693	5.649195	-2.467286
1	6.464514	4.588919	-1.922206
1	6.642626	6.356830	-1.812262
6	4.617634	6.845724	0.039477
1	3.784073	7.028390	-0.651452
1	5.320840	7.684280	-0.053670
1	4.213378	6.846090	1.059638
6	2.197173	-2.422784	2.577580
1	1.622388	-1.481264	2.639492
6	1.196512	-3.567563	2.884359
1	1.699268	-4.543568	2.865441
1	0.378937	-3.586857	2.155652
1	0.760396	-3.435347	3.884564
6	3.294372	-2.355771	3.671695
1	3.873778	-3.287430	3.701103
1	2.840101	-2.212605	4.661565
1	3.995868	-1.533385	3.490165
6	2.973932	-0.700767	-2.259304
1	2.360932	0.130575	-1.879897
6	2.206237	-1.317741	-3.457251
1	2.048940	-0.566476	-4.243516
1	1.223935	-1.696912	-3.145815
1	2.765015	-2.153219	-3.898188
6	4.317527	-0.078531	-2.718468
1	4.150248	0.658042	-3.516127
1	4.997974	-0.847088	-3.107449
1	4.816944	0.430052	-1.885218
6	-3.710493	1.284583	-2.703900
1	-4.531261	1.799668	-3.223325
6	-2.411835	1.736199	-3.424486
1	-2.471019	1.502037	-4.496331
1	-1.517658	1.232958	-3.032198
1	-2.262004	2.817208	-3.314827
6	-3.974967	-0.228819	-2.908223
1	-4.033500	-0.462726	-3.979609
1	-4.919288	-0.531789	-2.440119
1	-3.183206	-0.873343	-2.497694
6	-2.378601	1.288997	2.364476
1	-1.772844	0.422235	2.059351
6	-1.398553	2.381304	2.869184
1	-0.702672	2.695289	2.080656
1	-0.808767	2.008022	3.718142
1	-1.945559	3.271746	3.205880
6	-3.288165	0.804750	3.523396
1	-3.974632	0.020243	3.188085

1	-3.886106	1.628612	3.934769
1	-2.675937	0.399564	4.340699
6	-5.978464	4.376509	0.590041
1	-5.910710	4.643621	1.655308
6	-7.416235	3.854367	0.331426
1	-7.627838	2.966954	0.941473
1	-7.550834	3.577052	-0.722600
1	-8.159333	4.625844	0.574474
6	-5.700998	5.661849	-0.231389
1	-5.770223	5.465356	-1.309530
1	-4.696086	6.051672	-0.025353
1	-6.432071	6.443710	0.014807
6	4.961471	-5.114040	-0.731154
1	5.305453	-5.025836	-1.772685
6	6.221348	-5.209102	0.168098
1	6.843674	-4.310378	0.071821
1	6.828929	-6.081464	-0.108071
1	5.944542	-5.313738	1.225505
6	4.112227	-6.407930	-0.629584
1	3.238841	-6.360640	-1.292131
1	3.746262	-6.561396	0.394210
1	4.710309	-7.286165	-0.908193
15	-2.029775	-2.645075	0.571719
6	-2.351803	-3.608172	-1.029168
6	-2.643589	-5.152439	-3.403352
6	-3.603184	-4.163628	-1.382004
6	-1.244920	-3.848467	-1.884245
6	-1.390298	-4.606264	-3.059907
6	-3.745137	-4.930388	-2.555348
1	-4.464835	-4.009780	-0.739023
1	-0.260933	-3.460939	-1.622641
1	-0.526115	-4.776239	-3.698834
1	-4.716620	-5.354277	-2.801929
1	-2.756025	-5.745004	-4.308387
6	-3.743745	-2.492851	1.358026
6	-6.228240	-2.338053	2.729345
6	-4.835711	-1.789603	0.799851
6	-3.917159	-3.112546	2.618702
6	-5.147970	-3.037887	3.300042
6	-6.067152	-1.713090	1.476928
1	-4.723980	-1.285649	-0.154882
1	-3.086565	-3.656976	3.061937
1	-5.259726	-3.524121	4.266621
1	-6.891048	-1.159767	1.032038
1	-7.179521	-2.277624	3.253285

Rea-C=C-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.671721	0.485844	0.112153
6	-0.544036	-0.460949	-0.022325
6	0.577502	2.000008	0.059858
6	0.648686	4.939284	0.029592
6	-0.176691	2.795438	-0.907468
6	1.348023	2.785929	1.015993
6	1.374730	4.191907	0.962426
6	-0.118661	4.201890	-0.882063
1	1.969987	4.726385	1.698622
1	-0.688758	4.744387	-1.631108
6	-1.969693	-0.024138	0.020948
6	-4.768422	0.666225	0.236736
6	-2.502884	0.607621	1.204582
6	-2.885882	-0.287443	-1.071975
6	-4.241218	0.074879	-0.921940
6	-3.872089	0.924670	1.284442

1	-4.907496	-0.100796	-1.765001
1	-4.260025	1.366829	2.198646
6	2.073358	-0.125241	0.113447
6	4.820699	-1.072664	-0.082167
6	2.680169	-0.929923	1.165692
6	2.902030	0.141368	-1.043514
6	4.231214	-0.321662	-1.106686
6	4.013848	-1.367016	1.027441
1	4.824104	-0.092287	-1.989653
1	4.443979	-1.952177	1.835920
6	2.155159	2.194685	2.176378
1	1.889959	1.145518	2.256530
6	3.681077	2.304585	1.911512
1	3.962914	1.821174	0.971490
1	4.252543	1.835461	2.723539
1	3.980809	3.359959	1.855279
6	1.825469	2.856274	3.543302
1	0.748186	2.881759	3.730558
1	2.200930	3.885098	3.601121
1	2.302618	2.296890	4.359567
6	-1.037292	2.262538	-2.066232
1	-1.056850	1.180215	-2.013879
6	-2.497061	2.784293	-1.963850
1	-3.135849	2.274989	-2.696819
1	-2.544855	3.859724	-2.179442
1	-2.917123	2.619191	-0.968495
6	-0.488103	2.657854	-3.468103
1	-1.145418	2.252879	-4.250504
1	0.521438	2.280844	-3.647799
1	-0.463789	3.747727	-3.594152
6	0.692394	6.465041	0.018851
1	1.332651	6.781270	0.856347
6	1.329246	7.012829	-1.285432
1	0.728379	6.739319	-2.162914
1	2.339002	6.608718	-1.430820
1	1.397656	8.108821	-1.251764
6	-0.711564	7.083922	0.247343
1	-1.399184	6.816356	-0.565983
1	-0.649130	8.180016	0.287591
1	-1.151418	6.729086	1.188026
6	2.035560	-1.356175	2.510776
1	0.992033	-1.026528	2.529220
6	2.067143	-2.903877	2.687827
1	3.075873	-3.242193	2.960061
1	1.773636	-3.424087	1.772945
1	1.390482	-3.203425	3.498976
6	2.752218	-0.776067	3.767293
1	3.795733	-1.112870	3.813330
1	2.247860	-1.143601	4.671743
1	2.753946	0.311828	3.805480
6	2.414771	0.909816	-2.280388
1	1.348926	1.090391	-2.163954
6	2.591937	0.106788	-3.597552
1	2.182805	0.679695	-4.441229
1	2.065666	-0.853912	-3.559639
1	3.647987	-0.091687	-3.820534
6	3.126378	2.284365	-2.394275
1	2.756722	2.841313	-3.265435
1	4.210345	2.155117	-2.515807
1	2.952652	2.894338	-1.501465
6	-2.631651	-0.932674	-2.471387
1	-3.241554	-0.321286	-3.154283
6	-1.210190	-0.961783	-3.101437
1	-1.092058	-1.861071	-3.717473
1	-0.416756	-0.970042	-2.355513
1	-1.047848	-0.097472	-3.753982
6	-3.277209	-2.350297	-2.519729
1	-3.223808	-2.748637	-3.541763
1	-4.332082	-2.319467	-2.219455

1	-2.760040	-3.049939	-1.859799
6	-1.669100	0.845387	2.472050
1	-0.611154	0.730433	2.218832
6	-1.865913	2.272275	3.043798
1	-1.558983	3.036220	2.320079
1	-1.269093	2.398127	3.955710
1	-2.910760	2.461443	3.319598
6	-2.004016	-0.212298	3.561733
1	-1.830912	-1.232569	3.202160
1	-3.056428	-0.140680	3.868730
1	-1.381511	-0.049439	4.452717
6	-6.245817	1.034375	0.349628
1	-6.406952	1.447276	1.356615
6	-7.165043	-0.205381	0.200523
1	-6.918379	-0.971264	0.947281
1	-7.060787	-0.658597	-0.794210
1	-8.218442	0.076116	0.331902
6	-6.636156	2.134607	-0.672744
1	-6.510760	1.777218	-1.703513
1	-6.010766	3.027625	-0.549404
1	-7.686671	2.427966	-0.543353
6	6.270940	-1.542183	-0.179697
1	6.665211	-1.193585	-1.146141
6	7.152720	-0.916567	0.932937
1	7.107209	0.179365	0.903968
1	8.200970	-1.221576	0.811115
1	6.822090	-1.240374	1.928772
6	6.379791	-3.088995	-0.163562
1	5.785778	-3.535989	-0.970719
1	6.016814	-3.501807	0.786941
1	7.424782	-3.403346	-0.289078
15	-0.217568	-2.256451	0.261633
6	0.213665	-3.370219	-1.221934
6	0.964059	-5.048137	-3.381107
6	-0.589424	-4.473722	-1.587385
6	1.417874	-3.140829	-1.923377
6	1.783690	-3.966990	-3.001572
6	-0.218715	-5.303040	-2.661736
1	-1.501192	-4.693222	-1.040892
1	2.072308	-2.326650	-1.628383
1	2.709310	-3.769577	-3.537392
1	-0.857926	-6.139412	-2.936269
1	1.246316	-5.685506	-4.215833
6	-1.652450	-3.199936	1.064857
6	-3.521803	-4.810789	2.495210
6	-3.032693	-2.899968	1.046354
6	-1.230190	-4.329462	1.815743
6	-2.149873	-5.128147	2.517427
6	-3.953429	-3.695582	1.756267
1	-3.408631	-2.059379	0.482829
1	-0.175822	-4.588079	1.856558
1	-1.794133	-5.986193	3.083217
1	-5.009361	-3.436819	1.723435
1	-4.237176	-5.420033	3.043030

Rea-Si=Si-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-1.089589	0.193111	-0.311315
14	1.126470	-0.463348	0.390109
6	-1.759256	1.991424	-0.168784
6	-2.990096	4.600317	-0.090224
6	-1.368177	2.968719	0.810069
6	-2.760575	2.377231	-1.124149
6	-3.355546	3.652195	-1.056833

6	-1.986431	4.236232	0.823241
1	-4.119571	3.914706	-1.786034
1	-1.677031	4.957142	1.576406
6	2.581582	0.743187	0.067154
6	4.643196	2.707033	-0.354853
6	2.786758	1.337888	-1.221106
6	3.469829	1.116047	1.138088
6	4.465435	2.085802	0.894600
6	3.796883	2.309527	-1.398591
1	5.123400	2.359304	1.717361
1	3.931541	2.759740	-2.380324
6	-2.447778	-1.146353	-0.025832
6	-4.714945	-2.895219	0.269206
6	-2.767270	-2.119048	-1.033684
6	-3.255167	-1.118196	1.157864
6	-4.367685	-1.980301	1.274661
6	-3.888516	-2.955717	-0.866255
1	-4.979057	-1.937550	2.174503
1	-4.121559	-3.674164	-1.648697
6	-3.226647	1.454836	-2.254384
1	-2.603736	0.553572	-2.223156
6	-4.699029	1.013310	-2.060743
1	-4.828172	0.494096	-1.103953
1	-5.007474	0.328764	-2.862016
1	-5.375681	1.877881	-2.076500
6	-3.004869	2.090116	-3.650827
1	-1.957884	2.389951	-3.782906
1	-3.631946	2.978444	-3.797085
1	-3.257911	1.370286	-4.441378
6	-0.281529	2.739856	1.869998
1	0.067968	1.703055	1.798332
6	0.937395	3.667478	1.615312
1	1.725826	3.488579	2.357241
1	0.643921	4.723236	1.685204
1	1.366846	3.498105	0.621928
6	-0.809565	2.945461	3.316263
1	-0.023060	2.716106	4.047767
1	-1.670951	2.302358	3.528167
1	-1.118934	3.985015	3.484276
6	-3.667113	5.968979	-0.043834
1	-4.364876	6.019184	-0.893130
6	-4.501078	6.145757	1.252499
1	-3.858017	6.117685	2.142194
1	-5.247354	5.347495	1.352967
1	-5.026302	7.110479	1.245789
6	-2.649107	7.126272	-0.208669
1	-1.934116	7.146978	0.624283
1	-3.166432	8.094865	-0.230849
1	-2.077530	7.019203	-1.139241
6	-1.945801	-2.324028	-2.319056
1	-1.069105	-1.661079	-2.276226
6	-1.431421	-3.783697	-2.436051
1	-2.265208	-4.486425	-2.563339
1	-0.862282	-4.073683	-1.548585
1	-0.779710	-3.882772	-3.315981
6	-2.742497	-1.973264	-3.605598
1	-3.616178	-2.629319	-3.713393
1	-2.107561	-2.114445	-4.490996
1	-3.099054	-0.940058	-3.604545
6	-2.960380	-0.195232	2.348220
1	-2.055558	0.381581	2.117960
6	-2.659495	-1.007024	3.636437
1	-2.383477	-0.332442	4.458586
1	-1.833002	-1.711699	3.477040
1	-3.533724	-1.586889	3.959282
6	-4.107953	0.818398	2.593267
1	-3.876171	1.467951	3.448056
1	-5.051562	0.302355	2.814063
1	-4.264531	1.454461	1.714288

6	3.533829	0.501360	2.556818
1	4.197751	1.170249	3.123590
6	2.227665	0.430073	3.381563
1	2.458066	0.078376	4.396808
1	1.504799	-0.274093	2.950348
1	1.747759	1.410665	3.459608
6	4.239284	-0.881678	2.531280
1	4.434782	-1.225842	3.555623
1	5.199697	-0.822230	2.002397
1	3.619082	-1.641801	2.046949
6	1.970074	0.960192	-2.467543
1	1.288287	0.137663	-2.204260
6	1.102298	2.144355	-2.969858
1	0.386381	2.471560	-2.207222
1	0.538964	1.848554	-3.865563
1	1.729978	3.004988	-3.238617
6	2.879813	0.442637	-3.615597
1	3.503562	-0.396531	-3.289583
1	3.543998	1.236034	-3.984398
1	2.265896	0.107056	-4.462293
6	5.725269	3.764472	-0.571444
1	5.674445	4.080823	-1.624040
6	7.145245	3.191085	-0.324472
1	7.340373	2.326208	-0.971140
1	7.264718	2.865684	0.717387
1	7.910064	3.952685	-0.527657
6	5.478226	5.019995	0.305677
1	5.525119	4.770875	1.374093
1	4.490142	5.453338	0.105770
1	6.238638	5.786817	0.105375
6	-5.938998	-3.799446	0.415359
1	-6.416270	-3.558711	1.377195
6	-6.982752	-3.535260	-0.701269
1	-7.293106	-2.482732	-0.712166
1	-7.875870	-4.156761	-0.550523
1	-6.571125	-3.774075	-1.690944
6	-5.543122	-5.298700	0.454083
1	-4.826175	-5.497585	1.260444
1	-5.078292	-5.608904	-0.491061
1	-6.428486	-5.928512	0.615765
15	1.319179	-2.744862	-0.200383
6	1.888154	-3.557414	1.414287
6	2.517587	-4.920739	3.824794
6	2.970981	-4.461849	1.466407
6	1.115945	-3.355604	2.582917
6	1.429269	-4.026237	3.777690
6	3.282971	-5.136548	2.663744
1	3.573794	-4.640599	0.580531
1	0.267653	-2.673622	2.561307
1	0.825497	-3.853324	4.666092
1	4.122935	-5.827586	2.685244
1	2.760966	-5.440986	4.748308
6	2.826006	-2.897099	-1.335297
6	4.955205	-3.248974	-3.177973
6	4.110768	-2.378207	-1.057256
6	2.622235	-3.587570	-2.553144
6	3.677982	-3.764355	-3.468549
6	5.166899	-2.554226	-1.970389
1	4.289128	-1.833581	-0.136602
1	1.639803	-3.994328	-2.778042
1	3.502788	-4.304072	-4.396445
1	6.148290	-2.145776	-1.740795
1	5.773233	-3.385249	-3.881590

Rea-Ge=Ge-Triplet

Atomic Coordinates (Angstroms)

S- S21

Number	X	Y	Z
32	1.124325	0.217959	0.485817
32	-1.194849	-0.414515	-0.544215
6	1.972581	2.040782	0.297783
6	3.387898	4.544901	0.170928
6	1.613289	3.042487	-0.661906
6	3.027086	2.344489	1.220544
6	3.714625	3.572470	1.128276
6	2.324796	4.260310	-0.703287
1	4.521350	3.778329	1.829520
1	2.039850	5.004238	-1.443916
6	-2.715964	0.865775	-0.233960
6	-4.815815	2.786611	0.159774
6	-2.943921	1.452510	1.048594
6	-3.586828	1.228080	-1.320633
6	-4.607588	2.175162	-1.091983
6	-3.975814	2.404034	1.214127
1	-5.257979	2.439709	-1.924042
1	-4.132142	2.849596	2.194855
6	2.477172	-1.224248	0.087940
6	4.646073	-3.062400	-0.311001
6	2.763006	-2.241893	1.057401
6	3.256015	-1.188474	-1.109734
6	4.322381	-2.099429	-1.279671
6	3.841539	-3.124201	0.841000
1	4.916217	-2.055667	-2.191330
1	4.055238	-3.879857	1.593700
6	3.447961	1.396397	2.349037
1	2.804002	0.509724	2.300487
6	4.910419	0.910395	2.191980
1	5.050507	0.394248	1.234762
1	5.171435	0.209787	2.996559
1	5.617358	1.749377	2.235817
6	3.209792	2.034788	3.742479
1	2.163522	2.346704	3.857000
1	3.842979	2.918533	3.892866
1	3.443782	1.315401	4.539356
6	0.461849	2.890444	-1.664910
1	0.059890	1.873230	-1.581303
6	-0.689989	3.875302	-1.328732
1	-1.525151	3.753223	-2.029403
1	-0.343837	4.915529	-1.390380
1	-1.074841	3.705545	-0.316642
6	0.925456	3.079411	-3.133951
1	0.095434	2.885603	-3.824869
1	1.746706	2.398574	-3.386000
1	1.273220	4.104338	-3.315904
6	4.162263	5.860764	0.097482
1	4.915747	5.843890	0.899148
6	4.920561	6.003487	-1.248384
1	4.221022	6.041767	-2.093937
1	5.598195	5.155972	-1.411695
1	5.514541	6.927506	-1.260732
6	3.246589	7.086981	0.347060
1	2.479588	7.175393	-0.433821
1	3.835059	8.014520	0.345307
1	2.733494	7.006608	1.313712
6	1.944497	-2.444590	2.344698
1	1.084277	-1.759291	2.314592
6	1.380185	-3.885993	2.444114
1	2.186829	-4.623765	2.547453
1	0.785824	-4.139568	1.561344
1	0.732223	-3.976377	3.327445
6	2.760578	-2.124017	3.625948
1	3.624389	-2.795720	3.718000
1	2.133671	-2.260083	4.517907
1	3.135434	-1.096030	3.627432
6	2.975380	-0.208329	-2.256436

1	2.112639	0.409614	-1.976109
6	2.586800	-0.955793	-3.559794
1	2.333330	-0.237987	-4.352059
1	1.718450	-1.607766	-3.398216
1	3.412801	-1.579859	-3.924935
6	4.167653	0.751211	-2.504864
1	3.939514	1.447773	-3.322795
1	5.072597	0.195080	-2.782881
1	4.390473	1.340294	-1.607580
6	-3.543498	0.654756	-2.754930
1	-4.361617	1.159139	-3.289276
6	-2.257877	0.996182	-3.548754
1	-2.366121	0.669866	-4.592202
1	-1.373792	0.490630	-3.138252
1	-2.070241	2.075845	-3.544494
6	-3.860878	-0.860277	-2.832459
1	-3.943769	-1.172054	-3.882440
1	-4.813574	-1.089878	-2.337794
1	-3.077843	-1.474929	-2.375404
6	-2.122684	1.092456	2.295941
1	-1.429359	0.278032	2.036873
6	-1.265432	2.290009	2.784471
1	-0.563881	2.626873	2.012318
1	-0.683018	2.005210	3.671282
1	-1.902448	3.141891	3.058465
6	-3.018344	0.567211	3.449431
1	-3.638054	-0.275425	3.125447
1	-3.685125	1.354636	3.825752
1	-2.394170	0.232490	4.288916
6	-5.922468	3.819980	0.370226
1	-5.887097	4.131560	1.424882
6	-7.328446	3.219138	0.109607
1	-7.509771	2.346411	0.749712
1	-7.434463	2.898223	-0.935120
1	-8.110032	3.963637	0.312834
6	-5.695187	5.086127	-0.496772
1	-5.731517	4.844400	-1.567313
1	-4.717037	5.537380	-0.287767
1	-6.471503	5.836545	-0.294992
6	5.823710	-4.015943	-0.516114
1	6.295136	-3.757885	-1.476375
6	6.898182	-3.846807	0.589678
1	7.259200	-2.811544	0.635679
1	7.757233	-4.503785	0.397094
1	6.492935	-4.105281	1.577031
6	5.359071	-5.493030	-0.608060
1	4.624052	-5.627329	-1.411554
1	4.892472	-5.819722	0.330661
1	6.213298	-6.154543	-0.806798
15	-1.536245	-2.685855	0.410833
6	-1.879684	-3.701874	-1.150976
6	-2.196464	-5.319439	-3.465155
6	-3.033669	-4.498251	-1.319765
6	-0.878813	-3.737924	-2.152888
6	-1.036859	-4.534792	-3.299831
6	-3.189615	-5.299623	-2.468641
1	-3.810536	-4.499364	-0.560814
1	0.027981	-3.146345	-2.036980
1	-0.257481	-4.545129	-4.058719
1	-4.086204	-5.905778	-2.580372
1	-2.319750	-5.936728	-4.352044
6	-3.193325	-2.702840	1.322036
6	-5.569171	-2.839138	2.869564
6	-4.406813	-2.174984	0.826118
6	-3.187035	-3.293120	2.608286
6	-4.365499	-3.364587	3.376603
6	-5.585014	-2.242408	1.593202
1	-4.433627	-1.704085	-0.150655

1	-2.259976	-3.701813	3.003499
1	-4.341393	-3.827080	4.360729
1	-6.508299	-1.825825	1.197372
1	-6.480577	-2.891107	3.460933

Rea-Sn=Sn-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	1.313781	0.309584	0.696906
50	-1.330139	-0.269898	-0.598946
6	2.477506	2.138964	0.303756
6	4.111436	4.476552	-0.053430
6	2.114887	3.151317	-0.639475
6	3.660154	2.335226	1.085113
6	4.452052	3.487261	0.882761
6	2.933479	4.289605	-0.798503
1	5.356301	3.617734	1.475249
1	2.642915	5.045232	-1.525549
6	-2.941677	1.181410	-0.233765
6	-5.003597	3.118851	0.276626
6	-3.161610	1.692768	1.080366
6	-3.788367	1.645083	-1.297210
6	-4.793500	2.595307	-1.014361
6	-4.175591	2.651953	1.306873
1	-5.427904	2.933077	-1.832550
1	-4.327082	3.036855	2.314027
6	2.535386	-1.445110	0.199481
6	4.182702	-3.707556	-0.425212
6	2.797400	-2.450845	1.182664
6	3.096018	-1.600255	-1.103887
6	3.909126	-2.721151	-1.387397
6	3.611559	-3.554808	0.851819
1	4.340681	-2.828341	-2.381726
1	3.803263	-4.311098	1.610716
6	4.132254	1.345440	2.159410
1	3.403007	0.524734	2.220159
6	5.498625	0.708953	1.798114
1	5.442747	0.175606	0.841634
1	5.806068	-0.008889	2.570470
1	6.283544	1.472384	1.718665
6	4.171847	1.998318	3.565589
1	3.191922	2.412733	3.834918
1	4.904876	2.814050	3.608326
1	4.452248	1.255682	4.325038
6	0.852921	3.073870	-1.507028
1	0.364745	2.109175	-1.312301
6	-0.162893	4.183684	-1.128840
1	-1.087163	4.081476	-1.711718
1	0.253313	5.180867	-1.323557
1	-0.427140	4.132170	-0.065560
6	1.180503	3.118399	-3.022621
1	0.268538	2.981777	-3.617452
1	1.892427	2.330162	-3.297203
1	1.622846	4.081643	-3.307733
6	4.998080	5.706985	-0.249033
1	5.831551	5.629697	0.465105
6	5.609552	5.747767	-1.674402
1	4.824975	5.835586	-2.437677
1	6.181542	4.835357	-1.885131
1	6.282225	6.609510	-1.782115
6	4.239845	7.023603	0.061263
1	3.400495	7.169737	-0.631336
1	4.910878	7.887605	-0.038195
1	3.835874	7.016752	1.081438
6	2.234549	-2.389807	2.611399

1	1.621310	-1.476994	2.695121
6	1.304186	-3.589653	2.923453
1	1.849737	-4.540978	2.865302
1	0.465321	-3.631250	2.219425
1	0.895457	-3.499925	3.939912
6	3.357301	-2.282286	3.676373
1	3.988546	-3.180676	3.678088
1	2.923108	-2.176196	4.679876
1	4.006454	-1.418916	3.488895
6	2.861052	-0.586126	-2.231976
1	2.181894	0.194005	-1.857824
6	2.170843	-1.231784	-3.461724
1	1.971869	-0.474384	-4.232321
1	1.215170	-1.694695	-3.183441
1	2.803080	-2.008063	-3.911856
6	4.175473	0.127076	-2.642972
1	3.985743	0.862825	-3.436293
1	4.913522	-0.592579	-3.020704
1	4.618484	0.654146	-1.789530
6	-3.719146	1.186656	-2.770097
1	-4.516349	1.742443	-3.284711
6	-2.405126	1.584110	-3.489883
1	-2.478448	1.357580	-4.562537
1	-1.535758	1.034542	-3.102530
1	-2.207494	2.657163	-3.376256
6	-4.053191	-0.313391	-2.980648
1	-4.109419	-0.539535	-4.054240
1	-5.021852	-0.565751	-2.530208
1	-3.292658	-0.978931	-2.551430
6	-2.333843	1.249504	2.294581
1	-1.663384	0.433195	1.980122
6	-1.434907	2.398820	2.821095
1	-0.765693	2.775675	2.037425
1	-0.816593	2.050453	3.658997
1	-2.043812	3.241094	3.175303
6	-3.214421	0.678538	3.435771
1	-3.842497	-0.145067	3.079847
1	-3.872051	1.450543	3.856483
1	-2.580731	0.301567	4.249815
6	-6.101938	4.145143	0.555537
1	-6.040681	4.411608	1.621337
6	-7.513361	3.551389	0.305272
1	-7.675770	2.650911	0.911143
1	-7.644065	3.275547	-0.749616
1	-8.291620	4.283432	0.560374
6	-5.899999	5.447067	-0.262113
1	-5.970884	5.253043	-1.340565
1	-4.915352	5.889129	-0.064391
1	-6.668844	6.187723	-0.003639
6	5.071740	-4.905230	-0.764514
1	5.393095	-4.792472	-1.810994
6	6.350460	-4.938716	0.112770
1	6.921741	-4.006970	0.014914
1	6.999551	-5.774406	-0.182399
1	6.098334	-5.068291	1.173582
6	4.298051	-6.245399	-0.657617
1	3.412334	-6.244735	-1.305385
1	3.959172	-6.425575	0.371157
1	4.940444	-7.086591	-0.951922
15	-1.857008	-2.641389	0.550864
6	-2.045175	-3.758925	-0.969787
6	-2.146780	-5.496707	-3.217426
6	-3.250712	-4.401935	-1.329112
6	-0.885440	-4.010476	-1.745898
6	-0.936884	-4.866334	-2.860440
6	-3.299282	-5.264232	-2.443390
1	-4.150299	-4.240479	-0.741822
1	0.063035	-3.548673	-1.474066
1	-0.035611	-5.043048	-3.444261

1	-4.237586	-5.750672	-2.702661
1	-2.187325	-6.159446	-4.079354
6	-3.611490	-2.580167	1.261137
6	-6.160430	-2.577945	2.515229
6	-4.720077	-1.958884	0.642013
6	-3.800212	-3.197885	2.520902
6	-5.064466	-3.200626	3.142865
6	-5.983442	-1.955975	1.263610
1	-4.600835	-1.466796	-0.317991
1	-2.957495	-3.679449	3.011534
1	-5.189238	-3.684386	4.109135
1	-6.821691	-1.464971	0.774506
1	-7.136613	-2.574896	2.995314

Rea-Pb=Pb-Triplet

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	1.380033	0.267776	0.800197
82	-1.380805	-0.176690	-0.751153
6	2.771497	2.018969	0.260682
6	4.553940	4.221018	-0.187427
6	2.444352	3.042183	-0.680444
6	3.992405	2.127822	0.992727
6	4.859886	3.217265	0.746745
6	3.338063	4.115267	-0.888393
1	5.794196	3.287255	1.302606
1	3.076717	4.883913	-1.613703
6	-2.949529	1.404785	-0.219016
6	-4.855038	3.471532	0.401364
6	-3.096475	1.896247	1.112537
6	-3.793106	1.958943	-1.242162
6	-4.720137	2.970286	-0.908683
6	-4.034428	2.917794	1.394738
1	-5.350454	3.376255	-1.698897
1	-4.129006	3.287314	2.414906
6	2.526493	-1.627661	0.203627
6	3.977485	-4.007251	-0.468401
6	2.723748	-2.659479	1.172485
6	3.047260	-1.813275	-1.110263
6	3.764538	-2.993430	-1.418005
6	3.442976	-3.822603	0.820646
1	4.168039	-3.125954	-2.421466
1	3.589716	-4.598182	1.570698
6	4.420853	1.109064	2.059106
1	3.641878	0.336459	2.133690
6	5.731484	0.378592	1.670950
1	5.617354	-0.146221	0.714784
1	6.000810	-0.362416	2.436062
1	6.567676	1.083845	1.576930
6	4.535435	1.759270	3.462362
1	3.591298	2.238448	3.752445
1	5.320861	2.525781	3.484394
1	4.784042	1.001601	4.218420
6	1.139987	3.038540	-1.487802
1	0.598929	2.111784	-1.245009
6	0.217489	4.219715	-1.088464
1	-0.738442	4.167653	-1.626327
1	0.688199	5.183491	-1.323611
1	0.001286	4.205432	-0.012973
6	1.394542	3.030178	-3.017747
1	0.446431	2.953071	-3.566474
1	2.032316	2.185940	-3.308417
1	1.893246	3.952275	-3.343396
6	5.515737	5.386403	-0.424615
1	6.369022	5.253649	0.257418

6	6.073188	5.382268	-1.872341
1	5.267295	5.521438	-2.605256
1	6.572521	4.431965	-2.099956
1	6.798631	6.195683	-2.010585
6	4.862405	6.752871	-0.091427
1	4.008689	6.954420	-0.751955
1	5.586281	7.569268	-0.219842
1	4.497899	6.774683	0.943406
6	2.187209	-2.562525	2.609515
1	1.649339	-1.605864	2.708734
6	1.166965	-3.685568	2.927791
1	1.633686	-4.677216	2.861389
1	0.322778	-3.661602	2.227966
1	0.773497	-3.567970	3.947372
6	3.330101	-2.545955	3.657997
1	3.895075	-3.487242	3.644091
1	2.922734	-2.413320	4.669774
1	4.036742	-1.730111	3.461375
6	2.862917	-0.776568	-2.227264
1	2.275738	0.060283	-1.823888
6	2.070231	-1.355364	-3.428747
1	1.908210	-0.582561	-4.193100
1	1.089165	-1.733703	-3.111713
1	2.612922	-2.184517	-3.901229
6	4.218024	-0.183894	-2.693035
1	4.062790	0.571885	-3.475293
1	4.872130	-0.964352	-3.103686
1	4.741092	0.295802	-1.857164
6	-3.791795	1.535671	-2.726240
1	-4.546981	2.170082	-3.212818
6	-2.462177	1.837803	-3.465084
1	-2.579410	1.666097	-4.544211
1	-1.636032	1.192463	-3.129862
1	-2.158125	2.880988	-3.311654
6	-4.259081	0.074541	-2.961101
1	-4.368132	-0.121477	-4.036732
1	-5.230220	-0.105190	-2.481929
1	-3.545185	-0.661728	-2.569092
6	-2.262387	1.368583	2.288241
1	-1.654107	0.523136	1.929213
6	-1.278580	2.446474	2.814882
1	-0.610757	2.799761	2.018724
1	-0.658342	2.040112	3.625245
1	-1.822455	3.316212	3.206802
6	-3.142174	0.824473	3.443213
1	-3.833335	0.052373	3.087941
1	-3.736231	1.625411	3.903099
1	-2.510220	0.387272	4.228290
6	-5.864046	4.570649	0.735727
1	-5.752271	4.806763	1.804674
6	-7.323417	4.092264	0.515117
1	-7.538386	3.194869	1.109211
1	-7.502856	3.847981	-0.540461
1	-8.036061	4.876576	0.804818
6	-5.586462	5.872349	-0.060088
1	-5.703480	5.709373	-1.139739
1	-4.564997	6.232326	0.116063
1	-6.287670	6.663940	0.237311
6	4.765301	-5.267018	-0.833645
1	5.071865	-5.171242	-1.886310
6	6.056656	-5.403659	0.014754
1	6.694214	-4.516901	-0.091204
1	6.634439	-6.284160	-0.298323
1	5.818267	-5.520008	1.080304
6	3.895875	-6.546301	-0.717721
1	2.999435	-6.473871	-1.346500
1	3.566207	-6.707692	0.317179
1	4.466454	-7.431636	-1.030394
15	-2.167680	-2.651084	0.520036

6	-2.511129	-3.738743	-0.967824
6	-2.849090	-5.397691	-3.249597
6	-3.769827	-4.318802	-1.259782
6	-1.418713	-4.019395	-1.831456
6	-1.586495	-4.837998	-2.959834
6	-3.935806	-5.137599	-2.392583
1	-4.616473	-4.136302	-0.605091
1	-0.436589	-3.599990	-1.618979
1	-0.738273	-5.037671	-3.610267
1	-4.911434	-5.570404	-2.603679
1	-2.980910	-6.027710	-4.126545
6	-3.856223	-2.479043	1.342813
6	-6.304922	-2.218506	2.751535
6	-4.956128	-1.809297	0.757082
6	-3.998541	-3.008695	2.647554
6	-5.215880	-2.885989	3.344904
6	-6.169816	-1.677684	1.457468
1	-4.864838	-1.373054	-0.233620
1	-3.160540	-3.519810	3.116326
1	-5.309372	-3.305125	4.344196
1	-7.000867	-1.148276	0.997127
1	-7.243056	-2.115577	3.292001

TS1-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.464289	2.075597	0.129736
6	0.280996	4.946191	0.260724
6	0.892243	2.902992	-0.968659
6	-0.048107	2.727705	1.294523
6	-0.129416	4.137511	1.326534
6	0.796401	4.303589	-0.876534
1	-0.520045	4.618745	2.220537
1	1.132906	4.905551	-1.716776
6	-2.246130	-0.535706	-1.133581
6	-5.102981	-0.699816	-1.482737
6	-3.097685	0.582042	-0.844215
6	-2.861939	-1.717575	-1.705478
6	-4.264727	-1.767863	-1.844378
6	-4.493964	0.473019	-1.010046
1	-4.706912	-2.670430	-2.261972
1	-5.129553	1.318775	-0.765356
6	2.368983	-0.438778	-0.389263
6	5.138984	-1.253453	-0.635419
6	3.325180	-0.196475	0.659285
6	2.856516	-1.089220	-1.579166
6	4.212658	-1.476762	-1.660867
6	4.668552	-0.603155	0.515213
1	4.556835	-1.975229	-2.564094
1	5.360360	-0.407052	1.330626
6	-0.517303	2.011805	2.570140
1	-0.375892	0.933933	2.445551
6	0.319059	2.433198	3.809613
1	1.393229	2.330042	3.629596
1	0.054063	1.807429	4.672766
1	0.123297	3.477763	4.084396
6	-2.020010	2.266428	2.857571
1	-2.658315	1.777117	2.118204
1	-2.250014	3.339448	2.850243
1	-2.292974	1.874732	3.844759
6	1.510210	2.344229	-2.263016
1	1.345326	1.259441	-2.300786
6	0.878768	2.927615	-3.554690
1	1.277336	2.405278	-4.434927
1	1.115213	3.992487	-3.675123

1	-0.211064	2.822412	-3.558701
6	3.043823	2.585938	-2.270206
1	3.497358	2.186509	-3.186678
1	3.527458	2.106129	-1.412671
1	3.259744	3.661730	-2.229016
6	0.179994	6.466053	0.348019
1	-0.270943	6.711749	1.320956
6	1.581886	7.126130	0.303100
1	2.076734	6.933820	-0.658112
1	2.227488	6.730288	1.097356
1	1.503447	8.213903	0.431085
6	-0.744126	7.044550	-0.753527
1	-0.334003	6.855517	-1.754464
1	-0.854028	8.130689	-0.634642
1	-1.742250	6.590390	-0.709002
6	2.992160	0.506919	1.983793
1	1.924103	0.734637	2.010546
6	3.285424	-0.394880	3.212221
1	4.357702	-0.610490	3.308369
1	2.750236	-1.348545	3.140378
1	2.963575	0.106086	4.135083
6	3.757939	1.852974	2.097381
1	4.843681	1.694504	2.065198
1	3.525878	2.353131	3.046784
1	3.489365	2.531565	1.278946
6	2.029827	-1.446217	-2.827233
1	1.026497	-1.020157	-2.724906
6	1.859106	-2.983181	-2.944025
1	1.271123	-3.237031	-3.835204
1	1.338415	-3.382655	-2.068021
1	2.833227	-3.482852	-3.026950
6	2.625938	-0.876286	-4.141588
1	1.923323	-1.050409	-4.968141
1	3.571595	-1.365719	-4.408447
1	2.813465	0.201274	-4.071098
6	-2.133011	-2.955669	-2.288357
1	-2.939118	-3.583860	-2.694676
6	-1.251495	-2.578008	-3.510088
1	-0.814375	-3.481524	-3.958191
1	-0.426694	-1.916965	-3.220231
1	-1.849895	-2.062969	-4.273955
6	-1.386045	-3.872033	-1.281038
1	-1.086042	-4.802121	-1.784630
1	-2.034322	-4.141179	-0.436514
1	-0.485995	-3.400554	-0.879622
6	-2.518262	1.940661	-0.440710
1	-1.671059	1.765271	0.233233
6	-1.968645	2.649890	-1.707563
1	-1.208319	2.034672	-2.201356
1	-1.516866	3.613827	-1.443812
1	-2.780657	2.826957	-2.426188
6	-3.506051	2.886762	0.280154
1	-3.992121	2.402950	1.136604
1	-4.289818	3.246164	-0.399819
1	-2.965691	3.767629	0.646851
6	-6.618301	-0.792530	-1.644467
1	-7.051346	0.148045	-1.273043
6	-7.219640	-1.947973	-0.803936
1	-6.965438	-1.838141	0.258259
1	-6.842984	-2.922429	-1.141839
1	-8.313928	-1.961628	-0.895266
6	-7.016163	-0.933402	-3.137451
1	-6.635399	-1.872712	-3.559754
1	-6.607004	-0.107932	-3.733352
1	-8.108652	-0.931958	-3.248615
6	6.589914	-1.708243	-0.784169
1	6.686386	-2.176537	-1.775225
6	7.577908	-0.514585	-0.738326
1	7.331323	0.231912	-1.503829

1	8.606126	-0.859219	-0.913052
1	7.552705	-0.015690	0.239431
6	6.967488	-2.778380	0.272517
1	6.286889	-3.637876	0.225567
1	6.918591	-2.366432	1.289053
1	7.990752	-3.140598	0.104699
15	0.052106	-1.235750	1.980320
6	0.519375	-3.044009	1.679173
6	1.369056	-5.739791	1.365746
6	-0.310998	-4.115460	2.081346
6	1.793416	-3.344129	1.138641
6	2.209151	-4.677163	0.979389
6	0.110681	-5.449118	1.923172
1	-1.283398	-3.919639	2.520681
1	2.460099	-2.545006	0.833164
1	3.189010	-4.881863	0.553354
1	-0.548651	-6.256512	2.234676
1	1.690653	-6.770723	1.238193
6	-1.778553	-1.298668	2.492372
6	-4.453036	-1.310040	3.464411
6	-2.810782	-1.943038	1.773188
6	-2.109115	-0.682449	3.722666
6	-3.432936	-0.683403	4.203621
6	-4.133655	-1.947393	2.250440
1	-2.592397	-2.440241	0.836870
1	-1.327753	-0.211528	4.312502
1	-3.663534	-0.198123	5.149375
1	-4.908785	-2.437311	1.665880
1	-5.478114	-1.304856	3.828626
6	0.514603	0.162510	-0.191626
6	-0.354579	-0.787711	-0.801519

		1		
		A		
Frequencies	--	-173.0024		
Red. masses	--	8.6079		
Frc consts	--	0.1518		
IR Inten	--	58.0895		
Atom AN		X	Y	Z
1	6	-0.04	0.14	0.10
2	6	-0.02	0.07	0.03
3	6	-0.02	0.06	0.06
4	6	-0.02	0.12	0.08
5	6	-0.02	0.11	0.06
6	6	-0.02	0.06	0.03
7	1	-0.02	0.14	0.05
8	1	-0.01	0.05	0.03
9	6	0.19	-0.05	-0.01
10	6	0.09	-0.02	0.01
11	6	0.13	-0.05	0.01
12	6	0.09	-0.03	-0.01
13	6	0.09	-0.02	0.01
14	6	0.13	-0.04	0.02
15	1	0.08	-0.01	0.01
16	1	0.15	-0.03	0.03
17	6	-0.08	-0.15	-0.02
18	6	-0.02	-0.01	-0.02
19	6	-0.07	-0.06	-0.03
20	6	-0.03	-0.08	-0.02
21	6	-0.01	-0.02	-0.03
22	6	-0.05	0.00	-0.04
23	1	0.01	0.00	-0.04
24	1	-0.05	0.04	-0.04
25	6	-0.01	0.07	0.05
26	1	0.00	0.07	0.00
27	6	-0.01	0.03	0.05
28	1	-0.01	0.02	0.04
29	1	0.00	0.02	0.04

30	1	0.01	0.03	0.07
31	6	-0.02	0.04	0.05
32	1	-0.01	0.04	0.05
33	1	-0.03	0.04	0.06
34	1	-0.01	0.03	0.05
35	6	-0.02	0.02	0.07
36	1	-0.04	0.02	0.10
37	6	0.01	0.00	0.04
38	1	0.02	-0.02	0.06
39	1	0.02	0.00	0.03
40	1	0.00	0.02	0.02
41	6	-0.02	-0.01	0.05
42	1	-0.03	-0.03	0.06
43	1	-0.02	0.00	0.06
44	1	0.00	-0.01	0.04
45	6	0.00	0.07	0.00
46	1	0.00	0.10	-0.01
47	6	0.01	0.05	-0.01
48	1	0.00	0.02	-0.01
49	1	0.00	0.05	0.00
50	1	0.02	0.05	-0.03
51	6	0.00	0.05	-0.01
52	1	0.00	0.03	-0.01
53	1	0.00	0.05	-0.04
54	1	0.00	0.05	0.00
55	6	-0.05	-0.03	-0.03
56	1	-0.04	-0.01	-0.02
57	6	-0.03	-0.01	-0.02
58	1	-0.03	0.00	-0.03
59	1	-0.02	-0.02	0.00
60	1	-0.02	0.00	-0.02
61	6	-0.03	-0.03	-0.05
62	1	-0.03	-0.04	-0.05
63	1	-0.03	-0.03	-0.05
64	1	-0.04	-0.04	-0.05
65	6	-0.02	-0.06	-0.03
66	1	-0.02	-0.07	-0.01
67	6	0.00	-0.06	-0.05
68	1	0.01	-0.06	-0.06
69	1	0.01	-0.08	-0.06
70	1	0.01	-0.04	-0.05
71	6	-0.02	-0.02	-0.01
72	1	-0.02	0.00	-0.02
73	1	-0.02	0.00	-0.02
74	1	-0.03	-0.02	0.02
75	6	0.04	-0.04	-0.02
76	1	0.02	-0.03	0.00
77	6	0.01	-0.06	-0.05
78	1	-0.01	-0.07	-0.05
79	1	0.02	-0.07	-0.08
80	1	0.00	-0.07	-0.04
81	6	0.03	-0.05	-0.03
82	1	0.00	-0.07	-0.02
83	1	0.04	-0.02	-0.01
84	1	0.05	-0.08	-0.05
85	6	0.07	-0.02	0.01
86	1	0.09	0.02	0.00
87	6	0.03	-0.01	-0.01
88	1	0.05	0.01	-0.01
89	1	0.01	0.00	-0.01
90	1	0.02	-0.04	0.00
91	6	0.04	-0.04	-0.01
92	1	0.03	-0.05	-0.02
93	1	0.06	-0.04	-0.02
94	1	0.03	-0.05	0.01
95	6	0.08	0.01	0.02
96	1	0.11	0.02	0.03
97	6	0.06	0.02	0.02
98	1	0.06	0.00	0.02

99	1	0.04	0.01	0.01
100	1	0.06	0.04	0.01
101	6	0.06	0.02	0.02
102	1	0.04	0.01	0.02
103	1	0.06	0.01	0.01
104	1	0.06	0.03	0.04
105	6	-0.01	0.01	-0.01
106	1	0.00	0.01	-0.01
107	6	-0.02	0.01	0.00
108	1	-0.01	0.01	0.00
109	1	-0.02	0.01	0.01
110	1	-0.02	0.01	0.00
111	6	-0.02	0.01	-0.01
112	1	-0.01	0.01	-0.01
113	1	-0.02	0.01	-0.01
114	1	-0.01	0.01	0.00
115	15	0.01	0.05	-0.01
116	6	0.00	0.03	-0.02
117	6	-0.02	0.01	0.01
118	6	0.00	0.04	-0.01
119	6	0.01	0.01	0.00
120	6	-0.01	0.00	0.01
121	6	-0.01	0.03	0.00
122	1	0.00	0.05	-0.01
123	1	0.03	-0.01	0.01
124	1	0.00	-0.01	0.02
125	1	-0.02	0.04	0.01
126	1	-0.03	0.01	0.02
127	6	0.00	0.03	-0.01
128	6	0.00	0.00	0.01
129	6	0.01	0.01	0.00
130	6	0.00	0.02	-0.01
131	6	0.00	0.01	0.00
132	6	0.01	0.00	0.01
133	1	0.01	0.00	0.01
134	1	0.00	0.03	-0.01
135	1	0.00	0.00	0.00
136	1	0.01	-0.02	0.02
137	1	0.01	-0.02	0.01
138	6	-0.18	-0.33	0.01
139	6	-0.38	0.00	-0.22

TS1-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	0.800787	0.197754	-0.094418
14	-1.059609	-0.972177	-0.912202
6	1.276155	2.067635	0.113616
6	1.859296	4.887216	0.082488
6	1.821486	2.705445	-1.056859
6	1.040940	2.880334	1.266315
6	1.333284	4.261427	1.218292
6	2.101959	4.084032	-1.043543
1	1.150265	4.865923	2.104016
1	2.519822	4.539683	-1.937620
6	-2.839122	-0.242575	-1.141871
6	-5.657562	0.340955	-1.304136
6	-3.344955	1.071829	-0.868529
6	-3.783417	-1.242151	-1.602583
6	-5.156985	-0.925073	-1.651660
6	-4.729623	1.329469	-0.941300
1	-5.849644	-1.695062	-1.986144
1	-5.102012	2.322789	-0.709368
6	2.413476	-0.880709	-0.369158
6	4.847948	-2.409169	-0.735698

6	3.475814	-0.856459	0.602093
6	2.623310	-1.686274	-1.545452
6	3.821055	-2.422060	-1.686916
6	4.651581	-1.609915	0.400427
1	3.954176	-3.031248	-2.577935
1	5.429884	-1.569954	1.158452
6	0.498365	2.368283	2.609175
1	0.343587	1.287191	2.541274
6	1.506506	2.604795	3.767225
1	2.499769	2.213515	3.528023
1	1.152967	2.108238	4.681164
1	1.611575	3.674480	3.990112
6	-0.859671	3.023432	2.972626
1	-1.657340	2.690013	2.304735
1	-0.801339	4.117774	2.914841
1	-1.150421	2.759691	3.996531
6	2.172932	1.949299	-2.350763
1	1.728110	0.946264	-2.312913
6	1.620481	2.624372	-3.633944
1	1.801440	1.978752	-4.503966
1	2.117072	3.582647	-3.832612
1	0.543891	2.811351	-3.564574
6	3.711407	1.775885	-2.466810
1	3.974638	1.232607	-3.383716
1	4.116018	1.221536	-1.613304
1	4.203253	2.756886	-2.503850
6	2.165588	6.381868	0.084126
1	1.868953	6.778717	1.066387
6	3.683723	6.644805	-0.086607
1	4.037440	6.288257	-1.063103
1	4.261375	6.125823	0.688835
1	3.901944	7.718908	-0.019792
6	1.344495	7.137676	-0.991337
1	1.614544	6.805049	-2.002397
1	1.531326	8.218153	-0.931555
1	0.268678	6.966221	-0.858233
6	3.438629	-0.035141	1.899799
1	2.472254	0.468103	1.978427
6	3.577718	-0.930106	3.159947
1	4.560559	-1.417652	3.202774
1	2.808211	-1.710216	3.178729
1	3.468214	-0.323598	4.069004
6	4.535663	1.063710	1.884790
1	5.536734	0.622271	1.795493
1	4.514352	1.646783	2.814816
1	4.392873	1.754277	1.045039
6	1.640649	-1.863667	-2.716537
1	0.794047	-1.183305	-2.578543
6	1.066177	-3.304100	-2.729821
1	0.367013	-3.430355	-3.566238
1	0.526632	-3.514415	-1.800982
1	1.866904	-4.046835	-2.842255
6	2.264328	-1.527464	-4.097005
1	1.480528	-1.543855	-4.866788
1	3.026504	-2.260508	-4.391556
1	2.731514	-0.536016	-4.103214
6	-3.449097	-2.652335	-2.153557
1	-4.419477	-3.061176	-2.470951
6	-2.594003	-2.573040	-3.447718
1	-2.442995	-3.577992	-3.866621
1	-1.605811	-2.142377	-3.249482
1	-3.092815	-1.950443	-4.202967
6	-2.893814	-3.690701	-1.140725
1	-2.885875	-4.687280	-1.604878
1	-3.524474	-3.743000	-0.243253
1	-1.874322	-3.457912	-0.824555
6	-2.402180	2.244265	-0.583992
1	-1.581989	1.879260	0.045906
6	-1.783293	2.728967	-1.922665

1	-1.249388	1.914292	-2.424332
1	-1.076942	3.549095	-1.745740
1	-2.572540	3.084400	-2.599344
6	-3.051498	3.447446	0.137964
1	-3.581221	3.145895	1.050271
1	-3.763037	3.972686	-0.512927
1	-2.273853	4.168408	0.417008
6	-7.152224	0.645992	-1.366482
1	-7.295398	1.682355	-1.026455
6	-7.969478	-0.272771	-0.422491
1	-7.616283	-0.189741	0.613511
1	-7.886898	-1.325444	-0.723612
1	-9.033013	-0.000073	-0.445355
6	-7.684172	0.553036	-2.820968
1	-7.594807	-0.470400	-3.208545
1	-7.119645	1.215023	-3.489542
1	-8.743524	0.838973	-2.864613
6	6.114309	-3.237643	-0.945742
1	6.010323	-3.755871	-1.910846
6	7.380300	-2.347277	-1.032733
1	7.280386	-1.594892	-1.825191
1	8.266674	-2.958814	-1.249292
1	7.559864	-1.818992	-0.087105
6	6.277657	-4.324302	0.148255
1	5.394677	-4.974152	0.195109
1	6.414627	-3.871886	1.139212
1	7.155190	-4.951179	-0.060058
15	-0.211096	-1.165412	2.021707
6	-0.256306	-3.043829	1.801855
6	-0.166206	-5.879045	1.599705
6	-1.305002	-3.839412	2.318143
6	0.850756	-3.692883	1.203046
6	0.890732	-5.093874	1.099108
6	-1.259388	-5.242532	2.214950
1	-2.156625	-3.374931	2.803859
1	1.678073	-3.112281	0.809566
1	1.748214	-5.568325	0.626718
1	-2.081338	-5.832795	2.614481
1	-0.135544	-6.962738	1.514941
6	-1.950778	-0.719959	2.648242
6	-4.454472	0.017806	3.781851
6	-3.166522	-1.097638	2.034027
6	-2.015449	0.012775	3.857184
6	-3.253526	0.382451	4.417832
6	-4.404853	-0.731644	2.591133
1	-3.156617	-1.673696	1.117701
1	-1.096155	0.284340	4.368408
1	-3.277589	0.950650	5.345029
1	-5.322714	-1.022940	2.085926
1	-5.412225	0.309421	4.207449

		1		
		A		
Frequencies	--	-52.4829		
Red. masses	--	8.2271		
Frc consts	--	0.0134		
IR Inten	--	10.7791		
Atom AN		X	Y	Z
1	14	0.07	0.09	-0.12
2	14	0.03	-0.02	0.16
3	6	0.07	0.06	-0.06
4	6	0.04	0.06	-0.01
5	6	0.06	0.08	-0.05
6	6	0.05	0.03	-0.05
7	6	0.04	0.03	-0.02
8	6	0.04	0.08	-0.03
9	1	0.03	0.02	-0.01
10	1	0.04	0.11	-0.02

11	6	0.02	-0.02	0.11
12	6	0.02	-0.01	0.01
13	6	0.01	-0.02	0.06
14	6	0.03	-0.02	0.08
15	6	0.03	-0.02	0.04
16	6	0.02	-0.01	0.02
17	1	0.04	-0.02	0.02
18	1	0.01	-0.01	-0.01
19	6	0.03	0.04	-0.04
20	6	0.01	-0.01	0.00
21	6	0.02	0.02	-0.02
22	6	0.02	0.02	-0.03
23	6	0.01	0.00	-0.01
24	6	0.01	0.00	0.00
25	1	0.01	-0.01	0.00
26	1	0.00	-0.02	0.01
27	6	0.04	-0.01	-0.07
28	1	0.04	-0.01	-0.10
29	6	0.02	-0.03	-0.05
30	1	0.03	-0.01	-0.05
31	1	0.02	-0.06	-0.07
32	1	0.01	-0.04	-0.02
33	6	0.03	-0.03	-0.06
34	1	0.03	-0.02	-0.05
35	1	0.02	-0.03	-0.04
36	1	0.04	-0.04	-0.06
37	6	0.04	0.08	-0.06
38	1	0.03	0.08	-0.05
39	6	0.02	0.08	-0.05
40	1	0.01	0.09	-0.05
41	1	0.01	0.09	-0.05
42	1	0.02	0.07	-0.03
43	6	0.04	0.07	-0.07
44	1	0.02	0.07	-0.08
45	1	0.04	0.06	-0.08
46	1	0.04	0.07	-0.07
47	6	0.02	0.06	0.01
48	1	0.02	0.04	0.02
49	6	0.02	0.07	0.02
50	1	0.02	0.09	0.01
51	1	0.02	0.07	0.01
52	1	0.01	0.07	0.04
53	6	0.01	0.07	0.02
54	1	0.02	0.09	0.02
55	1	0.00	0.07	0.04
56	1	0.02	0.06	0.02
57	6	0.00	0.02	-0.02
58	1	0.01	0.04	-0.05
59	6	-0.06	0.01	-0.02
60	1	-0.08	-0.02	0.00
61	1	-0.09	0.03	-0.05
62	1	-0.07	0.00	-0.02
63	6	0.03	-0.01	0.01
64	1	0.02	-0.04	0.04
65	1	0.02	-0.02	0.02
66	1	0.07	0.00	0.01
67	6	0.02	0.02	-0.03
68	1	0.02	0.01	-0.03
69	6	0.02	0.02	-0.03
70	1	0.03	0.02	-0.03
71	1	0.01	0.03	-0.03
72	1	0.02	0.01	-0.02
73	6	0.03	0.02	-0.02
74	1	0.04	0.01	-0.03
75	1	0.04	0.02	-0.02
76	1	0.03	0.02	-0.02
77	6	0.05	-0.01	0.07
78	1	0.05	-0.02	0.06
79	6	0.04	0.03	0.07

80	1	0.08	0.04	0.05
81	1	0.03	0.06	0.07
82	1	0.03	0.02	0.07
83	6	0.07	-0.02	0.04
84	1	0.07	-0.01	0.03
85	1	0.10	-0.03	0.06
86	1	0.08	-0.01	0.02
87	6	0.01	-0.01	0.05
88	1	0.01	0.01	0.05
89	6	0.01	-0.03	0.04
90	1	0.01	-0.04	0.05
91	1	0.01	-0.03	0.02
92	1	0.01	-0.04	0.03
93	6	0.00	0.00	0.02
94	1	0.00	0.02	0.02
95	1	0.00	-0.01	0.01
96	1	0.00	0.01	0.01
97	6	0.02	-0.01	-0.02
98	1	0.02	-0.01	-0.03
99	6	0.01	0.00	-0.02
100	1	-0.01	0.01	-0.01
101	1	0.01	0.00	-0.01
102	1	0.01	0.00	-0.04
103	6	0.04	-0.03	-0.02
104	1	0.05	-0.03	-0.01
105	1	0.05	-0.03	-0.02
106	1	0.04	-0.03	-0.04
107	6	0.00	-0.02	0.01
108	1	0.00	-0.02	0.01
109	6	0.01	-0.02	0.01
110	1	0.01	-0.03	0.00
111	1	0.00	-0.03	0.01
112	1	0.01	-0.02	0.00
113	6	-0.01	-0.01	0.02
114	1	-0.01	0.00	0.02
115	1	-0.01	0.00	0.02
116	1	-0.01	-0.01	0.02
117	15	-0.18	-0.07	-0.16
118	6	-0.10	-0.08	0.01
119	6	-0.02	-0.08	0.08
120	6	-0.06	-0.09	0.06
121	6	-0.10	-0.06	0.00
122	6	-0.05	-0.06	0.03
123	6	-0.02	-0.10	0.09
124	1	-0.07	-0.10	0.06
125	1	-0.13	-0.04	-0.05
126	1	-0.05	-0.04	0.03
127	1	0.01	-0.11	0.12
128	1	0.01	-0.08	0.11
129	6	-0.12	-0.06	-0.02
130	6	-0.05	0.00	0.09
131	6	-0.16	-0.05	0.05
132	6	-0.05	-0.03	-0.03
133	6	-0.01	0.00	0.02
134	6	-0.12	-0.03	0.10
135	1	-0.21	-0.06	0.05
136	1	-0.01	-0.03	-0.09
137	1	0.04	0.02	0.01
138	1	-0.15	-0.02	0.15
139	1	-0.02	0.02	0.13

TS1-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.805425	0.192609	-0.028458

S-

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32	-1.184723	-1.082897	-0.919397
6	1.340398	2.146617	0.134798
6	1.969229	4.952205	0.013515
6	1.864899	2.740032	-1.065220
6	1.149830	2.989240	1.272003
6	1.464845	4.365084	1.181406
6	2.168637	4.114423	-1.097007
1	1.315515	4.995531	2.055888
1	2.569947	4.538655	-2.014267
6	-3.005911	-0.228345	-1.164312
6	-5.799595	0.458954	-1.191649
6	-3.443399	1.107245	-0.873179
6	-4.004685	-1.196568	-1.565232
6	-5.365938	-0.827785	-1.554105
6	-4.819845	1.416076	-0.881485
1	-6.103869	-1.573453	-1.843912
1	-5.143855	2.422699	-0.634529
6	2.484581	-0.918550	-0.367259
6	4.883951	-2.471704	-0.775445
6	3.564742	-0.888616	0.578395
6	2.650450	-1.733442	-1.538877
6	3.835672	-2.484514	-1.704747
6	4.727634	-1.656103	0.356618
1	3.941333	-3.104834	-2.592265
1	5.525455	-1.614993	1.094354
6	0.630827	2.507996	2.634668
1	0.450183	1.429984	2.580966
6	1.674583	2.730438	3.763055
1	2.640377	2.279609	3.513971
1	1.318674	2.281247	4.700294
1	1.839801	3.799841	3.947903
6	-0.705923	3.193499	3.019867
1	-1.515011	2.897613	2.346709
1	-0.616130	4.287004	2.985993
1	-1.000286	2.914120	4.038687
6	2.175311	1.937361	-2.340773
1	1.717059	0.943110	-2.255967
6	1.595401	2.573686	-3.630665
1	1.748416	1.897723	-4.482983
1	2.092230	3.521347	-3.874090
1	0.522070	2.769884	-3.538083
6	3.707553	1.734103	-2.487488
1	3.940516	1.166739	-3.398069
1	4.119826	1.187946	-1.632415
1	4.217171	2.704193	-2.554617
6	2.297614	6.443182	-0.040775
1	2.038310	6.875779	0.937131
6	3.813103	6.681039	-0.269486
1	4.131802	6.281643	-1.241496
1	4.410708	6.187804	0.507513
1	4.044460	7.754580	-0.254316
6	1.454526	7.179168	-1.114398
1	1.681216	6.803976	-2.121231
1	1.667683	8.256560	-1.102002
1	0.380447	7.038635	-0.938407
6	3.555344	-0.038891	1.858311
1	2.584977	0.457391	1.948792
6	3.731801	-0.900600	3.136099
1	4.713153	-1.392237	3.161380
1	2.958239	-1.674212	3.200230
1	3.651699	-0.269378	4.031328
6	4.637576	1.071753	1.787760
1	5.640546	0.640627	1.671722
1	4.638324	1.670779	2.707973
1	4.456855	1.746441	0.942394
6	1.625681	-1.900415	-2.675700
1	0.788541	-1.211902	-2.502416
6	1.046835	-3.340119	-2.692947
1	0.296974	-3.443281	-3.488738

1	0.568957	-3.585743	-1.738913
1	1.838774	-4.077466	-2.879363
6	2.201887	-1.546836	-4.072836
1	1.403029	-1.590864	-4.825949
1	2.982059	-2.255188	-4.380116
1	2.636490	-0.541331	-4.090590
6	-3.748330	-2.634648	-2.087972
1	-4.738903	-2.986507	-2.409381
6	-2.872861	-2.663189	-3.370286
1	-2.839370	-3.681984	-3.781355
1	-1.837521	-2.359032	-3.170065
1	-3.282627	-1.991795	-4.136743
6	-3.278686	-3.680022	-1.036152
1	-3.352559	-4.689056	-1.465913
1	-3.910806	-3.648211	-0.138824
1	-2.241095	-3.529020	-0.725038
6	-2.443947	2.243600	-0.620646
1	-1.609706	1.842111	-0.031690
6	-1.865061	2.733703	-1.976244
1	-1.398815	1.910098	-2.529397
1	-1.109273	3.511515	-1.809621
1	-2.665311	3.151981	-2.602593
6	-3.015807	3.456803	0.150016
1	-3.504979	3.158470	1.085767
1	-3.744173	4.013234	-0.454990
1	-2.202286	4.150167	0.394902
6	-7.285286	0.810439	-1.171724
1	-7.377857	1.855029	-0.839420
6	-8.067815	-0.072877	-0.165207
1	-7.657572	0.024804	0.848335
1	-8.018742	-1.133038	-0.446945
1	-9.126350	0.217932	-0.137183
6	-7.904060	0.711944	-2.591052
1	-7.856756	-0.317328	-2.970607
1	-7.367054	1.355040	-3.299654
1	-8.958548	1.017888	-2.576546
6	6.133533	-3.321324	-1.000822
1	6.002526	-3.850273	-1.956903
6	7.409804	-2.449909	-1.123909
1	7.307403	-1.712447	-1.930120
1	8.285811	-3.076416	-1.339854
1	7.608460	-1.904147	-0.192156
6	6.299973	-4.395990	0.105056
1	5.409741	-5.034227	0.172599
1	6.454422	-3.931766	1.087937
1	7.167248	-5.036151	-0.105776
15	-0.023061	-1.092683	2.231249
6	-0.149398	-2.964076	1.956983
6	-0.158992	-5.802669	1.709862
6	-1.197211	-3.739337	2.511269
6	0.906991	-3.640940	1.299285
6	0.898313	-5.041387	1.173231
6	-1.201897	-5.141578	2.385008
1	-2.009084	-3.258464	3.046869
1	1.734251	-3.079866	0.877407
1	1.718816	-5.533853	0.655605
1	-2.021964	-5.712516	2.816563
1	-0.166308	-6.885698	1.609283
6	-1.770116	-0.623995	2.814336
6	-4.289668	0.155752	3.889616
6	-2.980328	-1.001506	2.186508
6	-1.851334	0.133953	4.006782
6	-3.096184	0.524451	4.538279
6	-4.225923	-0.616302	2.713299
1	-2.962382	-1.605243	1.286087
1	-0.937466	0.406234	4.528730
1	-3.130948	1.110530	5.454054
1	-5.137064	-0.909790	2.196594

		1		
		A		
Frequencies	--	-36.7536		
Red. masses	--	7.7385		
Frc consts	--	0.0062		
IR Inten	--	3.7859		
Atom	AN	X	Y	Z
1	32	-0.03	-0.07	0.13
2	32	-0.02	0.02	-0.08
3	6	-0.05	-0.05	0.05
4	6	-0.05	-0.04	0.00
5	6	-0.05	-0.06	0.04
6	6	-0.03	-0.02	0.04
7	6	-0.04	-0.02	0.01
8	6	-0.06	-0.06	0.01
9	1	-0.03	-0.01	0.01
10	1	-0.06	-0.07	0.00
11	6	-0.01	0.03	-0.09
12	6	-0.01	0.02	-0.01
13	6	0.00	0.03	-0.07
14	6	-0.01	0.03	-0.06
15	6	-0.01	0.02	-0.02
16	6	0.00	0.03	-0.04
17	1	-0.02	0.02	0.00
18	1	0.00	0.03	-0.03
19	6	-0.01	-0.02	0.04
20	6	0.01	0.01	-0.01
21	6	0.01	0.00	0.02
22	6	-0.01	-0.01	0.03
23	6	-0.01	0.00	0.01
24	6	0.02	0.01	0.00
25	1	-0.01	0.01	0.01
26	1	0.03	0.02	-0.02
27	6	-0.02	0.00	0.05
28	1	-0.02	0.00	0.07
29	6	0.00	0.02	0.03
30	1	0.00	0.01	0.02
31	1	0.02	0.04	0.05
32	1	0.01	0.02	0.01
33	6	-0.01	0.01	0.06
34	1	-0.02	0.00	0.07
35	1	-0.01	0.01	0.04
36	1	0.00	0.03	0.06
37	6	-0.04	-0.07	0.04
38	1	-0.04	-0.07	0.05
39	6	-0.04	-0.08	0.03
40	1	-0.03	-0.09	0.04
41	1	-0.03	-0.08	0.03
42	1	-0.04	-0.08	0.02
43	6	-0.04	-0.05	0.05
44	1	-0.03	-0.06	0.06
45	1	-0.04	-0.04	0.06
46	1	-0.05	-0.05	0.04
47	6	-0.04	-0.04	-0.02
48	1	-0.04	-0.03	-0.03
49	6	-0.04	-0.05	-0.03
50	1	-0.04	-0.07	-0.02
51	1	-0.04	-0.04	-0.02
52	1	-0.04	-0.05	-0.04
53	6	-0.04	-0.05	-0.03
54	1	-0.04	-0.07	-0.03
55	1	-0.03	-0.05	-0.05
56	1	-0.04	-0.05	-0.03
57	6	0.03	0.00	0.02
58	1	0.03	-0.01	0.04
59	6	0.08	0.00	0.02

60	1	0.09	0.03	-0.01
61	1	0.10	-0.02	0.03
62	1	0.09	0.00	0.02
63	6	0.02	0.01	-0.01
64	1	0.02	0.03	-0.03
65	1	0.03	0.02	-0.01
66	1	-0.01	0.01	-0.01
67	6	-0.02	-0.02	0.05
68	1	-0.02	-0.01	0.05
69	6	-0.02	-0.02	0.06
70	1	-0.03	-0.02	0.06
71	1	-0.02	-0.01	0.06
72	1	-0.02	-0.02	0.06
73	6	-0.04	-0.02	0.04
74	1	-0.06	-0.02	0.05
75	1	-0.05	-0.03	0.03
76	1	-0.04	-0.02	0.03
77	6	-0.03	0.03	-0.07
78	1	-0.03	0.04	-0.07
79	6	-0.03	0.01	-0.07
80	1	-0.05	0.01	-0.07
81	1	-0.02	-0.01	-0.06
82	1	-0.01	0.02	-0.07
83	6	-0.04	0.02	-0.06
84	1	-0.06	0.02	-0.06
85	1	-0.04	0.03	-0.06
86	1	-0.04	0.01	-0.07
87	6	0.00	0.03	-0.10
88	1	0.04	0.03	-0.17
89	6	-0.09	0.08	-0.12
90	1	-0.14	0.10	-0.19
91	1	-0.07	0.06	-0.14
92	1	-0.13	0.11	-0.05
93	6	0.04	0.00	-0.03
94	1	0.08	-0.04	-0.01
95	1	0.01	0.03	0.03
96	1	0.05	-0.01	-0.04
97	6	-0.01	0.02	0.02
98	1	-0.01	0.02	0.03
99	6	0.01	0.01	0.03
100	1	0.03	0.00	0.02
101	1	0.01	0.01	0.02
102	1	0.01	0.00	0.05
103	6	-0.03	0.03	0.03
104	1	-0.04	0.03	0.02
105	1	-0.05	0.03	0.03
106	1	-0.03	0.02	0.05
107	6	0.01	0.02	-0.02
108	1	0.00	0.03	-0.03
109	6	0.01	0.03	-0.03
110	1	-0.01	0.03	-0.03
111	1	0.01	0.03	-0.04
112	1	0.01	0.02	-0.03
113	6	0.03	0.02	-0.03
114	1	0.03	0.01	-0.03
115	1	0.03	0.01	-0.03
116	1	0.03	0.02	-0.04
117	15	0.14	0.02	0.13
118	6	0.08	0.03	0.02
119	6	0.00	0.04	-0.06
120	6	0.06	0.04	0.01
121	6	0.05	0.02	0.00
122	6	0.01	0.03	-0.05
123	6	0.02	0.05	-0.03
124	1	0.08	0.05	0.03
125	1	0.07	0.01	0.00
126	1	0.00	0.02	-0.07
127	1	0.01	0.06	-0.04
128	1	-0.03	0.04	-0.09

129	6	0.11	0.03	0.02
130	6	0.04	0.02	-0.12
131	6	0.14	0.04	-0.05
132	6	0.03	0.02	0.03
133	6	0.00	0.01	-0.04
134	6	0.11	0.03	-0.12
135	1	0.20	0.03	-0.05
136	1	0.00	0.01	0.09
137	1	-0.05	0.00	-0.04
138	1	0.14	0.04	-0.18
139	1	0.02	0.01	-0.17

TS1-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.894975	0.251957	-0.030946
50	-1.296643	-1.239117	-0.825806
6	1.530824	2.310693	0.132619
6	2.200139	5.078166	-0.015184
6	2.053460	2.867863	-1.078463
6	1.343756	3.152123	1.263600
6	1.683044	4.520624	1.164210
6	2.381929	4.233811	-1.126305
1	1.542092	5.166025	2.029555
1	2.783239	4.647155	-2.048723
6	-3.154210	-0.156564	-1.151156
6	-5.887566	0.676057	-1.178985
6	-3.504224	1.202197	-0.857420
6	-4.192479	-1.068949	-1.553341
6	-5.531302	-0.633340	-1.543593
6	-4.862130	1.584410	-0.869699
1	-6.308771	-1.338081	-1.831536
1	-5.135616	2.606278	-0.623129
6	2.624525	-1.024988	-0.373376
6	4.929141	-2.681385	-0.753681
6	3.687157	-1.034199	0.582937
6	2.740040	-1.857637	-1.534051
6	3.887163	-2.664001	-1.691113
6	4.813477	-1.854478	0.377398
1	3.968416	-3.300295	-2.570301
1	5.610146	-1.848669	1.117917
6	0.794654	2.649013	2.606408
1	0.592744	1.573071	2.520989
6	1.826956	2.813262	3.752823
1	2.779999	2.334677	3.503262
1	1.444292	2.353834	4.674245
1	2.024263	3.872608	3.962243
6	-0.539647	3.340459	2.988954
1	-1.345109	3.059798	2.304066
1	-0.441947	4.433593	2.970641
1	-0.846947	3.047184	4.000102
6	2.311458	2.020316	-2.337330
1	1.810560	1.045404	-2.217714
6	1.722499	2.634620	-3.632454
1	1.842112	1.931804	-4.468456
1	2.236004	3.563636	-3.909844
1	0.655292	2.856788	-3.522636
6	3.825209	1.728196	-2.509156
1	4.003725	1.127031	-3.410503
1	4.221616	1.174465	-1.650949
1	4.388900	2.664697	-2.607610
6	2.567885	6.556761	-0.090980
1	2.323148	7.013075	0.879558
6	4.090632	6.733512	-0.324676
1	4.390437	6.306265	-1.290849

1	4.667000	6.223703	0.457898
1	4.367678	7.795788	-0.323832
6	1.742424	7.292454	-1.177632
1	1.956472	6.889552	-2.176446
1	1.980609	8.364193	-1.189154
1	0.665809	7.179555	-0.996378
6	3.667258	-0.162412	1.847148
1	2.702147	0.358109	1.900783
6	3.774114	-0.998299	3.147464
1	4.732429	-1.529606	3.209625
1	2.965900	-1.736211	3.207793
1	3.694886	-0.342725	4.025017
6	4.762971	0.933071	1.785908
1	5.762413	0.489086	1.693864
1	4.750299	1.545027	2.697467
1	4.604303	1.598291	0.928412
6	1.686732	-1.976103	-2.651606
1	0.887406	-1.248291	-2.457616
6	1.038739	-3.387076	-2.666425
1	0.255707	-3.442658	-3.435989
1	0.581438	-3.626297	-1.700547
1	1.786044	-4.159085	-2.890821
6	2.242289	-1.638601	-4.060072
1	1.425979	-1.657421	-4.795789
1	2.993959	-2.369964	-4.383111
1	2.704942	-0.645396	-4.085600
6	-3.983642	-2.514307	-2.087430
1	-4.978000	-2.813195	-2.444795
6	-3.071828	-2.564655	-3.346236
1	-3.044862	-3.583189	-3.756822
1	-2.030281	-2.286601	-3.127794
1	-3.439568	-1.880614	-4.121528
6	-3.600408	-3.614053	-1.048128
1	-3.792513	-4.605940	-1.480895
1	-4.195644	-3.520223	-0.130949
1	-2.544229	-3.594174	-0.761357
6	-2.440673	2.282894	-0.587648
1	-1.654582	1.840971	0.040244
6	-1.773348	2.723426	-1.919543
1	-1.312773	1.872535	-2.434842
1	-0.994616	3.472740	-1.724967
1	-2.519665	3.165070	-2.593849
6	-2.956569	3.543945	0.147251
1	-3.472276	3.296927	1.083658
1	-3.644428	4.125019	-0.481569
1	-2.109914	4.199617	0.385904
6	-7.351341	1.098625	-1.159903
1	-7.396699	2.147856	-0.832938
6	-8.163332	0.251653	-0.146813
1	-7.745548	0.345935	0.864263
1	-8.143658	-0.812287	-0.417476
1	-9.212350	0.573439	-0.118625
6	-7.958549	1.017410	-2.584212
1	-7.941316	-0.014946	-2.957768
1	-7.383025	1.634081	-3.286457
1	-9.000062	1.363255	-2.589356
6	6.143170	-3.578181	-0.967991
1	5.992775	-4.117002	-1.915446
6	7.439994	-2.741534	-1.106273
1	7.347803	-2.013046	-1.922221
1	8.302202	-3.388013	-1.315765
1	7.649937	-2.184752	-0.183648
6	6.263683	-4.636251	0.158017
1	5.347489	-5.236701	0.228911
1	6.424257	-4.157967	1.133044
1	7.106787	-5.313479	-0.031098
15	-0.099276	-1.066596	2.366371
6	-0.271874	-2.934484	2.110622
6	-0.368202	-5.765395	1.809419

6	-1.354713	-3.683600	2.630404
6	0.774856	-3.633657	1.458588
6	0.724122	-5.030278	1.307600
6	-1.402721	-5.081932	2.476218
1	-2.162151	-3.182683	3.155025
1	1.625638	-3.092248	1.054891
1	1.537216	-5.540335	0.795167
1	-2.249963	-5.633274	2.879320
1	-0.408813	-6.845406	1.688681
6	-1.821798	-0.512477	2.943502
6	-4.294234	0.435358	3.999004
6	-3.054045	-0.837822	2.327623
6	-1.860187	0.287540	4.110731
6	-3.080196	0.760580	4.631864
6	-4.275625	-0.371508	2.844834
1	-3.075684	-1.461656	1.439042
1	-0.929926	0.526334	4.619576
1	-3.079640	1.374727	5.529557
1	-5.202453	-0.627087	2.336349
1	-5.237720	0.801986	4.397015

		1		
		A		
Frequencies	--	-46.0483		
Red. masses	--	9.7420		
Frc consts	--	0.0122		
IR Inten	--	3.9209		
Atom AN		X	Y	Z
1	50	-0.04	-0.06	0.13
2	50	-0.03	0.01	-0.07
3	6	-0.05	-0.04	0.03
4	6	-0.03	-0.04	-0.01
5	6	-0.04	-0.06	0.02
6	6	-0.04	-0.01	0.02
7	6	-0.03	-0.02	0.00
8	6	-0.03	-0.06	0.01
9	1	-0.02	0.00	-0.01
10	1	-0.03	-0.08	0.00
11	6	-0.01	0.02	-0.09
12	6	-0.01	0.00	-0.01
13	6	-0.01	0.01	-0.05
14	6	-0.01	0.02	-0.08
15	6	-0.02	0.01	-0.04
16	6	-0.01	0.00	-0.01
17	1	-0.02	0.01	-0.03
18	1	-0.01	0.00	0.01
19	6	-0.02	-0.01	0.03
20	6	0.00	0.02	-0.02
21	6	0.01	0.01	0.01
22	6	-0.03	0.00	0.03
23	6	-0.02	0.01	0.00
24	6	0.01	0.02	-0.02
25	1	-0.03	0.02	0.00
26	1	0.03	0.03	-0.04
27	6	-0.03	0.02	0.03
28	1	-0.05	0.02	0.06
29	6	-0.02	0.03	0.02
30	1	-0.03	0.00	0.02
31	1	-0.02	0.05	0.03
32	1	0.00	0.03	0.00
33	6	-0.02	0.04	0.03
34	1	-0.03	0.05	0.03
35	1	-0.01	0.04	0.02
36	1	-0.03	0.06	0.03
37	6	-0.04	-0.07	0.03
38	1	-0.03	-0.07	0.04
39	6	-0.03	-0.08	0.02
40	1	-0.02	-0.08	0.03

41	1	-0.02	-0.08	0.02
42	1	-0.03	-0.07	0.01
43	6	-0.03	-0.06	0.04
44	1	-0.02	-0.06	0.05
45	1	-0.03	-0.04	0.05
46	1	-0.04	-0.05	0.03
47	6	-0.01	-0.04	-0.03
48	1	-0.01	-0.03	-0.04
49	6	-0.01	-0.06	-0.03
50	1	-0.02	-0.07	-0.03
51	1	-0.02	-0.05	-0.03
52	1	0.00	-0.06	-0.05
53	6	-0.01	-0.05	-0.04
54	1	-0.01	-0.06	-0.03
55	1	0.00	-0.05	-0.05
56	1	-0.01	-0.04	-0.04
57	6	0.03	0.01	0.01
58	1	0.03	-0.01	0.04
59	6	0.09	0.01	0.01
60	1	0.10	0.03	-0.02
61	1	0.11	-0.01	0.03
62	1	0.09	0.01	0.01
63	6	0.01	0.02	-0.02
64	1	0.02	0.04	-0.05
65	1	0.02	0.02	-0.02
66	1	-0.02	0.02	-0.02
67	6	-0.04	-0.01	0.04
68	1	-0.04	-0.01	0.06
69	6	-0.03	-0.02	0.05
70	1	-0.04	-0.03	0.06
71	1	-0.01	-0.02	0.06
72	1	-0.02	-0.01	0.04
73	6	-0.07	-0.01	0.03
74	1	-0.08	-0.01	0.05
75	1	-0.07	-0.01	0.02
76	1	-0.07	-0.01	0.03
77	6	-0.02	0.03	-0.10
78	1	-0.01	0.04	-0.12
79	6	0.00	0.03	-0.09
80	1	-0.01	0.04	-0.10
81	1	0.01	0.01	-0.06
82	1	0.03	0.05	-0.08
83	6	-0.04	0.01	-0.11
84	1	-0.06	0.02	-0.12
85	1	-0.04	0.01	-0.11
86	1	-0.04	-0.01	-0.11
87	6	-0.01	0.01	-0.04
88	1	-0.02	0.01	-0.03
89	6	0.01	0.01	-0.03
90	1	0.02	0.01	-0.02
91	1	0.00	0.01	-0.02
92	1	0.02	0.00	-0.04
93	6	-0.01	0.01	-0.04
94	1	-0.01	0.01	-0.04
95	1	-0.01	0.01	-0.04
96	1	-0.01	0.00	-0.03
97	6	-0.01	0.00	0.02
98	1	-0.01	-0.01	0.04
99	6	0.01	-0.02	0.02
100	1	0.02	-0.04	0.02
101	1	0.01	-0.02	0.01
102	1	0.01	-0.03	0.04
103	6	-0.04	0.02	0.03
104	1	-0.04	0.02	0.02
105	1	-0.05	0.03	0.03
106	1	-0.04	0.01	0.05
107	6	0.00	0.02	-0.04
108	1	-0.01	0.03	-0.04
109	6	0.00	0.02	-0.04

110	1	-0.01	0.03	-0.03
111	1	0.00	0.02	-0.05
112	1	0.01	0.02	-0.03
113	6	0.00	0.01	-0.04
114	1	0.00	0.01	-0.04
115	1	0.01	0.01	-0.04
116	1	0.00	0.02	-0.05
117	15	0.18	0.03	0.17
118	6	0.09	0.05	0.02
119	6	0.00	0.06	-0.09
120	6	0.06	0.06	-0.03
121	6	0.08	0.03	0.01
122	6	0.04	0.04	-0.04
123	6	0.02	0.07	-0.08
124	1	0.07	0.07	-0.01
125	1	0.11	0.02	0.05
126	1	0.03	0.03	-0.04
127	1	-0.01	0.09	-0.11
128	1	-0.03	0.07	-0.13
129	6	0.13	0.04	0.03
130	6	0.05	0.03	-0.13
131	6	0.17	0.04	-0.05
132	6	0.05	0.04	0.03
133	6	0.01	0.03	-0.05
134	6	0.13	0.03	-0.14
135	1	0.23	0.02	-0.04
136	1	0.01	0.04	0.09
137	1	-0.05	0.03	-0.05
138	1	0.17	0.03	-0.20
139	1	0.03	0.02	-0.19

TS1-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.904304	0.253754	0.050232
82	-1.418282	-1.265324	-0.751637
6	1.637130	2.372233	0.105625
6	2.383700	5.113897	-0.159470
6	2.143542	2.868147	-1.136732
6	1.506172	3.257831	1.210102
6	1.883833	4.612570	1.052702
6	2.510443	4.223398	-1.241584
1	1.786573	5.291567	1.898453
1	2.899813	4.590814	-2.188508
6	-3.281840	-0.066858	-1.128369
6	-5.976349	0.891317	-1.049042
6	-3.557639	1.308940	-0.835446
6	-4.377118	-0.931152	-1.474152
6	-5.695286	-0.436588	-1.413977
6	-4.896410	1.754033	-0.796020
1	-6.516071	-1.108905	-1.657070
1	-5.111158	2.789891	-0.549343
6	2.693956	-1.061337	-0.352778
6	4.946606	-2.775219	-0.787593
6	3.792370	-1.068528	0.560180
6	2.747538	-1.916176	-1.498070
6	3.870033	-2.752465	-1.686313
6	4.893021	-1.918922	0.327004
1	3.904459	-3.407538	-2.555313
1	5.719373	-1.914694	1.034787
6	0.983077	2.819435	2.585286
1	0.736435	1.750951	2.537869
6	2.060528	2.978134	3.690288
1	2.981364	2.445383	3.427281
1	1.690427	2.572534	4.641746

1	2.314164	4.034283	3.850611
6	-0.310778	3.573764	2.986360
1	-1.136653	3.333527	2.309307
1	-0.161264	4.661289	2.968608
1	-0.619390	3.292285	4.000684
6	2.352745	1.976268	-2.373443
1	1.844342	1.014788	-2.208080
6	1.739128	2.563242	-3.670180
1	1.819353	1.833292	-4.487593
1	2.262883	3.472316	-3.991166
1	0.680473	2.812433	-3.536564
6	3.857463	1.657209	-2.576410
1	4.004170	1.026067	-3.463059
1	4.267721	1.123636	-1.712117
1	4.432461	2.581293	-2.717789
6	2.788134	6.579845	-0.300316
1	2.586116	7.076540	0.660364
6	4.306097	6.713949	-0.588634
1	4.565927	6.244635	-1.546853
1	4.898330	6.223517	0.194308
1	4.603338	7.769886	-0.638461
6	1.949659	7.302440	-1.386438
1	2.118970	6.858340	-2.376365
1	2.221200	8.364995	-1.444308
1	0.876475	7.231725	-1.167841
6	3.841762	-0.165376	1.801511
1	2.887122	0.369128	1.882487
6	4.000401	-0.969611	3.116615
1	4.953753	-1.512849	3.147739
1	3.186385	-1.694188	3.235263
1	3.971316	-0.291102	3.979790
6	4.947134	0.913527	1.664591
1	5.937844	0.455335	1.548396
1	4.974505	1.552624	2.557390
1	4.762438	1.555043	0.794414
6	1.642906	-2.019940	-2.566081
1	0.873868	-1.266088	-2.340934
6	0.960718	-3.415045	-2.544417
1	0.140499	-3.458426	-3.275889
1	0.553296	-3.649899	-1.554425
1	1.679144	-4.202732	-2.804697
6	2.146412	-1.703065	-3.998843
1	1.306359	-1.723628	-4.707359
1	2.882468	-2.443130	-4.337197
1	2.615804	-0.714385	-4.050044
6	-4.251110	-2.393187	-1.979006
1	-5.259754	-2.646868	-2.331705
6	-3.340714	-2.534088	-3.230399
1	-3.394901	-3.556651	-3.627910
1	-2.277778	-2.338930	-3.018550
1	-3.648362	-1.834205	-4.017264
6	-3.929743	-3.475201	-0.901970
1	-4.193159	-4.469282	-1.288433
1	-4.503771	-3.302829	0.016842
1	-2.869361	-3.520765	-0.627138
6	-2.432270	2.336398	-0.614552
1	-1.651672	1.860269	-0.005145
6	-1.784498	2.729363	-1.970811
1	-1.385999	1.851919	-2.493918
1	-0.961418	3.437052	-1.806234
1	-2.525989	3.206454	-2.626204
6	-2.858629	3.627249	0.125009
1	-3.347832	3.411613	1.083157
1	-3.542725	4.235020	-0.482577
1	-1.973273	4.243733	0.323776
6	-7.417623	1.381237	-0.959097
1	-7.396627	2.436695	-0.650110
6	-8.210216	0.591452	0.114577
1	-7.737238	0.688524	1.100697

1	-8.250551	-0.477811	-0.131905
1	-9.241788	0.959544	0.188882
6	-8.110941	1.305447	-2.343677
1	-8.159959	0.268180	-2.700420
1	-7.554421	1.887707	-3.089172
1	-9.135783	1.695132	-2.292259
6	6.128187	-3.712340	-1.021313
1	5.932823	-4.264348	-1.953071
6	7.448224	-2.924023	-1.214289
1	7.359447	-2.211701	-2.044625
1	8.281643	-3.605359	-1.431067
1	7.703362	-2.354457	-0.311074
6	6.253124	-4.754060	0.120186
1	5.324193	-5.328660	0.229034
1	6.455417	-4.263369	1.081207
1	7.072379	-5.457052	-0.080856
15	0.118872	-0.946007	2.612388
6	-0.176625	-2.794062	2.301681
6	-0.429359	-5.613693	1.946360
6	-1.283232	-3.501124	2.835416
6	0.816534	-3.536861	1.612467
6	0.688524	-4.926015	1.434171
6	-1.409319	-4.891133	2.654435
1	-2.046683	-2.971548	3.396967
1	1.690044	-3.033854	1.206978
1	1.463492	-5.467453	0.895417
1	-2.271897	-5.407016	3.072028
1	-0.529573	-6.687433	1.805683
6	-1.596849	-0.316172	3.133088
6	-4.065795	0.761360	4.079059
6	-2.824061	-0.607937	2.490165
6	-1.642684	0.521566	4.274229
6	-2.859543	1.056783	4.741015
6	-4.042996	-0.079398	2.949175
1	-2.846411	-1.271849	1.628473
1	-0.720333	0.740709	4.806691
1	-2.863461	1.696832	5.620573
1	-4.962257	-0.314232	2.417605
1	-5.006127	1.175816	4.435244

1				
A				
Frequencies	--	-38.9966		
Red. masses	--	10.5073		
Frc consts	--	0.0094		
IR Inten	--	1.9106		
Atom AN		X	Y	Z
1	82	-0.03	-0.04	0.11
2	82	-0.02	0.00	-0.07
3	6	-0.05	-0.02	0.03
4	6	-0.03	-0.03	-0.01
5	6	-0.04	-0.04	0.02
6	6	-0.05	0.00	0.01
7	6	-0.04	-0.01	0.00
8	6	-0.03	-0.04	0.01
9	1	-0.03	0.00	-0.01
10	1	-0.03	-0.06	0.00
11	6	0.00	0.01	-0.08
12	6	0.00	0.01	0.00
13	6	0.00	0.00	-0.06
14	6	-0.01	0.01	-0.06
15	6	-0.01	0.01	-0.02
16	6	0.01	0.00	-0.02
17	1	-0.02	0.01	-0.01
18	1	0.01	0.00	-0.01
19	6	-0.01	0.00	0.02
20	6	0.00	0.02	-0.03
21	6	0.01	0.01	0.00

22	6	-0.02	0.01	0.02
23	6	-0.02	0.02	-0.01
24	6	0.01	0.02	-0.03
25	1	-0.03	0.02	-0.01
26	1	0.03	0.03	-0.04
27	6	-0.05	0.02	0.02
28	1	-0.08	0.03	0.03
29	6	-0.03	0.00	0.01
30	1	-0.05	-0.03	0.00
31	1	-0.03	0.02	0.02
32	1	0.00	0.00	0.00
33	6	-0.02	0.06	0.03
34	1	-0.03	0.08	0.03
35	1	0.01	0.05	0.03
36	1	-0.03	0.06	0.03
37	6	-0.04	-0.05	0.03
38	1	-0.03	-0.05	0.04
39	6	-0.02	-0.06	0.02
40	1	-0.02	-0.07	0.03
41	1	-0.02	-0.07	0.02
42	1	-0.02	-0.06	0.01
43	6	-0.03	-0.05	0.04
44	1	-0.03	-0.06	0.05
45	1	-0.03	-0.04	0.05
46	1	-0.04	-0.05	0.03
47	6	-0.02	-0.03	-0.02
48	1	-0.01	-0.02	-0.03
49	6	-0.01	-0.05	-0.02
50	1	-0.02	-0.06	-0.01
51	1	-0.02	-0.05	-0.01
52	1	-0.01	-0.05	-0.03
53	6	-0.01	-0.04	-0.03
54	1	-0.01	-0.05	-0.02
55	1	0.00	-0.04	-0.04
56	1	-0.01	-0.02	-0.03
57	6	0.03	0.02	-0.01
58	1	0.03	0.00	0.03
59	6	0.10	0.02	-0.01
60	1	0.11	0.05	-0.04
61	1	0.12	0.01	0.02
62	1	0.11	0.03	-0.01
63	6	0.01	0.04	-0.04
64	1	0.01	0.06	-0.07
65	1	0.02	0.04	-0.05
66	1	-0.03	0.03	-0.04
67	6	-0.04	0.00	0.03
68	1	-0.04	-0.01	0.05
69	6	-0.02	-0.01	0.05
70	1	-0.03	-0.03	0.06
71	1	0.00	-0.02	0.05
72	1	-0.01	0.00	0.04
73	6	-0.06	0.00	0.03
74	1	-0.07	-0.01	0.04
75	1	-0.06	0.01	0.01
76	1	-0.07	0.00	0.02
77	6	-0.03	0.01	-0.08
78	1	-0.03	0.03	-0.08
79	6	-0.03	0.01	-0.08
80	1	-0.04	0.02	-0.09
81	1	-0.03	-0.01	-0.07
82	1	-0.01	0.03	-0.07
83	6	-0.04	0.00	-0.09
84	1	-0.05	0.01	-0.10
85	1	-0.04	0.00	-0.09
86	1	-0.04	-0.01	-0.09
87	6	0.01	0.00	-0.07
88	1	0.02	-0.01	-0.09
89	6	-0.01	0.00	-0.08
90	1	-0.01	0.01	-0.08

91	1	-0.01	0.01	-0.09
92	1	-0.02	0.00	-0.07
93	6	0.03	-0.01	-0.06
94	1	0.04	-0.01	-0.05
95	1	0.02	0.00	-0.04
96	1	0.04	-0.01	-0.06
97	6	0.00	0.01	0.03
98	1	0.01	0.00	0.04
99	6	0.02	-0.01	0.03
100	1	0.03	-0.02	0.03
101	1	0.01	0.00	0.02
102	1	0.02	-0.01	0.05
103	6	-0.02	0.03	0.04
104	1	-0.03	0.03	0.03
105	1	-0.03	0.04	0.04
106	1	-0.02	0.03	0.06
107	6	0.00	0.03	-0.04
108	1	-0.01	0.03	-0.04
109	6	0.00	0.02	-0.04
110	1	-0.01	0.03	-0.04
111	1	0.00	0.02	-0.05
112	1	0.00	0.02	-0.04
113	6	0.00	0.02	-0.05
114	1	0.00	0.02	-0.05
115	1	0.01	0.01	-0.05
116	1	0.00	0.02	-0.06
117	15	0.17	0.03	0.13
118	6	0.10	0.05	0.03
119	6	0.00	0.07	-0.07
120	6	0.06	0.07	-0.02
121	6	0.09	0.04	0.03
122	6	0.04	0.05	-0.02
123	6	0.01	0.08	-0.07
124	1	0.07	0.08	-0.02
125	1	0.12	0.01	0.07
126	1	0.03	0.03	-0.02
127	1	-0.02	0.10	-0.11
128	1	-0.04	0.08	-0.11
129	6	0.14	0.05	0.03
130	6	0.08	0.05	-0.11
131	6	0.18	0.07	-0.06
132	6	0.07	0.03	0.04
133	6	0.04	0.03	-0.03
134	6	0.15	0.07	-0.13
135	1	0.22	0.07	-0.06
136	1	0.03	0.01	0.10
137	1	-0.01	0.01	-0.02
138	1	0.18	0.09	-0.20
139	1	0.06	0.04	-0.16

Int-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.508939	0.555526	-0.022116
6	-0.436612	-0.478409	-0.229490
6	-1.807336	-0.434425	-0.880912
6	-4.671873	-0.374025	-1.461771
6	-2.600355	-1.650814	-1.035240
6	-2.461775	0.752618	-1.445186
6	-3.856288	0.747317	-1.658619
6	-3.992222	-1.577173	-1.237974
1	-4.315625	1.665151	-2.013138
1	-4.562575	-2.500127	-1.268786
6	2.012230	0.152927	-0.070648
6	4.885845	-0.220843	-0.480597

6	2.967810	0.297422	1.012344
6	2.559651	-0.286103	-1.354160
6	3.958261	-0.451167	-1.500557
6	4.353081	0.140309	0.755366
1	4.330681	-0.762168	-2.473809
1	5.042146	0.294878	1.583774
6	0.211232	2.016158	0.320390
6	-0.049466	4.745804	1.294617
6	-0.753993	2.366896	1.352013
6	0.997086	3.105010	-0.223034
6	0.860651	4.410826	0.282154
6	-0.844167	3.706366	1.790213
1	1.478299	5.195259	-0.147711
1	-1.560106	3.940537	2.574115
15	0.237803	-1.926239	1.039650
6	1.970583	2.988823	-1.412191
1	1.977667	1.961693	-1.763033
6	3.427430	3.345861	-1.015989
1	3.778632	2.719749	-0.190634
1	3.511513	4.396805	-0.709042
1	4.099449	3.193011	-1.871430
6	1.527896	3.876667	-2.608541
1	0.499776	3.660992	-2.919379
1	2.188412	3.699428	-3.468635
1	1.584337	4.944589	-2.362824
6	-1.788371	2.010140	-2.044464
1	-0.722972	1.982109	-1.845875
6	-1.983498	1.993170	-3.592459
1	-1.671535	1.045011	-4.039060
1	-1.396455	2.800160	-4.053401
1	-3.035629	2.154644	-3.857177
6	-2.332482	3.363374	-1.516050
1	-2.244416	3.452492	-0.433120
1	-3.386403	3.505439	-1.787623
1	-1.767410	4.188668	-1.968737
6	-2.002741	-3.045291	-1.296742
1	-0.987963	-3.096471	-0.913240
6	-2.804985	-4.237977	-0.718888
1	-2.277865	-5.175976	-0.936651
1	-3.794035	-4.327691	-1.184010
1	-2.943396	-4.157446	0.363658
6	-1.898896	-3.220037	-2.844139
1	-1.373832	-4.154948	-3.083791
1	-1.351769	-2.391961	-3.306723
1	-2.898991	-3.259989	-3.295225
6	1.884627	-0.663465	-2.719180
1	2.679532	-0.458960	-3.449929
6	0.669315	0.088171	-3.281972
1	-0.253097	-0.159908	-2.764856
1	0.550252	-0.208320	-4.334497
1	0.802784	1.172447	-3.267572
6	1.632873	-2.193082	-2.811015
1	0.830482	-2.505606	-2.139800
1	2.528212	-2.766368	-2.548479
1	1.342676	-2.456792	-3.837784
6	-1.705870	1.419025	2.115144
1	-1.438310	0.389392	1.875983
6	-3.194624	1.640604	1.725652
1	-3.831849	0.961128	2.308947
1	-3.390187	1.468353	0.670323
1	-3.501521	2.667144	1.968545
6	-1.652726	1.576698	3.667151
1	-2.109737	0.691685	4.129875
1	-2.232843	2.449793	3.993954
1	-0.642182	1.682429	4.060107
6	2.786418	0.473189	2.548020
1	3.582389	1.173736	2.845608
6	3.102836	-0.881073	3.261076
1	3.120520	-0.728691	4.348857

1	4.072341	-1.292806	2.959180
1	2.326806	-1.617839	3.028996
6	1.489849	1.025052	3.126899
1	1.576915	1.047502	4.222506
1	0.647715	0.380172	2.874860
1	1.283315	2.039988	2.785328
6	-0.182733	6.170092	1.830073
1	-0.959011	6.157891	2.609683
6	-0.645043	7.159354	0.728399
1	0.098466	7.231264	-0.076558
1	-0.784398	8.165227	1.147142
1	-1.594211	6.837917	0.281282
6	1.132713	6.659209	2.490888
1	1.950217	6.703080	1.759060
1	1.442514	5.986358	3.300358
1	1.002637	7.666036	2.910409
6	-6.191093	-0.323779	-1.598775
1	-6.566133	-1.350644	-1.473023
6	-6.638573	0.167641	-3.000360
1	-6.320539	1.203368	-3.178523
1	-7.733002	0.135170	-3.087840
1	-6.210854	-0.457474	-3.794255
6	-6.829268	0.546676	-0.483891
1	-6.493353	1.589391	-0.559109
1	-6.554670	0.177119	0.512143
1	-7.924766	0.537279	-0.564991
6	6.391055	-0.361902	-0.696080
1	6.883770	-0.129742	0.259909
6	6.782588	-1.812077	-1.083013
1	6.319530	-2.106617	-2.033964
1	6.459974	-2.526544	-0.314536
1	7.871330	-1.900329	-1.197331
6	6.915663	0.649060	-1.748981
1	6.469967	0.460368	-2.734642
1	8.006192	0.567927	-1.851660
1	6.672491	1.679693	-1.461699
6	1.097444	-3.516668	0.389797
6	2.670805	-5.796981	-0.264913
6	0.499098	-4.782475	0.201392
6	2.504420	-3.422119	0.272411
6	3.282726	-4.546482	-0.057931
6	1.274514	-5.910536	-0.124676
1	-0.566987	-4.907033	0.341980
1	2.997870	-2.473310	0.453223
1	4.362468	-4.444568	-0.142327
1	0.788186	-6.874200	-0.260971
1	3.270854	-6.668858	-0.515978
6	-1.221896	-2.641827	2.022115
6	-3.122981	-3.612214	3.919349
6	-2.503653	-2.058966	2.133986
6	-0.905538	-3.711092	2.902555
6	-1.842950	-4.194544	3.830773
6	-3.442053	-2.540424	3.067559
1	-2.797684	-1.246910	1.483989
1	0.080248	-4.166883	2.872152
1	-1.570151	-5.019039	4.486004
1	-4.423843	-2.074788	3.120129
1	-3.849755	-3.983956	4.637865

Int-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	0.895911	0.189093	0.325738
14	-0.613310	-1.372193	-1.388178
6	-2.517839	-1.081254	-1.246114

6	-5.346759	-0.776188	-1.181052
6	-3.356169	-2.187553	-0.961032
6	-3.111393	0.136508	-1.652987
6	-4.518075	0.266123	-1.598457
6	-4.753145	-2.003793	-0.894813
1	-4.987921	1.196164	-1.906932
1	-5.401792	-2.845811	-0.666596
6	2.741558	0.477544	-0.103535
6	5.588211	0.863034	-0.569390
6	3.652214	0.852182	0.971658
6	3.320197	0.312376	-1.423684
6	4.724789	0.503924	-1.592653
6	5.037568	1.029356	0.689358
1	5.166910	0.353599	-2.578491
1	5.719747	1.292367	1.498999
6	-0.154808	1.786184	0.614402
6	-1.583155	4.255722	1.246682
6	-1.302485	1.811645	1.497533
6	0.215749	3.067921	0.037654
6	-0.496089	4.248732	0.389156
6	-1.971492	3.037099	1.777093
1	-0.182000	5.203852	-0.028496
1	-2.826928	3.036281	2.451394
15	0.610039	-1.900806	0.628695
6	1.356142	3.332006	-0.956649
1	1.771029	2.394096	-1.284380
6	2.501058	4.147195	-0.342017
1	2.890541	3.677929	0.563294
1	2.187914	5.162914	-0.078071
1	3.332453	4.233130	-1.050664
6	0.883166	4.018040	-2.251516
1	0.089891	3.439478	-2.732691
1	1.712243	4.098158	-2.963832
1	0.507664	5.032356	-2.086037
6	-2.296813	1.264032	-2.270546
1	-1.317886	1.275118	-1.796651
6	-2.107892	1.010741	-3.770369
1	-1.630690	0.043126	-3.958176
1	-1.476622	1.785939	-4.217855
1	-3.067524	1.011061	-4.300014
6	-2.884766	2.668414	-2.063429
1	-3.153453	2.837573	-1.016836
1	-3.779689	2.835277	-2.672892
1	-2.163410	3.437209	-2.355145
6	-2.800213	-3.602967	-0.908600
1	-1.769071	-3.548394	-0.568144
6	-3.533553	-4.544925	0.055913
1	-2.967279	-5.474293	0.183498
1	-4.524689	-4.827738	-0.314590
1	-3.659717	-4.085900	1.041921
6	-2.784802	-4.215673	-2.314286
1	-2.330682	-5.212356	-2.296618
1	-2.206940	-3.599890	-3.012163
1	-3.797815	-4.313359	-2.720939
6	2.673650	-0.083557	-2.770613
1	3.409758	0.182724	-3.545562
6	1.463278	0.692305	-3.267531
1	0.653076	0.728807	-2.550729
1	1.071091	0.257743	-4.193779
1	1.750289	1.720703	-3.502975
6	2.531719	-1.588537	-2.960697
1	1.689174	-1.984363	-2.407990
1	3.437197	-2.119849	-2.650673
1	2.357691	-1.828479	-4.016036
6	-1.899211	0.613066	2.245246
1	-1.445002	-0.296588	1.869401
6	-3.410809	0.440062	2.024727
1	-3.723365	-0.569045	2.315650
1	-3.682408	0.596940	0.983794

1	-4.003951	1.142608	2.620483
6	-1.659194	0.734397	3.759218
1	-2.055149	-0.140585	4.284329
1	-2.159261	1.610488	4.187494
1	-0.598419	0.828835	3.999321
6	3.387720	1.039007	2.486762
1	4.224908	1.644921	2.866222
6	3.496764	-0.291201	3.237232
1	3.401033	-0.140383	4.317995
1	4.465988	-0.769165	3.056294
1	2.721851	-0.992550	2.928077
6	2.191609	1.847654	2.974314
1	2.346487	2.150914	4.017299
1	1.275930	1.262790	2.972616
1	2.049653	2.762008	2.396598
6	-2.336524	5.524245	1.593310
1	-3.139803	5.273883	2.299026
6	-3.000817	6.135952	0.357003
1	-2.264075	6.465162	-0.383893
1	-3.604451	7.006546	0.635422
1	-3.662767	5.411470	-0.130420
6	-1.434013	6.545759	2.290278
1	-0.634686	6.904176	1.632612
1	-0.964665	6.110630	3.179680
1	-2.015546	7.417085	2.610500
6	-6.854056	-0.620479	-1.099626
1	-7.280527	-1.550599	-0.700865
6	-7.469973	-0.395820	-2.482424
1	-7.136772	0.546427	-2.931007
1	-8.562924	-0.364740	-2.416654
1	-7.198260	-1.205972	-3.168325
6	-7.254224	0.498558	-0.133887
1	-6.925683	1.482563	-0.485574
1	-6.816372	0.335135	0.857282
1	-8.342861	0.534729	-0.017794
6	7.075946	1.052975	-0.792136
1	7.537355	1.353487	0.158023
6	7.749225	-0.252472	-1.223753
1	7.388684	-0.596936	-2.199137
1	7.558371	-1.050190	-0.497106
1	8.833937	-0.119539	-1.298525
6	7.359435	2.172735	-1.797028
1	6.989282	1.929395	-2.798839
1	8.436822	2.353912	-1.876701
1	6.884168	3.109074	-1.483817
6	1.858257	-3.042781	0.078417
6	3.761842	-4.940103	-0.758644
6	3.187000	-2.958801	0.501799
6	1.498237	-4.104930	-0.765009
6	2.441078	-5.045509	-1.183202
6	4.134799	-3.895805	0.082890
1	3.509483	-2.158765	1.155628
1	0.474079	-4.190818	-1.118881
1	2.143290	-5.853676	-1.845378
1	5.165925	-3.805454	0.413888
1	4.499729	-5.666995	-1.085771
6	-0.155584	-2.591159	2.047115
6	-1.169375	-3.836486	4.381757
6	-0.778044	-3.842165	1.999780
6	0.015163	-2.022952	3.314124
6	-0.495508	-2.625733	4.468875
6	-1.299367	-4.453071	3.144757
1	-0.818206	-4.392846	1.066828
1	0.563040	-1.094242	3.426430
1	-0.357364	-2.149347	5.436025
1	-1.783334	-5.423087	3.067011
1	-1.565095	-4.310816	5.275094

Int-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.759354	0.386694	-0.141151
32	-0.794193	-1.400177	-1.555375
6	-2.763789	-0.934918	-1.230358
6	-5.607121	-0.512141	-1.293958
6	-3.668017	-1.947369	-0.780067
6	-3.318299	0.283091	-1.746176
6	-4.715119	0.471180	-1.762436
6	-5.060558	-1.713918	-0.815440
1	-5.115477	1.403490	-2.153086
1	-5.739012	-2.490125	-0.465770
6	2.807395	0.548187	-0.264706
6	5.675067	0.901620	-0.574593
6	3.671536	0.699658	0.880825
6	3.434820	0.547270	-1.571817
6	4.831678	0.731343	-1.681534
6	5.066734	0.875650	0.682022
1	5.268831	0.733775	-2.677885
1	5.698172	0.999052	1.561289
6	-0.088156	2.025056	0.773154
6	-1.401147	4.411607	1.735707
6	-1.167742	1.949565	1.712047
6	0.317832	3.333001	0.331080
6	-0.335200	4.481322	0.825905
6	-1.794707	3.135147	2.158480
1	0.002475	5.456534	0.482710
1	-2.615116	3.057559	2.868740
15	0.463891	-2.108404	0.671321
6	1.468193	3.601332	-0.653987
1	1.828906	2.652767	-1.053877
6	2.676940	4.261996	0.061244
1	3.043583	3.632896	0.880015
1	2.404029	5.240441	0.478187
1	3.504299	4.410542	-0.645684
6	1.025779	4.460668	-1.866958
1	0.184480	3.999227	-2.398148
1	1.859063	4.573305	-2.573960
1	0.716944	5.468042	-1.561565
6	-2.431211	1.371283	-2.365940
1	-1.415791	1.242099	-1.966457
6	-2.359839	1.196080	-3.909118
1	-2.010296	0.192511	-4.183842
1	-1.674186	1.931383	-4.352440
1	-3.351731	1.339780	-4.358227
6	-2.862570	2.814171	-2.007881
1	-2.923706	2.952736	-0.922221
1	-3.836163	3.069085	-2.446379
1	-2.131477	3.532925	-2.400200
6	-3.188467	-3.328912	-0.311647
1	-2.102191	-3.282144	-0.159689
6	-3.805067	-3.761414	1.042399
1	-3.373658	-4.716320	1.369168
1	-4.892060	-3.895492	0.969199
1	-3.605752	-3.017525	1.823126
6	-3.459865	-4.400929	-1.403193
1	-3.073906	-5.381472	-1.090216
1	-2.981755	-4.128864	-2.353121
1	-4.537144	-4.505212	-1.588329
6	2.787741	0.298033	-2.962245
1	3.570513	0.587442	-3.677448
6	1.574559	1.165388	-3.372261
1	0.689419	0.995724	-2.752669
1	1.293581	0.919861	-4.405666
1	1.822558	2.231850	-3.337723

6	2.551646	-1.214159	-3.219240
1	1.766615	-1.630429	-2.585258
1	3.470919	-1.784228	-3.036049
1	2.249368	-1.372618	-4.264093
6	-1.702335	0.653283	2.339320
1	-1.148516	-0.197390	1.922460
6	-3.205763	0.424118	2.032612
1	-3.525429	-0.549875	2.425654
1	-3.407941	0.439594	0.960097
1	-3.823794	1.194935	2.511660
6	-1.506098	0.648002	3.882306
1	-1.834266	-0.311662	4.300898
1	-2.108017	1.437807	4.348858
1	-0.462864	0.816840	4.170533
6	3.363409	0.633783	2.405270
1	4.157491	1.240832	2.862989
6	3.564489	-0.807191	2.956015
1	3.543368	-0.792853	4.054583
1	4.528522	-1.226204	2.642143
1	2.767190	-1.476505	2.616726
6	2.052498	1.213549	2.955887
1	2.119608	1.251333	4.052942
1	1.192894	0.591123	2.703165
1	1.853906	2.224667	2.592288
6	-2.105718	5.665359	2.253741
1	-2.906101	5.336605	2.933568
6	-2.770739	6.468587	1.105827
1	-2.019892	6.835023	0.393322
1	-3.308561	7.339242	1.505028
1	-3.484619	5.847062	0.550788
6	-1.144119	6.568049	3.070194
1	-0.326606	6.945020	2.441386
1	-0.697387	6.015494	3.906364
1	-1.681453	7.435230	3.477507
6	-7.120714	-0.295160	-1.314348
1	-7.589397	-1.201986	-0.903113
6	-7.658474	-0.108569	-2.757228
1	-7.237871	0.792801	-3.222304
1	-8.752156	-0.004452	-2.751657
1	-7.397170	-0.965755	-3.390563
6	-7.543817	0.894639	-0.413602
1	-7.118855	1.838374	-0.780266
1	-7.198959	0.750160	0.618044
1	-8.637329	1.000367	-0.401148
6	7.181290	1.108987	-0.725140
1	7.603672	1.206103	0.286350
6	7.863898	-0.108740	-1.400965
1	7.495727	-0.250671	-2.425610
1	7.667329	-1.032789	-0.842525
1	8.951193	0.038237	-1.451930
6	7.505157	2.417024	-1.493287
1	7.118754	2.377965	-2.520386
1	8.591033	2.573200	-1.548296
1	7.056776	3.287586	-0.998184
6	1.753195	-3.244492	-0.133342
6	3.608030	-5.049159	-1.297655
6	3.137122	-3.101791	0.100515
6	1.312467	-4.290935	-0.975618
6	2.229475	-5.191540	-1.548075
6	4.057767	-3.997430	-0.478187
1	3.504163	-2.289715	0.714761
1	0.254229	-4.391045	-1.205605
1	1.869000	-5.991721	-2.190515
1	5.121120	-3.868311	-0.289693
1	4.319887	-5.741260	-1.742089
6	0.040528	-3.053799	2.253948
6	-0.567275	-4.505520	4.615745
6	-0.307767	-4.423330	2.189051
6	0.082070	-2.424474	3.516233

6	-0.224004	-3.143258	4.688263
6	-0.603328	-5.143464	3.360042
1	-0.338319	-4.934416	1.231006
1	0.370477	-1.382288	3.593275
1	-0.182832	-2.640399	5.651840
1	-0.862866	-6.197490	3.290588
1	-0.798736	-5.062408	5.520677

Int-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.863568	0.380625	-0.183189
50	-1.020425	-1.579817	-1.671625
6	-3.065912	-0.847289	-1.203922
6	-5.840760	-0.115351	-1.073849
6	-4.021683	-1.706034	-0.580241
6	-3.532374	0.377958	-1.778685
6	-4.897921	0.722128	-1.700527
6	-5.381395	-1.325535	-0.526073
1	-5.232766	1.659219	-2.140657
1	-6.102950	-1.986321	-0.047972
6	3.094989	0.446363	-0.223562
6	5.972136	0.738477	-0.467302
6	3.932860	0.576696	0.939554
6	3.751059	0.417217	-1.512853
6	5.153278	0.574668	-1.595313
6	5.336096	0.724364	0.777390
1	5.614390	0.558770	-2.581041
1	5.949084	0.832079	1.671965
6	0.065275	2.224595	0.788911
6	-1.096879	4.692755	1.717571
6	-1.001969	2.222909	1.739263
6	0.542878	3.493630	0.320460
6	-0.037209	4.688967	0.795602
6	-1.557509	3.448828	2.173351
1	0.350216	5.638243	0.430917
1	-2.373728	3.431612	2.893252
15	0.344727	-2.252425	0.742695
6	1.696652	3.651049	-0.682432
1	2.017676	2.659606	-1.018362
6	2.941295	4.299863	-0.020935
1	3.298582	3.696156	0.821436
1	2.712668	5.306423	0.353019
1	3.760723	4.384142	-0.747292
6	1.274051	4.444796	-1.945692
1	0.420607	3.971765	-2.447322
1	2.106935	4.499490	-2.659781
1	0.985818	5.473301	-1.695389
6	-2.590441	1.317648	-2.546215
1	-1.554228	1.026876	-2.310036
6	-2.781351	1.160609	-4.079949
1	-2.631499	0.120537	-4.397773
1	-2.069357	1.793566	-4.627596
1	-3.796673	1.456043	-4.375798
6	-2.728686	2.803200	-2.129309
1	-2.574181	2.929966	-1.051689
1	-3.719225	3.201576	-2.384264
1	-1.984007	3.415951	-2.654978
6	-3.630281	-3.074856	-0.004897
1	-2.532370	-3.118949	0.054642
6	-4.152946	-3.303486	1.435568
1	-3.770617	-4.252054	1.833807
1	-5.249551	-3.345761	1.465295
1	-3.825380	-2.500333	2.106475
6	-4.095530	-4.222343	-0.942924

1	-3.771955	-5.198312	-0.554773
1	-3.686685	-4.099896	-1.954578
1	-5.190377	-4.236841	-1.025535
6	3.109209	0.148401	-2.900025
1	3.928080	0.310923	-3.614600
6	1.998046	1.116281	-3.379083
1	1.057831	1.014536	-2.823055
1	1.764580	0.901031	-4.431088
1	2.327209	2.159228	-3.314346
6	2.709927	-1.340224	-3.075325
1	1.894990	-1.639055	-2.411320
1	3.563222	-1.996466	-2.864979
1	2.378042	-1.523998	-4.106698
6	-1.593903	0.955740	2.372048
1	-1.085558	0.076987	1.947236
6	-3.107367	0.801341	2.072774
1	-3.482750	-0.141141	2.492013
1	-3.308097	0.796450	0.998637
1	-3.681044	1.620026	2.526721
6	-1.371917	0.935635	3.910223
1	-1.763174	0.004308	4.338879
1	-1.901621	1.770206	4.386468
1	-0.311882	1.024651	4.173996
6	3.557839	0.500923	2.444314
1	4.363928	1.047442	2.954471
6	3.634924	-0.960299	2.970744
1	3.568142	-0.968145	4.067563
1	4.579710	-1.439085	2.684604
1	2.807625	-1.565158	2.583963
6	2.254982	1.156704	2.927767
1	2.261732	1.192070	4.026600
1	1.370108	0.584590	2.633863
1	2.133050	2.177606	2.555774
6	-1.729351	5.993535	2.213513
1	-2.541714	5.722321	2.904419
6	-2.358661	6.807244	1.052835
1	-1.593665	7.123336	0.331330
1	-2.851645	7.710552	1.437175
1	-3.104163	6.211203	0.511467
6	-0.716065	6.860200	3.006072
1	0.118272	7.177617	2.366506
1	-0.296506	6.302563	3.852905
1	-1.202904	7.764560	3.395799
6	-7.319864	0.266017	-0.992505
1	-7.842378	-0.551520	-0.473202
6	-7.959462	0.406537	-2.398381
1	-7.493613	1.223560	-2.965172
1	-9.032745	0.625808	-2.314713
1	-7.840130	-0.516061	-2.980300
6	-7.535793	1.556900	-0.159795
1	-7.047638	2.418838	-0.633607
1	-7.119591	1.449316	0.849848
1	-8.606944	1.784382	-0.069693
6	7.485718	0.914860	-0.584278
1	7.885781	1.018461	0.435605
6	8.159957	-0.326239	-1.225546
1	7.812430	-0.476954	-2.256183
1	7.932610	-1.237504	-0.657899
1	9.250856	-0.201083	-1.253731
6	7.854843	2.204314	-1.363168
1	7.493905	2.157130	-2.399196
1	8.944669	2.338448	-1.392946
1	7.411484	3.090967	-0.892746
6	1.569078	-3.494445	-0.011842
6	3.348642	-5.420789	-1.103241
6	2.963137	-3.376338	0.177480
6	1.081961	-4.582461	-0.773348
6	1.960985	-5.541911	-1.309706
6	3.845884	-4.331378	-0.364090

1	3.365883	-2.537146	0.730897
1	0.015292	-4.674237	-0.966856
1	1.563790	-6.371399	-1.890409
1	4.916646	-4.219444	-0.209260
1	4.030962	-6.158614	-1.519473
6	-0.153983	-3.103294	2.357219
6	-0.902579	-4.360172	4.790544
6	-0.565367	-4.456648	2.373266
6	-0.118501	-2.392490	3.576656
6	-0.495381	-3.013489	4.783562
6	-0.930701	-5.080738	3.579820
1	-0.591483	-5.028940	1.450183
1	0.220676	-1.361875	3.591688
1	-0.458547	-2.448741	5.712515
1	-1.238229	-6.124201	3.573307
1	-1.188473	-4.842449	5.722417

Int-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	1.658746	0.065577	-0.244661
82	-1.881646	-0.951146	0.416618
6	-3.451303	-0.659909	-1.223195
6	-5.480347	-0.653592	-3.246870
6	-4.689538	-1.333153	-1.017102
6	-3.247297	0.026899	-2.454470
6	-4.258553	0.022106	-3.439866
6	-5.677275	-1.324715	-2.026496
1	-4.090201	0.553692	-4.375229
1	-6.620401	-1.844503	-1.861779
6	2.945496	-1.803511	0.069825
6	4.731631	-4.054071	0.340208
6	3.537759	-2.126455	1.326741
6	3.182679	-2.700590	-1.025750
6	4.071949	-3.785943	-0.875715
6	4.427161	-3.225568	1.429277
1	4.244545	-4.438606	-1.730702
1	4.888541	-3.436982	2.394745
6	3.101825	1.860293	-0.385327
6	4.614679	4.297050	-0.647628
6	2.543913	3.123003	0.002111
6	4.445291	1.846100	-0.886158
6	5.166928	3.053374	-1.005071
6	3.305801	4.306173	-0.140942
1	6.186116	3.018496	-1.385185
1	2.869347	5.258127	0.157250
15	-2.277342	1.303973	1.948149
6	5.182278	0.556306	-1.270388
1	4.473096	-0.273639	-1.224911
6	6.304699	0.228972	-0.248944
1	5.896124	0.124094	0.763431
1	7.064963	1.021224	-0.228469
1	6.799951	-0.715336	-0.512556
6	5.763383	0.603136	-2.707812
1	4.996488	0.876287	-3.444554
1	6.176303	-0.377120	-2.983502
1	6.575330	1.336923	-2.791249
6	-1.944467	0.781791	-2.748762
1	-1.294808	0.697768	-1.861682
6	-1.173103	0.156988	-3.940817
1	-0.961161	-0.904850	-3.761991
1	-0.220473	0.679499	-4.105389
1	-1.758041	0.229486	-4.866836
6	-2.182072	2.296233	-2.984031
1	-2.680528	2.759052	-2.123363

1	-2.810438	2.464675	-3.868201
1	-1.228571	2.816522	-3.146728
6	-4.983237	-2.087151	0.289105
1	-4.142251	-1.917649	0.991643
6	-6.244951	-1.550258	1.012349
1	-6.382930	-2.058857	1.976424
1	-7.145914	-1.727414	0.411172
1	-6.166373	-0.472305	1.192533
6	-5.075582	-3.619149	0.064903
1	-5.233097	-4.144335	1.016617
1	-4.161211	-4.009873	-0.399604
1	-5.915503	-3.862265	-0.598490
6	2.443511	-2.640442	-2.378737
1	2.969391	-3.341475	-3.043033
6	2.460497	-1.283526	-3.120646
1	1.797930	-0.525562	-2.663613
1	2.071829	-1.410907	-4.139828
1	3.468332	-0.866140	-3.188059
6	0.993184	-3.177794	-2.234083
1	0.395755	-2.544181	-1.564909
1	0.996086	-4.189304	-1.810744
1	0.489770	-3.211273	-3.210172
6	1.147806	3.279956	0.627920
1	0.643728	2.304186	0.655934
6	0.226184	4.213629	-0.197111
1	-0.776995	4.238805	0.247169
1	0.136100	3.865152	-1.234026
1	0.613060	5.240563	-0.222057
6	1.237179	3.762417	2.100350
1	0.235560	3.788353	2.547566
1	1.668257	4.770111	2.160879
1	1.870039	3.094048	2.699514
6	3.200941	-1.461177	2.676266
1	4.110243	-1.525833	3.293432
6	2.099289	-2.291594	3.396431
1	1.881272	-1.876047	4.389642
1	2.407460	-3.336523	3.517923
1	1.167403	-2.282663	2.814684
6	2.798794	0.024722	2.656110
1	2.759284	0.413481	3.682292
1	1.768600	0.168016	2.274325
1	3.494918	0.648580	2.087579
6	5.405869	5.597654	-0.795777
1	4.764762	6.416231	-0.435461
6	5.747853	5.894361	-2.279550
1	6.401846	5.117439	-2.697369
1	6.268916	6.857246	-2.370463
1	4.839701	5.934542	-2.894178
6	6.689933	5.595849	0.073807
1	7.383391	4.806785	-0.245797
1	6.451183	5.424819	1.131122
1	7.213832	6.557642	-0.010402
6	-6.568236	-0.658792	-4.322700
1	-7.406511	-1.260941	-3.941179
6	-6.080644	-1.324580	-5.635988
1	-5.251895	-0.759408	-6.082817
1	-6.894226	-1.365634	-6.372993
1	-5.728871	-2.347711	-5.452982
6	-7.110934	0.767773	-4.599302
1	-6.322594	1.420551	-4.997053
1	-7.496414	1.227992	-3.680833
1	-7.924658	0.735766	-5.336653
6	5.726187	-5.206968	0.480703
1	6.065427	-5.222938	1.527447
6	5.071779	-6.580973	0.183438
1	4.727159	-6.639761	-0.857465
1	4.205868	-6.755509	0.834437
1	5.792483	-7.394370	0.343533
6	6.977955	-4.990188	-0.409864

1	6.706894	-4.972231	-1.473941
1	7.704398	-5.800792	-0.261158
1	7.470794	-4.038761	-0.172858
6	-2.193664	0.450629	3.641746
6	-1.891771	-0.850028	6.157041
6	-1.011209	0.603492	4.403860
6	-3.224681	-0.366649	4.167213
6	-3.078445	-1.005700	5.412184
6	-0.857757	-0.043098	5.646666
1	-0.217751	1.247551	4.030610
1	-4.148349	-0.494773	3.606635
1	-3.885269	-1.626112	5.796850
1	0.058621	0.094845	6.217093
1	-1.778353	-1.345956	7.118367
6	-4.047882	1.956732	1.872567
6	-6.607430	3.196534	1.694761
6	-4.736732	2.375751	3.038404
6	-4.664482	2.178592	0.617273
6	-5.928446	2.791005	0.529665
6	-6.002655	2.984682	2.949398
1	-4.283619	2.236016	4.015992
1	-4.168470	1.860703	-0.295264
1	-6.380558	2.944053	-0.447975
1	-6.510190	3.298068	3.859613
1	-7.585009	3.668467	1.627215

TS2-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.390251	0.010583	0.441555
6	-0.652571	-1.118578	0.206106
1	-0.680297	-2.035617	1.166155
6	1.705433	0.064644	-0.547616
6	4.117301	0.274746	-2.188801
6	2.778829	1.001910	-0.234154
6	1.907261	-0.743833	-1.717445
6	3.089613	-0.617303	-2.483704
6	3.921478	1.074475	-1.058413
1	3.201250	-1.251549	-3.358684
1	4.688593	1.795828	-0.792930
6	-0.134036	1.519434	0.557792
6	-0.755256	4.362830	0.526871
6	-0.326366	2.265392	1.779973
6	-0.385635	2.235413	-0.672233
6	-0.672804	3.616244	-0.653603
6	-0.603437	3.650366	1.720656
1	-0.834293	4.116753	-1.604573
1	-0.707429	4.194134	2.656751
15	1.533927	-0.707412	2.064538
6	2.437065	-2.268000	1.446710
6	4.014327	-4.546989	0.808421
6	1.928737	-3.575441	1.622817
6	3.751902	-2.124047	0.943765
6	4.531127	-3.250213	0.624001
6	2.709043	-4.703909	1.309790
1	0.932002	-3.726736	2.021201
1	4.171576	-1.133856	0.801282
1	5.538836	-3.113088	0.238715
1	2.295945	-5.698737	1.461238
1	4.618802	-5.419111	0.569654
6	0.232146	-1.589508	3.084160
6	-1.828342	-2.916835	4.467828
6	-0.935633	-1.974438	2.424301
6	0.396905	-1.897098	4.452322
6	-0.632354	-2.576003	5.136012

6	-1.990125	-2.607353	3.099959
1	1.310708	-1.622653	4.976299
1	-0.505431	-2.835608	6.185410
1	-2.909404	-2.873906	2.583848
1	-2.624635	-3.427074	5.006013
6	-2.072066	-1.140982	-0.320599
6	-4.477862	-1.252976	-1.942721
6	-3.156811	-0.195691	-0.145030
6	-2.390330	-2.306004	-1.144993
6	-3.540019	-2.295890	-1.958972
6	-4.293643	-0.255167	-0.975139
1	-3.724700	-3.137409	-2.619590
1	-5.069183	0.493551	-0.840477
6	0.957064	-1.799058	-2.301622
1	0.051599	-1.809074	-1.699395
6	0.556779	-1.495844	-3.773092
1	1.417468	-1.550961	-4.451642
1	0.109846	-0.502696	-3.882336
1	-0.178186	-2.231682	-4.122151
6	1.609156	-3.205416	-2.211108
1	2.575712	-3.225779	-2.728778
1	0.971723	-3.962390	-2.678767
1	1.787501	-3.491928	-1.170367
6	2.863901	2.015286	0.934874
1	1.993278	1.915033	1.568443
6	4.103238	1.783157	1.841607
1	5.046465	1.903793	1.294609
1	4.091052	0.783409	2.289645
1	4.103533	2.518745	2.657982
6	2.875430	3.479658	0.417000
1	3.787223	3.698490	-0.154224
1	2.839750	4.174649	1.267011
1	2.013961	3.682536	-0.223952
6	5.372622	0.360837	-3.053044
1	5.257328	-0.364744	-3.872568
6	6.643455	-0.035339	-2.257043
1	7.528692	-0.020396	-2.907201
1	6.544268	-1.043619	-1.834587
1	6.823220	0.661653	-1.427755
6	5.538794	1.762706	-3.694449
1	6.418512	1.784892	-4.351979
1	5.673884	2.536161	-2.926903
1	4.656919	2.031020	-4.289741
6	-0.393969	1.620175	-2.087101
6	-1.759051	1.808746	-2.803041
1	-1.729032	1.318073	-3.786178
1	-1.987701	2.868644	-2.972910
1	-2.580485	1.368592	-2.232923
6	0.727911	2.218146	-2.978804
1	0.747646	1.715884	-3.954983
1	1.713779	2.109073	-2.519879
1	0.551717	3.286562	-3.161170
1	-0.232124	0.548076	-2.009446
6	-0.289285	1.720038	3.229727
1	-0.233133	0.634695	3.210782
6	-1.586865	2.051233	4.023472
1	-2.487741	1.724158	3.499287
1	-1.682156	3.126158	4.222652
1	-1.556440	1.538191	4.994298
6	0.918915	2.251008	4.051432
1	1.876284	1.911687	3.648501
1	0.848612	1.896169	5.088796
1	0.924458	3.349000	4.075238
6	-1.029899	5.865249	0.522089
1	-1.043425	6.202843	1.569620
6	0.090902	6.651166	-0.207055
1	0.149063	6.363639	-1.265277
1	1.070542	6.456545	0.247031
1	-0.102105	7.731689	-0.162629

6	-2.416242	6.196029	-0.090699
1	-2.460918	5.900964	-1.147540
1	-2.616161	7.274794	-0.035158
1	-3.219608	5.668670	0.438926
6	-1.620271	-3.641202	-1.104958
1	-0.593513	-3.452656	-0.793173
6	-1.605210	-4.412052	-2.451459
1	-0.891393	-5.243146	-2.390978
1	-1.318468	-3.775449	-3.294553
1	-2.585353	-4.851364	-2.678038
6	-2.258395	-4.574796	-0.033991
1	-1.760108	-5.554386	-0.053588
1	-3.325644	-4.733276	-0.240729
1	-2.158976	-4.168219	0.975606
6	-3.274167	0.772216	1.036886
1	-2.315218	0.807142	1.549131
6	-4.333705	0.223283	2.039698
1	-5.313523	0.125445	1.554248
1	-4.450814	0.918473	2.883250
1	-4.049654	-0.756117	2.441874
6	-3.677619	2.213201	0.635375
1	-4.710762	2.251574	0.264523
1	-3.019665	2.618308	-0.135514
1	-3.619407	2.875061	1.508052
6	-5.672195	-1.254663	-2.893810
1	-5.598565	-2.160188	-3.514356
6	-5.631091	-0.031160	-3.847210
1	-6.463849	-0.072147	-4.562187
1	-4.691869	-0.002628	-4.413706
1	-5.713156	0.909043	-3.286230
6	-7.023465	-1.318011	-2.135594
1	-7.859032	-1.373305	-2.846076
1	-7.172377	-0.425830	-1.513396
1	-7.069912	-2.197547	-1.481072

1				
A				
Frequencies	--	-1091.0935		
Red. masses	--	1.2779		
Frc consts	--	0.8964		
IR Inten	--	114.4451		
Atom AN		X	Y	Z
1	6	-0.02	0.01	-0.01
2	6	0.04	0.03	-0.13
3	1	-0.50	-0.03	0.85
4	6	0.00	0.00	0.00
5	6	0.00	0.00	0.00
6	6	0.00	0.00	0.00
7	6	0.00	0.00	0.00
8	6	0.00	0.00	0.00
9	6	0.00	0.00	0.00
10	1	0.00	0.00	0.00
11	1	0.00	0.00	0.00
12	6	0.01	0.01	0.00
13	6	0.00	0.00	0.00
14	6	0.00	0.00	0.00
15	6	0.00	0.00	0.00
16	6	0.00	0.00	0.00
17	6	0.00	0.00	0.00
18	1	0.00	0.00	0.00
19	1	0.00	0.00	0.00
20	15	0.00	0.00	0.00
21	6	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
26	6	0.00	0.00	0.00

27	1	0.00	0.00	-0.01
28	1	0.00	0.00	0.00
29	1	0.00	0.00	0.00
30	1	0.00	0.00	0.00
31	1	0.00	0.00	0.00
32	6	0.00	0.00	0.01
33	6	-0.01	0.01	0.01
34	6	0.02	-0.05	0.01
35	6	0.00	0.01	0.00
36	6	0.00	0.00	0.00
37	6	0.00	0.00	0.01
38	1	0.00	0.00	0.01
39	1	0.00	-0.01	0.00
40	1	0.02	-0.03	-0.01
41	1	0.00	0.00	0.01
42	6	0.01	0.01	0.01
43	6	0.00	0.00	0.00
44	6	-0.01	0.00	0.00
45	6	0.00	0.00	0.00
46	6	0.00	0.00	0.00
47	6	0.00	0.00	0.00
48	1	0.00	0.00	0.00
49	1	0.00	0.00	0.00
50	6	0.00	0.00	0.00
51	1	0.02	0.00	0.02
52	6	0.00	0.00	0.00
53	1	0.00	0.00	0.00
54	1	0.00	0.00	0.00
55	1	0.00	0.00	0.00
56	6	0.00	0.00	0.00
57	1	0.00	0.00	0.00
58	1	0.00	0.00	0.00
59	1	0.00	0.00	0.00
60	6	0.00	0.00	0.00
61	1	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	1	0.00	0.00	0.00
64	1	0.00	0.00	0.00
65	1	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	1	0.00	0.00	0.00
68	1	0.00	0.00	0.00
69	1	0.00	0.00	0.00
70	6	0.00	0.00	0.00
71	1	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	1	0.00	0.00	0.00
74	1	0.00	0.00	0.00
75	1	0.00	0.00	0.00
76	6	0.00	0.00	0.00
77	1	0.00	0.00	0.00
78	1	0.00	0.00	0.00
79	1	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	1	0.00	0.00	0.00
83	1	0.00	0.00	0.00
84	1	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	1	0.00	0.00	0.00
87	1	0.00	0.00	0.00
88	1	0.00	0.00	0.00
89	1	0.00	0.00	0.00
90	6	0.00	0.00	0.00
91	1	0.00	0.00	0.00
92	6	0.00	0.00	0.00
93	1	0.00	0.00	0.00
94	1	0.00	0.00	0.00

95	1	0.00	0.00	0.00
96	6	0.00	0.00	0.00
97	1	0.00	0.00	0.00
98	1	0.00	0.00	0.00
99	1	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	6	0.00	0.00	0.00
103	1	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	6	0.00	0.00	0.00
107	1	0.00	0.00	0.00
108	1	0.00	0.00	0.00
109	1	0.00	0.00	0.00
110	6	0.00	0.00	0.00
111	1	-0.01	0.03	0.02
112	6	0.00	0.00	0.00
113	1	0.00	0.00	0.00
114	1	0.00	0.00	0.00
115	1	0.00	0.00	0.00
116	6	0.00	0.00	0.00
117	1	0.00	0.00	0.00
118	1	0.00	0.00	0.00
119	1	0.00	0.00	0.00
120	6	0.00	0.00	0.00
121	1	0.00	0.00	0.00
122	6	0.00	0.00	0.00
123	1	0.00	0.00	0.00
124	1	0.00	0.00	0.00
125	1	0.00	0.00	0.00
126	6	0.00	0.00	0.00
127	1	0.00	0.00	0.00
128	1	0.00	0.00	0.00
129	1	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	1	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	6	0.00	0.00	0.00
137	1	0.00	0.00	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00

TS2-Si

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	14	0.726625	0.067919	0.459941
2	14	-0.970197	-1.573973	0.149190
3	1	-0.821497	-2.592180	1.410382
4	6	2.311460	0.010606	-0.685135
5	6	4.775133	-0.006539	-2.199181
6	6	3.430812	0.837150	-0.309584
7	6	2.462848	-0.806691	-1.851980
8	6	3.682668	-0.802348	-2.565149
9	6	4.617735	0.813554	-1.070664
10	1	3.779004	-1.440966	-3.440527
11	1	5.440167	1.456615	-0.766248
12	6	0.106999	1.916585	0.497246
13	6	-0.700419	4.684332	0.341912
14	6	-0.070485	2.703695	1.680197
15	6	-0.174587	2.545197	-0.766506
16	6	-0.556757	3.900678	-0.814349

17	6	-0.462903	4.057414	1.572704
18	1	-0.751572	4.350995	-1.785092
19	1	-0.582656	4.641721	2.483130
20	15	1.658804	-0.939502	2.464154
21	6	2.446939	-2.554266	1.827664
22	6	3.827306	-4.919945	1.063393
23	6	1.847848	-3.824986	1.982577
24	6	3.753575	-2.489097	1.289262
25	6	4.435254	-3.659581	0.908215
26	6	2.529837	-4.995819	1.604180
27	1	0.852086	-3.915324	2.404385
28	1	4.245119	-1.528623	1.166531
29	1	5.439324	-3.583754	0.497198
30	1	2.044677	-5.961441	1.730561
31	1	4.354793	-5.825409	0.772413
32	6	0.085004	-1.627496	3.250260
33	6	-2.145688	-2.782541	4.570084
34	6	-1.071625	-1.995648	2.509391
35	6	0.096158	-1.825113	4.648922
36	6	-1.002952	-2.412705	5.308522
37	6	-2.183572	-2.571422	3.176999
38	1	0.979543	-1.542451	5.218151
39	1	-0.957482	-2.593899	6.381374
40	1	-3.050366	-2.896544	2.604393
41	1	-2.989167	-3.250421	5.075113
42	6	-2.778846	-1.316356	-0.477174
43	6	-5.380669	-1.105695	-1.701052
44	6	-3.734728	-0.346283	-0.025295
45	6	-3.167152	-2.187633	-1.560905
46	6	-4.446970	-2.058842	-2.137707
47	6	-5.002347	-0.264971	-0.641997
48	1	-4.725456	-2.717962	-2.955827
49	1	-5.707710	0.480856	-0.283316
50	6	1.378317	-1.732905	-2.419157
51	1	0.443765	-1.546076	-1.878777
52	6	1.087300	-1.475424	-3.920996
53	1	1.941803	-1.744779	-4.554371
54	1	0.848563	-0.422427	-4.111049
55	1	0.233885	-2.084483	-4.245228
56	6	1.738798	-3.222293	-2.182887
57	1	2.672613	-3.484133	-2.697958
58	1	0.945199	-3.876873	-2.568333
59	1	1.870065	-3.433964	-1.117074
60	6	3.435014	1.808179	0.886763
61	1	2.510795	1.686710	1.454160
62	6	4.596236	1.532377	1.878151
63	1	5.577747	1.665469	1.406006
64	1	4.544192	0.514607	2.282064
65	1	4.539570	2.229343	2.725340
66	6	3.474378	3.283492	0.405388
67	1	4.388583	3.488735	-0.166958
68	1	3.454267	3.966795	1.265086
69	1	2.612996	3.514385	-0.230795
70	6	6.071918	-0.030000	-3.007594
71	1	5.942178	-0.763811	-3.817323
72	6	7.278619	-0.491373	-2.149726
73	1	8.187798	-0.551844	-2.763189
74	1	7.095128	-1.479282	-1.708356
75	1	7.473196	0.212765	-1.330033
76	6	6.360926	1.343599	-3.667862
77	1	7.265826	1.290898	-4.288416
78	1	6.518744	2.121772	-2.909396
79	1	5.524746	1.659863	-4.304115
80	6	-0.093921	1.823861	-2.123880
81	6	-1.460835	1.808916	-2.859390
82	1	-1.371175	1.263036	-3.808666
83	1	-1.804363	2.824937	-3.092585
84	1	-2.235375	1.317858	-2.259027
85	6	1.005213	2.438577	-3.030731

86	1	1.060370	1.900527	-3.986369
87	1	1.989487	2.383025	-2.552950
88	1	0.791093	3.491897	-3.254173
89	1	0.180508	0.778170	-1.958297
90	6	0.135122	2.181149	3.110829
91	1	0.469666	1.142659	3.066724
92	6	-1.186265	2.187793	3.923724
93	1	-1.952638	1.574777	3.439581
94	1	-1.582989	3.205667	4.033989
95	1	-1.013385	1.781958	4.929316
96	6	1.230114	2.970729	3.876655
97	1	2.181817	2.968856	3.334088
98	1	1.400654	2.518799	4.862776
99	1	0.933787	4.015978	4.033668
100	6	-1.101135	6.157752	0.269305
101	1	-1.170003	6.533241	1.301422
102	6	-0.028023	7.005140	-0.463897
103	1	0.074620	6.690872	-1.511116
104	1	0.953592	6.901348	0.015274
105	1	-0.304467	8.068314	-0.457592
106	6	-2.492431	6.348748	-0.389361
107	1	-2.484151	6.015472	-1.435641
108	1	-2.781910	7.408345	-0.377964
109	1	-3.263654	5.774894	0.139743
110	6	-2.263275	-3.305862	-2.112262
111	1	-1.223711	-3.047220	-1.884253
112	6	-2.362848	-3.497913	-3.646067
113	1	-1.567097	-4.174662	-3.985377
114	1	-2.254691	-2.545422	-4.180623
115	1	-3.318157	-3.947899	-3.946553
116	6	-2.551928	-4.642731	-1.379415
117	1	-1.901711	-5.440501	-1.763904
118	1	-3.596542	-4.950326	-1.521762
119	1	-2.366169	-4.543288	-0.302852
120	6	-3.472606	0.631646	1.125459
121	1	-2.442029	0.485998	1.469029
122	6	-4.418346	0.350513	2.324818
123	1	-5.468657	0.496971	2.039489
124	1	-4.200881	1.038043	3.152925
125	1	-4.306587	-0.674872	2.694414
126	6	-3.621558	2.108691	0.676578
127	1	-4.648379	2.327027	0.353438
128	1	-2.945705	2.346189	-0.150167
129	1	-3.381974	2.783519	1.507406
130	6	-6.748312	-0.995039	-2.375571
131	1	-6.810543	-1.797206	-3.126147
132	6	-6.906464	0.353680	-3.126936
133	1	-7.873164	0.392917	-3.647335
134	1	-6.110274	0.488750	-3.869899
135	1	-6.863621	1.201619	-2.430780
136	6	-7.911041	-1.205883	-1.372255
137	1	-8.877698	-1.179898	-1.893071
138	1	-7.921782	-0.419270	-0.606569
139	1	-7.821682	-2.172636	-0.860867

1				
A				
Frequencies	--	-529.6250		
Red. masses	--	2.9230		
Frc consts	--	0.4831		
IR Inten	--	241.2758		
Atom	AN	X	Y	Z
1	14	0.02	-0.02	0.00
2	14	-0.05	0.03	0.20
3	1	0.30	-0.51	-0.72
4	6	0.00	0.00	0.00
5	6	0.00	0.00	0.00
6	6	0.00	0.00	0.00

7	6	0.00	0.00	0.00
8	6	0.00	0.00	0.00
9	6	0.00	0.00	0.00
10	1	0.00	0.00	0.00
11	1	0.00	0.00	0.00
12	6	-0.02	-0.02	0.00
13	6	0.00	0.00	0.00
14	6	0.00	-0.01	0.00
15	6	0.00	-0.01	0.00
16	6	0.00	0.00	0.00
17	6	0.01	-0.01	0.00
18	1	0.01	0.00	0.00
19	1	0.01	-0.01	0.00
20	15	0.00	0.00	0.00
21	6	0.00	0.00	-0.01
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
26	6	0.00	0.00	0.00
27	1	0.01	0.00	0.02
28	1	0.00	0.00	0.00
29	1	0.00	0.00	0.00
30	1	0.00	0.00	0.01
31	1	0.00	0.00	0.00
32	6	-0.02	0.01	-0.05
33	6	0.03	-0.02	-0.06
34	6	-0.04	0.15	-0.14
35	6	0.00	-0.03	-0.04
36	6	0.00	-0.01	-0.02
37	6	0.02	0.03	-0.07
38	1	0.01	-0.03	-0.05
39	1	-0.01	0.02	-0.02
40	1	-0.04	0.09	-0.02
41	1	0.02	-0.02	-0.08
42	6	0.00	-0.04	0.00
43	6	0.00	0.00	0.00
44	6	0.02	-0.01	0.00
45	6	0.00	0.00	-0.01
46	6	0.00	0.00	0.00
47	6	0.01	0.00	0.00
48	1	0.00	0.00	0.00
49	1	0.02	0.00	0.00
50	6	0.00	0.00	0.00
51	1	0.00	0.02	-0.01
52	6	0.00	0.00	0.00
53	1	0.00	0.00	0.00
54	1	0.00	0.00	0.00
55	1	0.00	0.00	0.00
56	6	0.00	0.00	0.00
57	1	0.00	0.00	0.01
58	1	0.00	0.00	0.00
59	1	0.00	0.00	0.00
60	6	0.00	0.00	0.00
61	1	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	1	0.00	0.00	0.00
64	1	0.00	0.00	0.00
65	1	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	1	0.00	0.00	0.00
68	1	0.00	0.00	0.00
69	1	0.00	0.00	0.00
70	6	0.00	0.00	0.00
71	1	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	1	0.00	0.00	0.00
74	1	0.00	0.00	0.00
75	1	0.00	0.00	0.00

76	6	0.00	0.00	0.00
77	1	0.00	0.00	0.00
78	1	0.00	0.00	0.00
79	1	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	1	0.00	0.00	0.00
83	1	0.00	0.00	0.00
84	1	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	1	0.00	0.00	0.00
87	1	0.00	0.00	0.00
88	1	0.00	0.00	0.00
89	1	0.00	0.00	0.00
90	6	0.00	0.00	0.00
91	1	-0.01	0.00	0.01
92	6	0.00	0.00	0.00
93	1	0.00	0.00	0.00
94	1	0.00	0.00	0.00
95	1	0.00	0.00	0.00
96	6	0.00	0.00	0.00
97	1	0.00	0.00	0.00
98	1	0.00	0.00	0.00
99	1	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	6	0.00	0.00	0.00
103	1	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	6	0.00	0.00	0.00
107	1	0.00	0.00	0.00
108	1	0.00	0.00	0.00
109	1	0.00	0.00	0.00
110	6	0.00	0.00	0.01
111	1	0.01	0.02	0.00
112	6	0.01	0.00	0.00
113	1	0.01	0.00	0.00
114	1	0.00	0.00	0.00
115	1	0.01	0.00	0.01
116	6	0.00	0.00	0.00
117	1	0.01	0.00	0.01
118	1	0.01	0.00	-0.01
119	1	-0.01	-0.01	0.01
120	6	0.00	0.00	0.00
121	1	0.00	0.00	0.02
122	6	0.00	0.00	0.00
123	1	0.00	0.00	0.00
124	1	0.00	0.00	0.00
125	1	0.00	0.00	0.00
126	6	0.00	0.00	0.00
127	1	0.00	0.00	0.00
128	1	0.00	0.00	0.00
129	1	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	1	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	6	0.00	0.00	0.00
137	1	0.00	0.00	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00

TS2-Ge

S-

S68

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.785166	0.101428	0.460406
32	-1.025480	-1.589963	0.143607
1	-0.849485	-2.674776	1.373994
6	2.411471	0.017621	-0.731451
6	4.860610	-0.056687	-2.239553
6	3.543544	0.813725	-0.346366
6	2.530174	-0.798583	-1.899407
6	3.748335	-0.822441	-2.613863
6	4.729466	0.763549	-1.106496
1	3.829121	-1.457932	-3.493346
1	5.569929	1.381993	-0.799701
6	0.165698	2.023440	0.486729
6	-0.579651	4.796372	0.337130
6	0.002548	2.802200	1.673804
6	-0.096651	2.651176	-0.777568
6	-0.451295	4.014181	-0.822895
6	-0.359605	4.164462	1.569571
1	-0.634890	4.472097	-1.792330
1	-0.469615	4.750062	2.480601
15	1.661760	-0.973228	2.532444
6	2.409050	-2.593192	1.860018
6	3.726539	-4.974356	1.031321
6	1.792401	-3.855312	2.017413
6	3.702953	-2.545388	1.288084
6	4.353278	-3.723155	0.875696
6	2.442594	-5.033379	1.606325
1	0.807063	-3.930269	2.467365
1	4.210103	-1.593121	1.162246
1	5.347328	-3.660084	0.438459
1	1.943880	-5.991879	1.734548
1	4.229306	-5.885356	0.714748
6	0.022719	-1.599213	3.244707
6	-2.308793	-2.617452	4.505793
6	-1.132690	-1.909214	2.462165
6	-0.024618	-1.777651	4.645452
6	-1.174624	-2.292585	5.277968
6	-2.288005	-2.427118	3.111834
1	0.852086	-1.530633	5.240852
1	-1.176140	-2.451424	6.354933
1	-3.153927	-2.713504	2.517140
1	-3.194693	-3.028398	4.986805
6	-2.889486	-1.246002	-0.513626
6	-5.455676	-0.915032	-1.756365
6	-3.798170	-0.238954	-0.056492
6	-3.288469	-2.082022	-1.613978
6	-4.557006	-1.898459	-2.200863
6	-5.055191	-0.099575	-0.684943
1	-4.852853	-2.533707	-3.031978
1	-5.732697	0.672225	-0.326975
6	1.409855	-1.688493	-2.456517
1	0.486674	-1.466868	-1.910001
6	1.112729	-1.420312	-3.955281
1	1.954137	-1.711499	-4.596406
1	0.901000	-0.360631	-4.140688
1	0.239590	-2.005127	-4.273078
6	1.718148	-3.190456	-2.224262
1	2.635941	-3.486205	-2.749585
1	0.896203	-3.814433	-2.601448
1	1.853926	-3.409474	-1.160234
6	3.550878	1.772537	0.858811
1	2.616850	1.658606	1.415621
6	4.694047	1.467349	1.861378
1	5.682942	1.584966	1.400755
1	4.618007	0.447333	2.256111
1	4.640249	2.158294	2.713562
6	3.613394	3.252029	0.393974

1	4.532381	3.449999	-0.173075
1	3.599089	3.926317	1.260840
1	2.757315	3.502023	-0.242417
6	6.156974	-0.111190	-3.045543
1	6.009857	-0.837237	-3.859178
6	7.346405	-0.609341	-2.184582
1	8.257066	-0.691807	-2.792927
1	7.132694	-1.593869	-1.749144
1	7.554831	0.084706	-1.359742
6	6.480673	1.258547	-3.696947
1	7.385301	1.188809	-4.315886
1	6.654005	2.028171	-2.933187
1	5.652939	1.597773	-4.332547
6	-0.023425	1.921558	-2.130634
6	-1.389062	1.923266	-2.868738
1	-1.305546	1.374363	-3.816763
1	-1.717952	2.943620	-3.103977
1	-2.171789	1.444196	-2.268963
6	1.088260	2.511480	-3.038201
1	1.133226	1.969214	-3.991976
1	2.071011	2.436714	-2.559702
1	0.896015	3.568259	-3.264704
1	0.234502	0.871489	-1.958378
6	0.191587	2.254240	3.096209
1	0.496801	1.206671	3.034283
6	-1.131352	2.283288	3.905998
1	-1.912247	1.698222	3.409625
1	-1.501192	3.309513	4.031453
1	-0.972528	1.856367	4.905067
6	1.308241	3.000794	3.872722
1	2.260538	2.973679	3.331137
1	1.462624	2.533462	4.854235
1	1.044555	4.053324	4.039307
6	-0.944110	6.278938	0.265013
1	-1.009309	6.654841	1.297124
6	0.155170	7.098411	-0.461153
1	0.255943	6.781569	-1.507770
1	1.130763	6.968079	0.023884
1	-0.092774	8.168488	-0.455979
6	-2.326320	6.503809	-0.401461
1	-2.320171	6.169950	-1.447535
1	-2.590228	7.569973	-0.391794
1	-3.113982	5.948585	0.123344
6	-2.405480	-3.214799	-2.169597
1	-1.360353	-2.982678	-1.928708
6	-2.483965	-3.380070	-3.707044
1	-1.705141	-4.077901	-4.043005
1	-2.333695	-2.423094	-4.223095
1	-3.448570	-3.792176	-4.030646
6	-2.730580	-4.555356	-1.459189
1	-2.092915	-5.361889	-1.846200
1	-3.779805	-4.837646	-1.617894
1	-2.557367	-4.475659	-0.378746
6	-3.493731	0.721100	1.100503
1	-2.469875	0.530096	1.443082
6	-4.447882	0.475231	2.300561
1	-5.491605	0.668025	2.018746
1	-4.197707	1.147796	3.131943
1	-4.378479	-0.555504	2.664541
6	-3.577651	2.206408	0.661326
1	-4.593201	2.470822	0.337357
1	-2.889529	2.422131	-0.161490
1	-3.312129	2.864395	1.497959
6	-6.812141	-0.741702	-2.439207
1	-6.901508	-1.532854	-3.198663
6	-6.908299	0.620199	-3.176780
1	-7.867936	0.705774	-3.704513
1	-6.100566	0.729534	-3.911551
1	-6.835338	1.457987	-2.470859

6	-7.987912	-0.916122	-1.444479
1	-8.950251	-0.849367	-1.969498
1	-7.972394	-0.136137	-0.672088
1	-7.937145	-1.889631	-0.940521

1
A

Frequencies -- -925.6207
 Red. masses -- 1.1725
 Frc consts -- 0.5919
 IR Inten -- 894.0856

Atom	AN	X	Y	Z
1	32	0.00	0.00	0.00
2	32	0.01	-0.01	-0.03
3	1	-0.20	0.50	0.84
4	6	0.00	0.00	0.00
5	6	0.00	0.00	0.00
6	6	0.00	0.00	0.00
7	6	0.00	0.00	0.00
8	6	0.00	0.00	0.00
9	6	0.00	0.00	0.00
10	1	0.00	0.00	0.00
11	1	0.00	0.00	0.00
12	6	0.01	0.01	0.00
13	6	0.00	0.00	0.00
14	6	0.00	0.00	0.00
15	6	0.00	0.00	0.00
16	6	0.00	0.00	0.00
17	6	0.00	0.00	0.00
18	1	0.00	0.00	0.00
19	1	0.00	0.00	0.00
20	15	0.00	0.00	0.00
21	6	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
26	6	0.00	0.00	0.00
27	1	0.00	-0.01	0.00
28	1	0.00	0.00	0.00
29	1	0.00	0.00	0.00
30	1	0.00	0.00	0.00
31	1	0.00	0.00	0.00
32	6	0.01	0.00	0.01
33	6	-0.01	0.01	0.01
34	6	0.02	-0.08	0.03
35	6	0.00	0.01	0.00
36	6	0.00	0.00	0.00
37	6	-0.01	-0.01	0.02
38	1	0.00	0.01	0.00
39	1	0.01	-0.02	0.00
40	1	0.02	-0.05	-0.01
41	1	-0.01	0.01	0.01
42	6	-0.01	0.02	0.01
43	6	0.00	0.00	0.00
44	6	-0.01	0.00	0.00
45	6	0.00	0.00	0.00
46	6	0.00	0.00	0.00
47	6	-0.01	0.00	0.00
48	1	0.00	0.00	0.00
49	1	-0.01	0.00	0.00
50	6	0.00	0.00	0.00
51	1	0.00	-0.01	0.01
52	6	0.00	0.00	0.00
53	1	0.00	0.00	0.00
54	1	0.00	0.00	0.00
55	1	0.00	0.00	0.00
56	6	0.00	0.00	0.00

57	1	0.00	0.00	-0.01
58	1	0.00	0.00	0.00
59	1	0.00	0.00	0.00
60	6	0.00	0.00	0.00
61	1	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	1	0.00	0.00	0.00
64	1	0.00	0.00	0.00
65	1	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	1	0.00	0.00	0.00
68	1	0.00	0.00	0.00
69	1	0.00	0.00	0.00
70	6	0.00	0.00	0.00
71	1	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	1	0.00	0.00	0.00
74	1	0.00	0.00	0.00
75	1	0.00	0.00	0.00
76	6	0.00	0.00	0.00
77	1	0.00	0.00	0.00
78	1	0.00	0.00	0.00
79	1	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	1	0.00	0.00	0.00
83	1	0.00	0.00	0.00
84	1	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	1	0.00	0.00	0.00
87	1	0.00	0.00	0.00
88	1	0.00	0.00	0.00
89	1	0.00	0.00	0.00
90	6	0.00	0.00	0.00
91	1	0.00	0.00	0.00
92	6	0.00	0.00	0.00
93	1	0.00	0.00	0.00
94	1	0.00	0.00	0.00
95	1	0.00	0.00	0.00
96	6	0.00	0.00	0.00
97	1	0.00	0.00	0.00
98	1	0.00	0.00	0.00
99	1	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	6	0.00	0.00	0.00
103	1	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	6	0.00	0.00	0.00
107	1	0.00	0.00	0.00
108	1	0.00	0.00	0.00
109	1	0.00	0.00	0.00
110	6	0.00	0.00	0.00
111	1	-0.01	-0.01	0.01
112	6	0.00	0.00	0.00
113	1	0.00	0.00	0.00
114	1	0.00	0.00	0.00
115	1	0.00	0.00	-0.01
116	6	0.00	0.00	0.00
117	1	0.00	0.00	0.00
118	1	0.00	0.00	0.00
119	1	0.01	0.01	0.00
120	6	0.00	0.00	0.00
121	1	0.00	0.00	-0.01
122	6	0.00	0.00	0.00
123	1	0.00	0.00	0.00
124	1	0.00	0.00	0.00
125	1	0.00	0.00	0.00

126	6	0.00	0.00	0.00
127	1	0.00	0.00	0.00
128	1	0.00	0.00	0.00
129	1	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	1	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	6	0.00	0.00	0.00
137	1	0.00	0.00	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00

TS2-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.883147	0.112027	0.471740
50	-1.176701	-1.740002	0.122599
1	-0.974084	-2.938850	1.428035
6	2.621231	0.016638	-0.824094
6	5.040425	-0.085408	-2.352190
6	3.776986	0.755158	-0.414153
6	2.687917	-0.750930	-2.025715
6	3.896513	-0.791229	-2.754895
6	4.955783	0.693265	-1.183799
1	3.946577	-1.388309	-3.663678
1	5.823656	1.264982	-0.861610
6	0.249373	2.194906	0.537640
6	-0.412947	4.980985	0.479172
6	0.108373	2.931549	1.750553
6	0.006290	2.861827	-0.706261
6	-0.310651	4.234983	-0.708833
6	-0.213234	4.306976	1.694505
1	-0.481214	4.731183	-1.662072
1	-0.305967	4.867635	2.623409
15	1.664981	-1.154971	2.676605
6	2.354715	-2.749944	1.891144
6	3.570325	-5.099831	0.841651
6	1.717280	-4.006808	2.000075
6	3.621080	-2.693981	1.259390
6	4.220913	-3.855217	0.738475
6	2.316509	-5.168572	1.478680
1	0.753404	-4.087159	2.493667
1	4.146839	-1.747304	1.167836
1	5.191756	-3.783411	0.253075
1	1.800180	-6.122208	1.567164
1	4.031396	-5.997594	0.436186
6	-0.035080	-1.720881	3.323822
6	-2.442889	-2.565515	4.588243
6	-1.206337	-1.974317	2.534051
6	-0.110878	-1.873562	4.728986
6	-1.296301	-2.296018	5.362689
6	-2.391856	-2.413302	3.193464
1	0.772992	-1.671673	5.330132
1	-1.317106	-2.425833	6.442487
1	-3.269749	-2.663088	2.598311
1	-3.360787	-2.901652	5.066255
6	-3.136853	-1.176990	-0.622992
6	-5.633644	-0.574489	-1.880085
6	-3.956465	-0.115997	-0.129208
6	-3.564883	-1.906885	-1.780311
6	-4.804070	-1.595159	-2.375611
6	-5.187750	0.156829	-0.765608

1	-5.130851	-2.152409	-3.250483
1	-5.806358	0.965065	-0.381215
6	1.509690	-1.561109	-2.585761
1	0.613339	-1.304055	-2.007773
6	1.187528	-1.222552	-4.064524
1	2.000034	-1.523657	-4.737674
1	1.017387	-0.147758	-4.202353
1	0.281296	-1.756767	-4.381813
6	1.731725	-3.085748	-2.410939
1	2.615341	-3.419132	-2.971160
1	0.862020	-3.645265	-2.783129
1	1.881685	-3.349569	-1.358601
6	3.792020	1.662248	0.828916
1	2.845047	1.540875	1.372243
6	4.910729	1.293385	1.835671
1	5.907953	1.404165	1.391891
1	4.805893	0.260472	2.188657
1	4.859747	1.952304	2.712800
6	3.876468	3.159291	0.430181
1	4.803756	3.370039	-0.118200
1	3.858372	3.796268	1.324691
1	3.030377	3.445988	-0.204633
6	6.328849	-0.158510	-3.168639
1	6.150065	-0.845934	-4.008983
6	7.499375	-0.736559	-2.332415
1	8.405479	-0.831120	-2.945526
1	7.246556	-1.728089	-1.935481
1	7.735316	-0.084950	-1.480870
6	6.699905	1.222824	-3.767652
1	7.599850	1.145971	-4.392332
1	6.901174	1.955749	-2.975210
1	5.882601	1.614857	-4.386316
6	0.069150	2.156848	-2.072187
6	-1.290092	2.201547	-2.819644
1	-1.211358	1.672108	-3.779050
1	-1.596670	3.233560	-3.032879
1	-2.087034	1.725375	-2.235931
6	1.204451	2.726628	-2.961490
1	1.240649	2.198338	-3.923512
1	2.180011	2.612675	-2.475848
1	1.046521	3.792559	-3.170663
1	0.298338	1.094115	-1.914941
6	0.283524	2.301599	3.139100
1	0.551958	1.246612	3.011237
6	-1.035848	2.325232	3.954620
1	-1.834803	1.790406	3.428443
1	-1.375149	3.353711	4.135806
1	-0.889046	1.839450	4.928082
6	1.433296	2.959292	3.945146
1	2.379844	2.920309	3.392479
1	1.575296	2.435223	4.899319
1	1.215015	4.012100	4.166762
6	-0.721888	6.477650	0.450239
1	-0.778323	6.825914	1.492413
6	0.413821	7.272724	-0.246992
1	0.508518	6.980572	-1.301384
1	1.380378	7.089505	0.239116
1	0.209415	8.351378	-0.213610
6	-2.090015	6.774137	-0.216606
1	-2.090492	6.468396	-1.271270
1	-2.312779	7.848968	-0.179536
1	-2.901573	6.235670	0.289008
6	-2.726709	-3.045122	-2.391415
1	-1.672177	-2.868846	-2.126893
6	-2.771939	-3.108726	-3.937096
1	-2.024144	-3.827739	-4.298154
1	-2.552412	-2.130645	-4.384535
1	-3.749425	-3.441684	-4.308910
6	-3.107650	-4.413689	-1.769192

1	-2.485612	-5.215754	-2.189550
1	-4.161421	-4.651976	-1.963739
1	-2.955088	-4.404022	-0.682386
6	-3.568616	0.768816	1.064935
1	-2.554971	0.490450	1.384833
6	-4.516372	0.543052	2.272817
1	-5.548166	0.820570	2.018933
1	-4.202312	1.161018	3.124961
1	-4.513825	-0.504327	2.593815
6	-3.541616	2.274898	0.692021
1	-4.537310	2.631899	0.397180
1	-2.849838	2.474980	-0.132410
1	-3.213295	2.873126	1.551223
6	-6.969900	-0.269708	-2.555638
1	-7.109739	-1.009891	-3.357712
6	-6.969713	1.134196	-3.215799
1	-7.918619	1.315196	-3.738718
1	-6.152732	1.228095	-3.942573
1	-6.842175	1.924384	-2.464145
6	-8.156213	-0.420375	-1.569486
1	-9.112561	-0.267772	-2.087367
1	-8.091774	0.316732	-0.758406
1	-8.165143	-1.419296	-1.114959

		1		
		A		
Frequencies	--	-1197.1853		
Red. masses	--	1.0760		
Frc consts	--	0.9086		
IR Inten	--	1144.2840		
Atom AN		X	Y	Z
1	50	0.00	0.00	0.00
2	50	0.00	0.00	-0.01
3	1	-0.09	0.57	0.81
4	6	0.00	0.00	0.00
5	6	0.00	0.00	0.00
6	6	0.00	0.00	0.00
7	6	0.00	0.00	0.00
8	6	0.00	0.00	0.00
9	6	0.00	0.00	0.00
10	1	0.00	0.00	0.00
11	1	0.00	0.00	0.00
12	6	0.01	0.00	0.00
13	6	0.00	0.00	0.00
14	6	0.00	0.00	0.00
15	6	0.00	0.00	0.00
16	6	0.00	0.00	0.00
17	6	0.00	0.00	0.00
18	1	0.00	0.00	0.00
19	1	0.00	0.00	0.00
20	15	0.00	0.00	0.00
21	6	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
26	6	0.00	0.00	0.00
27	1	0.00	-0.01	0.00
28	1	0.00	0.00	0.00
29	1	0.00	0.00	0.00
30	1	0.00	0.00	0.00
31	1	0.00	0.00	0.00
32	6	0.01	0.00	0.01
33	6	-0.01	0.01	0.00
34	6	0.01	-0.07	0.00
35	6	0.00	0.01	0.00
36	6	0.00	0.00	0.00
37	6	-0.01	0.00	0.01

38	1	0.00	0.01	0.00
39	1	0.00	-0.01	0.00
40	1	0.01	-0.04	-0.01
41	1	0.00	0.01	0.00
42	6	0.00	0.01	0.01
43	6	0.00	0.00	0.00
44	6	0.00	0.00	0.00
45	6	0.00	0.00	0.00
46	6	0.00	0.00	0.00
47	6	0.00	0.00	0.00
48	1	0.00	0.00	0.00
49	1	0.00	0.00	0.00
50	6	0.00	0.00	0.00
51	1	0.00	-0.01	0.01
52	6	0.00	0.00	0.00
53	1	0.00	0.00	0.00
54	1	0.00	0.00	0.00
55	1	0.00	0.00	0.00
56	6	0.00	0.00	0.00
57	1	0.00	0.00	0.00
58	1	0.00	0.00	0.00
59	1	0.00	0.00	0.00
60	6	0.00	0.00	0.00
61	1	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	1	0.00	0.00	0.00
64	1	0.00	0.00	0.00
65	1	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	1	0.00	0.00	0.00
68	1	0.00	0.00	0.00
69	1	0.00	0.00	0.00
70	6	0.00	0.00	0.00
71	1	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	1	0.00	0.00	0.00
74	1	0.00	0.00	0.00
75	1	0.00	0.00	0.00
76	6	0.00	0.00	0.00
77	1	0.00	0.00	0.00
78	1	0.00	0.00	0.00
79	1	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	1	0.00	0.00	0.00
83	1	0.00	0.00	0.00
84	1	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	1	0.00	0.00	0.00
87	1	0.00	0.00	0.00
88	1	0.00	0.00	0.00
89	1	0.00	0.00	0.00
90	6	0.00	0.00	0.00
91	1	0.00	0.00	0.00
92	6	0.00	0.00	0.00
93	1	0.00	0.00	0.00
94	1	0.00	0.00	0.00
95	1	0.00	0.00	0.00
96	6	0.00	0.00	0.00
97	1	0.00	0.00	0.00
98	1	0.00	0.00	0.00
99	1	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	6	0.00	0.00	0.00
103	1	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	6	0.00	0.00	0.00

107	1	0.00	0.00	0.00
108	1	0.00	0.00	0.00
109	1	0.00	0.00	0.00
110	6	0.00	0.00	0.00
111	1	-0.01	-0.01	0.00
112	6	0.00	0.00	0.00
113	1	0.00	0.00	0.00
114	1	0.00	0.00	0.00
115	1	0.00	0.00	-0.01
116	6	0.00	0.00	0.00
117	1	0.00	0.00	0.00
118	1	0.00	0.00	0.00
119	1	0.01	0.01	0.00
120	6	0.00	0.00	0.00
121	1	0.00	0.00	-0.01
122	6	0.00	0.00	0.00
123	1	0.00	0.00	0.00
124	1	0.00	0.00	0.00
125	1	0.00	0.00	0.00
126	6	0.00	0.00	0.00
127	1	0.00	0.00	0.00
128	1	0.00	0.00	0.00
129	1	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	1	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	6	0.00	0.00	0.00
137	1	0.00	0.00	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00

TS2-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.895029	0.163928	0.485581
82	-1.170993	-1.686078	0.067222
1	-1.059681	-2.959449	1.305663
6	2.599337	0.070797	-0.893871
6	4.975567	-0.062937	-2.438689
6	3.761769	0.785352	-0.479273
6	2.616992	-0.680353	-2.102641
6	3.814802	-0.737820	-2.845422
6	4.927656	0.707805	-1.262844
1	3.844179	-1.322766	-3.762841
1	5.812123	1.255837	-0.945606
6	0.278877	2.289329	0.538463
6	-0.279458	5.076170	0.521383
6	0.178060	3.000332	1.765467
6	0.058080	2.964468	-0.700431
6	-0.208928	4.347655	-0.680236
6	-0.095867	4.385503	1.729784
1	-0.366478	4.864574	-1.624593
1	-0.162260	4.938525	2.665297
15	1.713133	-1.171361	2.667086
6	2.324903	-2.739811	1.776863
6	3.438860	-5.091365	0.623845
6	1.628752	-3.968846	1.818625
6	3.590180	-2.708377	1.139787
6	4.141599	-3.871989	0.571899
6	2.176392	-5.131180	1.246282
1	0.659631	-4.024880	2.304327
1	4.154305	-1.780812	1.084961

1	5.117774	-3.823667	0.094219
1	1.615521	-6.062230	1.289361
1	3.867183	-5.993080	0.192000
6	0.002266	-1.707326	3.304667
6	-2.393796	-2.576188	4.572994
6	-1.191710	-1.882226	2.532236
6	-0.045935	-1.936877	4.702106
6	-1.223665	-2.380131	5.333264
6	-2.371807	-2.327656	3.191362
1	0.855556	-1.790955	5.292667
1	-1.218496	-2.587936	6.400200
1	-3.269012	-2.515297	2.601387
1	-3.305173	-2.935177	5.046486
6	-3.128589	-0.955579	-0.663012
6	-5.593239	-0.283436	-1.901766
6	-3.901480	0.128374	-0.155121
6	-3.555130	-1.651680	-1.835778
6	-4.786032	-1.307623	-2.425237
6	-5.127450	0.434415	-0.786475
1	-5.126239	-1.842949	-3.308308
1	-5.727831	1.252277	-0.393656
6	1.404590	-1.448357	-2.652852
1	0.523907	-1.160678	-2.065165
6	1.072878	-1.092289	-4.125581
1	1.869949	-1.406879	-4.810537
1	0.923904	-0.013437	-4.253688
1	0.151013	-1.603766	-4.435343
6	1.576348	-2.981327	-2.490729
1	2.448347	-3.337472	-3.054449
1	0.689889	-3.510247	-2.869415
1	1.720327	-3.262374	-1.441686
6	3.795805	1.672886	0.778434
1	2.845306	1.570242	1.318264
6	4.896311	1.255522	1.784924
1	5.898360	1.332981	1.346056
1	4.749619	0.224382	2.128269
1	4.864169	1.906777	2.668707
6	3.909810	3.175046	0.409416
1	4.833455	3.379120	-0.146694
1	3.915264	3.791962	1.318182
1	3.060343	3.492776	-0.206070
6	6.255460	-0.157159	-3.258978
1	6.059041	-0.827878	-4.108484
6	7.403683	-0.777057	-2.423297
1	8.312471	-0.891347	-3.027847
1	7.115724	-1.764612	-2.039789
1	7.647586	-0.143461	-1.560566
6	6.647092	1.228039	-3.832458
1	7.541716	1.153230	-4.463804
1	6.859512	1.941330	-3.025210
1	5.829426	1.643012	-4.435954
6	0.090656	2.269185	-2.073523
6	-1.268812	2.367939	-2.815828
1	-1.207951	1.850667	-3.783390
1	-1.543686	3.411840	-3.013694
1	-2.078333	1.906578	-2.237864
6	1.239933	2.806912	-2.965588
1	1.243600	2.292948	-3.936212
1	2.215444	2.643968	-2.494360
1	1.124238	3.881387	-3.157433
1	0.282498	1.198772	-1.925868
6	0.351997	2.333644	3.137047
1	0.586379	1.273968	2.982332
6	-0.955706	2.372218	3.968812
1	-1.770377	1.862615	3.442578
1	-1.270987	3.404091	4.171529
1	-0.807582	1.864934	4.931003
6	1.531832	2.936389	3.941681
1	2.470938	2.874150	3.378544

1	1.665230	2.389468	4.884166
1	1.352819	3.991711	4.184481
6	-0.543484	6.579165	0.512754
1	-0.578393	6.916826	1.559127
6	0.609325	7.343529	-0.188859
1	0.682723	7.059035	-1.246998
1	1.573824	7.119442	0.284474
1	0.444003	8.427948	-0.141116
6	-1.911986	6.911893	-0.134556
1	-1.929454	6.618453	-1.192527
1	-2.116252	7.989258	-0.080563
1	-2.725936	6.378806	0.373289
6	-2.720327	-2.787134	-2.459328
1	-1.660237	-2.595027	-2.232082
6	-2.789977	-2.861306	-4.001878
1	-2.042111	-3.577849	-4.367953
1	-2.579813	-1.884518	-4.455975
1	-3.770403	-3.201229	-4.356431
6	-3.068437	-4.155502	-1.817948
1	-2.446767	-4.954158	-2.245153
1	-4.123691	-4.404584	-1.984074
1	-2.892267	-4.138492	-0.734754
6	-3.479263	0.995944	1.042736
1	-2.465108	0.699388	1.342645
6	-4.409189	0.773054	2.264899
1	-5.443527	1.053318	2.025428
1	-4.082235	1.392530	3.111225
1	-4.402311	-0.273456	2.587840
6	-3.438585	2.507889	0.691098
1	-4.432214	2.881306	0.409747
1	-2.750058	2.716363	-0.133480
1	-3.098787	3.089082	1.557972
6	-6.937752	0.034439	-2.547023
1	-7.096461	-0.697742	-3.352686
6	-6.938315	1.444007	-3.191364
1	-7.891677	1.638704	-3.700089
1	-6.128697	1.536760	-3.926783
1	-6.791839	2.224444	-2.433082
6	-8.096502	-0.128425	-1.531369
1	-9.068027	0.024847	-2.018782
1	-8.009222	0.598936	-0.713732
1	-8.086111	-1.132112	-1.087002

```

          1
          A
Frequencies -- -1237.1219
Red. masses  --   1.0625
Frc consts   --   0.9581
IR Inten     --  1081.0995
Atom AN      X      Y      Z
  1  82      0.00   0.00   0.00
  2  82      0.00   0.00   0.00
  3   1     -0.01   0.57   0.81
  4   6      0.00   0.00   0.00
  5   6      0.00   0.00   0.00
  6   6      0.00   0.00   0.00
  7   6      0.00   0.00   0.00
  8   6      0.00   0.00   0.00
  9   6      0.00   0.00   0.00
 10   1      0.00   0.00   0.00
 11   1      0.00   0.00   0.00
 12   6      0.01   0.00   0.00
 13   6      0.00   0.00   0.00
 14   6      0.00   0.00   0.00
 15   6      0.00   0.00   0.00
 16   6      0.00   0.00   0.00
 17   6      0.00   0.00   0.00
 18   1      0.00   0.00   0.00

```

19	1	0.00	0.00	0.00
20	15	0.00	0.00	0.00
21	6	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
26	6	0.00	0.00	0.00
27	1	0.00	-0.01	0.00
28	1	0.00	0.00	0.00
29	1	0.00	0.00	0.00
30	1	0.00	0.00	0.00
31	1	0.00	0.00	0.00
32	6	0.01	0.00	0.00
33	6	-0.01	0.01	0.00
34	6	0.01	-0.06	0.00
35	6	0.00	0.01	0.00
36	6	0.00	0.00	0.00
37	6	-0.01	0.00	0.01
38	1	0.00	0.01	-0.01
39	1	0.00	-0.01	0.00
40	1	0.01	-0.03	-0.01
41	1	0.00	0.00	0.00
42	6	0.00	0.01	0.01
43	6	0.00	0.00	0.00
44	6	0.00	0.00	0.00
45	6	0.00	0.00	0.00
46	6	0.00	0.00	0.00
47	6	0.00	0.00	0.00
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49	1	-0.01	0.00	0.00
50	6	0.00	0.00	0.00
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56	6	0.00	0.00	0.00
57	1	0.00	0.00	0.00
58	1	0.00	0.00	0.00
59	1	0.00	0.00	0.00
60	6	0.00	0.00	0.00
61	1	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	1	0.00	0.00	0.00
64	1	0.00	0.00	0.00
65	1	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	1	0.00	0.00	0.00
68	1	0.00	0.00	0.00
69	1	0.00	0.00	0.00
70	6	0.00	0.00	0.00
71	1	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	1	0.00	0.00	0.00
74	1	0.00	0.00	0.00
75	1	0.00	0.00	0.00
76	6	0.00	0.00	0.00
77	1	0.00	0.00	0.00
78	1	0.00	0.00	0.00
79	1	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	1	0.00	0.00	0.00
83	1	0.00	0.00	0.00
84	1	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	1	0.00	0.00	0.00

87	1	0.00	0.00	0.00
88	1	0.00	0.00	0.00
89	1	0.00	0.00	0.00
90	6	0.00	0.00	0.00
91	1	0.00	0.00	0.00
92	6	0.00	0.00	0.00
93	1	0.00	0.00	0.00
94	1	0.00	0.00	0.00
95	1	0.00	0.00	0.00
96	6	0.00	0.00	0.00
97	1	0.00	0.00	0.00
98	1	0.00	0.00	0.00
99	1	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	6	0.00	0.00	0.00
103	1	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	6	0.00	0.00	0.00
107	1	0.00	0.00	0.00
108	1	0.00	0.00	0.00
109	1	0.00	0.00	0.00
110	6	0.00	0.00	0.00
111	1	0.00	-0.01	0.00
112	6	0.00	0.00	0.00
113	1	0.00	0.00	0.00
114	1	0.00	0.00	0.00
115	1	0.00	0.00	0.00
116	6	0.00	0.00	0.00
117	1	0.00	0.00	0.00
118	1	0.00	0.00	0.00
119	1	0.01	0.01	0.00
120	6	0.00	0.00	0.00
121	1	0.00	0.00	-0.01
122	6	0.00	0.00	0.00
123	1	0.00	0.00	0.00
124	1	0.00	0.00	0.00
125	1	0.00	0.00	0.00
126	6	0.00	0.00	0.00
127	1	0.00	0.00	0.00
128	1	0.00	0.00	0.00
129	1	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	1	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	6	0.00	0.00	0.00
137	1	0.00	0.00	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00

Pro-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.474331	0.028765	0.540444
6	-0.774149	-1.109374	0.620584
1	-0.236764	-2.011542	0.313923
6	1.732060	-0.065461	-0.488836
6	4.176193	-0.125543	-2.108744
6	2.859844	0.833459	-0.242969
6	1.903637	-0.974165	-1.588278
6	3.102795	-0.980707	-2.341556

6	4.011715	0.776905	-1.053192
1	3.190093	-1.691312	-3.158416
1	4.813834	1.476809	-0.838634
6	-0.020960	1.545738	0.508456
6	-0.498273	4.406946	0.211455
6	-0.187992	2.412639	1.654219
6	-0.228110	2.161899	-0.785938
6	-0.441617	3.552241	-0.894413
6	-0.396700	3.797878	1.465338
1	-0.567839	3.972307	-1.888585
1	-0.482225	4.427939	2.347393
15	1.512240	-0.567637	2.209626
6	2.327624	-2.230067	1.722517
6	3.769287	-4.647360	1.293507
6	1.741705	-3.486318	2.004001
6	3.651975	-2.209791	1.223727
6	4.363546	-3.403338	1.007066
6	2.454730	-4.682635	1.793746
1	0.735552	-3.542148	2.407753
1	4.133772	-1.262993	1.003573
1	5.380115	-3.358809	0.622752
1	1.983147	-5.635445	2.024426
1	4.322063	-5.570571	1.134707
6	-0.014433	-1.252338	3.014835
6	-2.436011	-2.266656	3.958546
6	-1.085890	-1.393143	2.114305
6	-0.136919	-1.601174	4.369614
6	-1.357432	-2.111926	4.850103
6	-2.301420	-1.914238	2.602632
1	0.708773	-1.477388	5.042479
1	-1.465294	-2.384660	5.897136
1	-3.140585	-2.055771	1.931919
1	-3.383628	-2.663911	4.315717
6	-2.111277	-1.120759	-0.204044
6	-4.488687	-1.234387	-1.859987
6	-3.143792	-0.119575	-0.110136
6	-2.443926	-2.305065	-0.969205
6	-3.586736	-2.304126	-1.799094
6	-4.270129	-0.185998	-0.958890
1	-3.798330	-3.181128	-2.402240
1	-5.008531	0.607809	-0.890690
6	0.905524	-2.022058	-2.112476
1	-0.038766	-1.926268	-1.587983
6	0.568391	-1.831129	-3.619530
1	1.442342	-1.990822	-4.261927
1	0.178927	-0.829334	-3.824853
1	-0.197486	-2.555260	-3.923840
6	1.478071	-3.449107	-1.882132
1	2.445803	-3.562604	-2.384216
1	0.808121	-4.213196	-2.287975
1	1.642136	-3.653215	-0.818856
6	2.994821	1.936057	0.840441
1	2.117483	1.941584	1.472859
6	4.214085	1.715272	1.777689
1	5.166510	1.737390	1.233771
1	4.144389	0.760854	2.311146
1	4.248608	2.517097	2.528314
6	3.090317	3.349343	0.202502
1	4.017877	3.471228	-0.372196
1	3.084369	4.113537	0.991716
1	2.246855	3.543473	-0.464651
6	5.443874	-0.176299	-2.958140
1	5.300896	-0.960934	-3.716673
6	6.685172	-0.566311	-2.113561
1	7.576779	-0.648463	-2.749931
1	6.532398	-1.529636	-1.610018
1	6.891183	0.188208	-1.342695
6	5.689592	1.157586	-3.710174
1	6.576469	1.080641	-4.353846

1	5.856995	1.983814	-3.006553
1	4.829495	1.421067	-4.338497
6	-0.261006	1.432846	-2.147160
6	-1.609029	1.629238	-2.893498
1	-1.587830	1.067893	-3.838361
1	-1.789011	2.682609	-3.143780
1	-2.455353	1.265163	-2.306853
6	0.893657	1.902578	-3.074759
1	0.895677	1.322123	-4.006683
1	1.871375	1.788165	-2.600599
1	0.767851	2.958962	-3.346960
1	-0.157087	0.364551	-1.979397
6	-0.184980	2.014192	3.151065
1	-0.167841	0.933739	3.242905
6	-1.481658	2.463797	3.884853
1	-2.384603	2.116535	3.376023
1	-1.543700	3.555201	3.978287
1	-1.485225	2.045291	4.900363
6	1.036925	2.573709	3.930589
1	1.980693	2.159175	3.566901
1	0.948511	2.315314	4.994749
1	1.087899	3.667944	3.856004
6	-0.694168	5.915143	0.070341
1	-0.701136	6.343454	1.084240
6	0.473284	6.577270	-0.706943
1	0.527436	6.197669	-1.735947
1	1.437000	6.373941	-0.223537
1	0.335322	7.665946	-0.757451
6	-2.055051	6.261242	-0.589135
1	-2.103551	5.880141	-1.617880
1	-2.199710	7.349539	-0.627614
1	-2.890069	5.822016	-0.029006
6	-1.762885	-3.690918	-0.821591
1	-0.717794	-3.582309	-0.527069
6	-1.784746	-4.552087	-2.113076
1	-1.119152	-5.415530	-1.988337
1	-1.460940	-3.991649	-2.995875
1	-2.786770	-4.951224	-2.313389
6	-2.455655	-4.515821	0.303754
1	-2.032627	-5.529435	0.335086
1	-3.533142	-4.604046	0.110827
1	-2.318964	-4.065319	1.289606
6	-3.239021	0.981056	0.965597
1	-2.301813	1.015987	1.517233
6	-4.385493	0.659973	1.972154
1	-5.346477	0.570820	1.449732
1	-4.479513	1.476583	2.701095
1	-4.214100	-0.264054	2.528963
6	-3.517551	2.395146	0.394299
1	-4.534892	2.464943	-0.013290
1	-2.812712	2.668972	-0.390318
1	-3.436529	3.140248	1.195300
6	-5.677662	-1.253436	-2.819603
1	-5.644840	-2.208412	-3.365566
6	-5.573085	-0.114066	-3.867440
1	-6.402338	-0.170932	-4.585704
1	-4.629610	-0.175282	-4.424281
1	-5.612837	0.870556	-3.382891
6	-7.035994	-1.190674	-2.074288
1	-7.869307	-1.261129	-2.786416
1	-7.145273	-0.245528	-1.526151
1	-7.130458	-2.011611	-1.352199

Pro-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

S-

S83

14	0.000000	0.000000	0.000000
14	0.000000	0.000000	2.360100
15	2.307808	0.000000	2.383060
6	2.579935	-0.834170	0.760855
6	1.659002	-0.868130	-0.249767
1	0.274583	1.299380	-0.336326
6	-0.392232	1.484251	3.501469
6	-0.890667	-1.517252	3.121381
6	2.689817	1.756665	1.950626
6	-1.364343	-0.636335	-1.165703
6	-0.868816	3.747976	5.328784
6	-0.055662	1.451978	4.932583
6	-1.003776	2.746017	3.075967
6	-1.209827	3.818514	3.971769
6	-0.300443	2.547596	5.785376
1	-1.655836	4.737551	3.597536
1	-0.035770	2.454718	6.836110
6	-2.452553	-3.682105	4.350677
6	-0.290259	-2.776315	3.563924
6	-2.340291	-1.451271	3.307696
6	-3.065696	-2.498009	3.910687
6	-1.070316	-3.797158	4.153482
1	-4.140329	-2.382289	4.032099
1	-0.576220	-4.712094	4.474519
6	3.519338	4.483131	1.430417
6	3.129008	2.200358	0.650016
6	2.689151	2.778211	2.968320
6	3.089401	4.102928	2.716512
6	3.537668	3.524705	0.399767
1	3.153615	1.478113	-0.160190
1	2.369848	2.506267	3.970020
1	3.069639	4.831267	3.524157
1	3.867963	3.803215	-0.598728
1	3.836614	5.505334	1.236588
6	3.260127	-2.028218	-1.781149
6	3.929247	-1.446113	0.483910
6	4.228686	-2.032194	-0.760371
6	1.995129	-1.458906	-1.543111
1	4.680529	-1.435696	1.270485
1	5.205705	-2.478915	-0.930717
1	1.254066	-1.459922	-2.339876
1	3.485192	-2.466870	-2.751009
6	-3.332987	-1.608891	-3.068913
6	-1.709719	-2.038686	-1.263811
6	-2.064899	0.259375	-2.066035
6	-3.012155	-0.245082	-2.982252
6	-2.668946	-2.484821	-2.197190
1	-3.517801	0.445635	-3.651443
1	-2.898415	-3.546626	-2.239379
6	-1.444250	2.991141	1.626617
1	-1.380139	2.043669	1.083582
6	-2.917857	3.464816	1.516646
1	-3.058054	4.460054	1.956291
1	-3.601615	2.774670	2.024573
1	-3.214355	3.527020	0.461756
6	-0.499594	4.001539	0.924127
1	-0.529987	4.975107	1.430850
1	-0.804203	4.156968	-0.119924
1	0.538349	3.653253	0.932684
6	0.562722	0.210821	5.602778
1	0.788451	-0.535822	4.839178
6	1.902904	0.522415	6.319729
1	1.772907	1.246992	7.133478
1	2.648281	0.921324	5.621685
1	2.316322	-0.396189	6.757551
6	-0.439389	-0.445289	6.590266
1	-0.708677	0.246457	7.399297
1	0.003720	-1.340983	7.045932

1	-1.359129	-0.746595	6.076878
6	-1.120106	4.928638	6.266343
1	-1.545137	5.744713	5.662776
6	0.194477	5.453450	6.899973
1	-0.004028	6.332505	7.527973
1	0.919578	5.739333	6.127434
1	0.661536	4.687694	7.533234
6	-2.156273	4.575584	7.365617
1	-2.365297	5.451438	7.994740
1	-1.783383	3.774903	8.018011
1	-3.101196	4.235380	6.923558
6	-3.167878	-0.234875	2.855367
6	-4.236364	-0.615167	1.795757
1	-4.788814	0.280745	1.480713
1	-4.965588	-1.330949	2.196438
1	-3.778020	-1.058903	0.904603
6	-3.828189	0.484252	4.061524
1	-4.397258	1.359946	3.722122
1	-3.075126	0.826649	4.779812
1	-4.525015	-0.182034	4.586611
1	-2.503995	0.490377	2.376123
6	1.208542	-3.089639	3.426992
1	1.719841	-2.223790	3.005211
6	1.465773	-4.273729	2.457800
1	1.067409	-4.064602	1.459626
1	1.002220	-5.199511	2.823408
1	2.544651	-4.452243	2.358837
6	1.882779	-3.370816	4.796561
1	1.731262	-2.542086	5.497031
1	2.963989	-3.506427	4.661373
1	1.485913	-4.282348	5.261859
6	-3.250464	-4.803776	5.014867
1	-2.548208	-5.620619	5.239779
6	-3.872990	-4.341956	6.358700
1	-4.601057	-3.535416	6.199554
1	-3.101883	-3.967601	7.043714
1	-4.395317	-5.174651	6.849078
6	-4.341692	-5.374696	4.072104
1	-5.092271	-4.611497	3.827266
1	-4.862476	-6.215474	4.550023
1	-3.904830	-5.730292	3.130382
6	-1.776735	1.770940	-2.129685
1	-1.406671	2.098704	-1.156038
6	-3.021858	2.641250	-2.434616
1	-2.772307	3.701549	-2.293778
1	-3.858928	2.394210	-1.769381
1	-3.365857	2.526738	-3.470299
6	-0.658464	2.060208	-3.168811
1	-0.429699	3.134109	-3.203937
1	-0.974242	1.743632	-4.172012
1	0.265614	1.524316	-2.920601
6	-1.068331	-3.126313	-0.386430
1	-0.364469	-2.654485	0.309624
6	-0.273128	-4.154855	-1.236539
1	-0.939937	-4.696910	-1.919708
1	0.207310	-4.896269	-0.584492
1	0.506812	-3.673994	-1.834097
6	-2.122428	-3.876868	0.468472
1	-2.836302	-4.416860	-0.167421
1	-2.683853	-3.192039	1.109557
1	-1.627229	-4.610976	1.115943
6	-4.379530	-2.104340	-4.067095
1	-4.701595	-1.238777	-4.665216
6	-5.634003	-2.660490	-3.342380
1	-6.397430	-2.965627	-4.070848
1	-6.073594	-1.905961	-2.677906
1	-5.380221	-3.537564	-2.732455
6	-3.798641	-3.156868	-5.046114
1	-4.555741	-3.455691	-5.783579

1	-3.477221	-4.060601	-4.511961
1	-2.930367	-2.758846	-5.586321

Pro-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.841563	0.101325	0.413642
32	-1.121286	-1.486083	0.300688
1	-0.563923	-2.827560	-0.219132
6	2.528016	-0.026953	-0.686464
6	5.025839	-0.186900	-2.105728
6	3.662373	0.752623	-0.276330
6	2.670913	-0.872918	-1.828521
6	3.911176	-0.939681	-2.501376
6	4.872474	0.659573	-0.994455
1	4.008637	-1.597438	-3.362858
1	5.715840	1.265824	-0.671495
6	0.241609	2.033116	0.435738
6	-0.560617	4.791593	0.232857
6	0.086509	2.840494	1.606171
6	-0.032732	2.635448	-0.839052
6	-0.414652	3.990310	-0.911961
6	-0.311114	4.190591	1.474582
1	-0.607461	4.424999	-1.890320
1	-0.423913	4.793010	2.374008
15	1.511934	-0.951249	2.569227
6	2.284475	-2.584244	1.959956
6	3.640241	-4.981798	1.250247
6	1.631633	-3.835207	2.040557
6	3.629092	-2.555139	1.516618
6	4.298626	-3.739887	1.161010
6	2.304621	-5.022371	1.692644
1	0.602571	-3.891415	2.381831
1	4.159400	-1.609539	1.449501
1	5.330640	-3.690783	0.820757
1	1.783269	-5.974312	1.767320
1	4.159230	-5.899535	0.982801
6	-0.206811	-1.564328	3.128062
6	-2.616551	-2.629616	4.164897
6	-1.304905	-1.799216	2.254005
6	-0.342513	-1.837254	4.509004
6	-1.537841	-2.367492	5.029534
6	-2.497089	-2.340208	2.792613
1	0.496162	-1.645511	5.174633
1	-1.621428	-2.577502	6.093513
1	-3.339247	-2.544561	2.134011
1	-3.541635	-3.049952	4.553870
6	-2.891068	-1.169233	-0.577961
6	-5.524907	-0.913815	-1.702184
6	-3.827333	-0.219432	-0.054096
6	-3.286265	-1.957231	-1.710324
6	-4.589543	-1.816364	-2.233575
6	-5.116075	-0.118339	-0.619857
1	-4.886515	-2.425322	-3.083868
1	-5.812249	0.605629	-0.202709
6	1.542911	-1.750468	-2.385999
1	0.616441	-1.483628	-1.866784
6	1.291493	-1.511387	-3.897999
1	2.145208	-1.835757	-4.505961
1	1.111397	-0.451108	-4.112086
1	0.414826	-2.082488	-4.229776
6	1.813878	-3.252615	-2.110722
1	2.729595	-3.581287	-2.620035
1	0.982454	-3.869115	-2.479347
1	1.938103	-3.447333	-1.040238

6	3.647355	1.735850	0.908082
1	2.691571	1.651239	1.432545
6	4.749775	1.430213	1.955513
1	5.756094	1.521276	1.527521
1	4.643337	0.419287	2.366657
1	4.679343	2.138183	2.792189
6	3.759378	3.202374	0.411962
1	4.700349	3.365791	-0.129618
1	3.733567	3.898316	1.261284
1	2.929933	3.455779	-0.257885
6	6.348358	-0.283647	-2.866490
1	6.213208	-1.022742	-3.670422
6	7.500737	-0.788201	-1.959442
1	8.427444	-0.898897	-2.538695
1	7.255931	-1.760356	-1.513044
1	7.698700	-0.082520	-1.141916
6	6.725513	1.064919	-3.533977
1	7.648237	0.960445	-4.120718
1	6.893399	1.845973	-2.780617
1	5.928494	1.410946	-4.204049
6	0.067429	1.883776	-2.177839
6	-1.287217	1.849975	-2.934145
1	-1.182694	1.283343	-3.869616
1	-1.628620	2.860047	-3.194343
1	-2.069996	1.370908	-2.334481
6	1.183978	2.476452	-3.077635
1	1.252753	1.920076	-4.021906
1	2.160041	2.425744	-2.581884
1	0.978753	3.526488	-3.323288
1	0.338820	0.840330	-1.984110
6	0.319094	2.345023	3.041335
1	0.710032	1.326115	3.008392
6	-1.002635	2.296857	3.852818
1	-1.737628	1.638875	3.376608
1	-1.448551	3.296046	3.947051
1	-0.813021	1.913513	4.864068
6	1.378457	3.190895	3.796755
1	2.323518	3.235462	3.243112
1	1.580914	2.746420	4.780167
1	1.034805	4.220600	3.959203
6	-0.970608	6.261257	0.139342
1	-1.045886	6.648937	1.166451
6	0.100502	7.106565	-0.598932
1	0.211490	6.779702	-1.641389
1	1.079952	7.015874	-0.112675
1	-0.183362	8.167710	-0.607624
6	-2.360680	6.434001	-0.526213
1	-2.346766	6.087993	-1.568235
1	-2.658220	7.491359	-0.528390
1	-3.129082	5.860625	0.007511
6	-2.371743	-2.998305	-2.380782
1	-1.331931	-2.750785	-2.148703
6	-2.477205	-3.013833	-3.927157
1	-1.700487	-3.668799	-4.344451
1	-2.342904	-2.009547	-4.348573
1	-3.444125	-3.400221	-4.272397
6	-2.648147	-4.415697	-1.809749
1	-1.978217	-5.156325	-2.267486
1	-3.683903	-4.718772	-2.013707
1	-2.495547	-4.444419	-0.724123
6	-3.507498	0.751427	1.093779
1	-2.491245	0.552468	1.455849
6	-4.471502	0.583183	2.298167
1	-5.502917	0.831640	2.016269
1	-4.179429	1.258047	3.113644
1	-4.462053	-0.439956	2.686316
6	-3.538388	2.223811	0.604866
1	-4.541111	2.499628	0.252596
1	-2.830668	2.391100	-0.212444

1	-3.268810	2.900746	1.424902
6	-6.928904	-0.802523	-2.297022
1	-6.989434	-1.512815	-3.135275
6	-7.204138	0.612948	-2.867897
1	-8.195665	0.652007	-3.338879
1	-6.454343	0.888881	-3.619961
1	-7.179736	1.371985	-2.074903
6	-8.019367	-1.202756	-1.269160
1	-9.015678	-1.167223	-1.730321
1	-8.022644	-0.519493	-0.409538
1	-7.851739	-2.218635	-0.889657

Pro-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.975862	0.105231	0.380996
50	-1.265152	-1.604315	0.127443
1	-0.779765	-3.113814	-0.539161
6	2.832343	-0.011722	-0.752149
6	5.333623	-0.100568	-2.156873
6	3.961837	0.737199	-0.287303
6	2.978579	-0.803674	-1.930390
6	4.222326	-0.833695	-2.600846
6	5.178862	0.681268	-0.998055
1	4.326271	-1.445294	-3.495548
1	6.024101	1.262191	-0.634846
6	0.354510	2.197483	0.501132
6	-0.512328	4.935711	0.458356
6	0.188765	2.928405	1.715876
6	0.070464	2.861230	-0.736709
6	-0.347928	4.207668	-0.733761
6	-0.240057	4.274703	1.666078
1	-0.553591	4.694185	-1.685195
1	-0.365354	4.822406	2.598596
15	1.478869	-1.173234	2.649114
6	2.238916	-2.779162	1.963954
6	3.569104	-5.149028	1.121499
6	1.563279	-4.020886	1.946857
6	3.593559	-2.746071	1.550643
6	4.250730	-3.916145	1.130799
6	2.223622	-5.194034	1.532287
1	0.526784	-4.080887	2.264741
1	4.141858	-1.807751	1.560385
1	5.290635	-3.863346	0.816063
1	1.684451	-6.139032	1.531854
1	4.077811	-6.055995	0.802682
6	-0.279325	-1.769208	3.128797
6	-2.713143	-2.790178	4.173333
6	-1.384560	-1.985148	2.252422
6	-0.424737	-2.043842	4.511566
6	-1.627702	-2.552018	5.035103
6	-2.587050	-2.501008	2.801502
1	0.417364	-1.867611	5.177088
1	-1.711127	-2.761513	6.099230
1	-3.441246	-2.685682	2.151226
1	-3.647324	-3.190139	4.562270
6	-3.187762	-1.083755	-0.734518
6	-5.834931	-0.639854	-1.751521
6	-4.088500	-0.190576	-0.069498
6	-3.612423	-1.692465	-1.957965
6	-4.927234	-1.472524	-2.425389
6	-5.385903	0.008122	-0.587204
1	-5.250726	-1.957765	-3.344456
1	-6.058375	0.687123	-0.067674
6	1.847610	-1.654417	-2.522857

1	0.932038	-1.449303	-1.954197
6	1.544141	-1.291807	-3.999966
1	2.390702	-1.531476	-4.655896
1	1.326984	-0.221957	-4.111848
1	0.674876	-1.858977	-4.359114
6	2.139896	-3.170385	-2.375386
1	3.040089	-3.452368	-2.937682
1	1.299624	-3.763187	-2.761443
1	2.299881	-3.444735	-1.326685
6	3.920872	1.638963	0.957546
1	2.947196	1.522309	1.450697
6	4.990797	1.251133	2.010851
1	6.008092	1.378662	1.619474
1	4.878824	0.208286	2.330975
1	4.893251	1.886927	2.900863
6	4.049469	3.136490	0.571841
1	5.007638	3.333931	0.073468
1	3.998054	3.770639	1.467073
1	3.242462	3.441089	-0.104583
6	6.660711	-0.155655	-2.914653
1	6.522654	-0.829572	-3.773326
6	7.798546	-0.744106	-2.040168
1	8.730221	-0.818120	-2.617295
1	7.539025	-1.746153	-1.675860
1	7.994622	-0.109143	-1.166055
6	7.060709	1.234659	-3.474162
1	7.986187	1.162593	-4.061389
1	7.233893	1.953027	-2.661887
1	6.273336	1.642434	-4.120531
6	0.204445	2.176985	-2.107100
6	-1.136948	2.151872	-2.885729
1	-1.013232	1.620029	-3.839187
1	-1.485602	3.166978	-3.114284
1	-1.924187	1.646713	-2.312823
6	1.329454	2.820692	-2.958639
1	1.423792	2.306479	-3.924554
1	2.295865	2.758624	-2.444898
1	1.116088	3.878425	-3.159965
1	0.493645	1.127355	-1.955770
6	0.437669	2.329482	3.106740
1	0.834410	1.316320	2.988600
6	-0.877845	2.205176	3.920238
1	-1.613147	1.586400	3.392126
1	-1.328353	3.190495	4.100009
1	-0.681346	1.738072	4.894074
6	1.500153	3.123629	3.910611
1	2.443047	3.199648	3.355349
1	1.705314	2.620661	4.864762
1	1.159242	4.142704	4.134702
6	-0.974374	6.393395	0.450033
1	-1.041569	6.724469	1.497273
6	0.046776	7.317199	-0.264021
1	0.148993	7.049258	-1.323965
1	1.039075	7.242908	0.198302
1	-0.279433	8.364878	-0.212788
6	-2.384798	6.546378	-0.177000
1	-2.381196	6.254363	-1.235540
1	-2.721953	7.590139	-0.118163
1	-3.118577	5.916863	0.342013
6	-2.705397	-2.587242	-2.818585
1	-1.682508	-2.529210	-2.430944
6	-2.636449	-2.110601	-4.293257
1	-1.911750	-2.718410	-4.852047
1	-2.325229	-1.059887	-4.355149
1	-3.605264	-2.204880	-4.799523
6	-3.134530	-4.075506	-2.738484
1	-2.462444	-4.705636	-3.336686
1	-4.155841	-4.211416	-3.118307
1	-3.109750	-4.437734	-1.703130

6	-3.694577	0.634912	1.165157
1	-2.707347	0.303679	1.514208
6	-4.673253	0.455195	2.353962
1	-5.668537	0.852996	2.117195
1	-4.301377	0.996163	3.234135
1	-4.784405	-0.599806	2.627091
6	-3.567367	2.137855	0.797777
1	-4.525539	2.533480	0.435847
1	-2.815702	2.296443	0.016800
1	-3.266087	2.723265	1.675611
6	-7.251463	-0.432292	-2.289302
1	-7.355893	-1.053016	-3.191822
6	-7.496879	1.041083	-2.708266
1	-8.501407	1.157891	-3.137025
1	-6.763014	1.367135	-3.456074
1	-7.419542	1.715904	-1.845513
6	-8.326129	-0.901625	-1.274554
1	-9.332794	-0.791740	-1.700113
1	-8.284907	-0.307782	-0.351944
1	-8.180571	-1.954641	-1.002408

Pro-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	1.023424	0.142017	0.363590
82	-1.317628	-1.527457	0.041214
1	-0.907649	-3.086605	-0.660433
6	2.932455	-0.005417	-0.804518
6	5.415392	-0.137810	-2.218907
6	4.074848	0.710759	-0.330026
6	3.044940	-0.788802	-1.988742
6	4.284164	-0.837625	-2.667918
6	5.287610	0.631381	-1.047931
1	4.368290	-1.439191	-3.571658
1	6.149513	1.184709	-0.680758
6	0.453499	2.312942	0.498102
6	-0.325658	5.067792	0.502500
6	0.312689	3.019427	1.727128
6	0.192917	2.996283	-0.730133
6	-0.184858	4.355558	-0.702625
6	-0.073735	4.379642	1.700046
1	-0.376692	4.864448	-1.645292
1	-0.181446	4.915911	2.641390
15	1.451288	-1.212640	2.665295
6	2.174075	-2.819481	1.951243
6	3.451504	-5.196762	1.051047
6	1.468891	-4.044003	1.898351
6	3.531249	-2.807611	1.543957
6	4.162734	-3.981363	1.096106
6	2.103039	-5.220792	1.454844
1	0.429464	-4.086459	2.209569
1	4.100341	-1.882096	1.580065
1	5.204965	-3.945269	0.786825
1	1.541788	-6.152408	1.426447
1	3.939712	-6.106771	0.709631
6	-0.333011	-1.766757	3.107907
6	-2.809372	-2.720200	4.118320
6	-1.432687	-1.947749	2.220383
6	-0.504900	-2.042010	4.488369
6	-1.728091	-2.517975	4.994677
6	-2.657937	-2.428236	2.749175
1	0.333587	-1.892210	5.165316
1	-1.830674	-2.729856	6.056619
1	-3.509842	-2.582110	2.087979
1	-3.759887	-3.094097	4.493625

6	-3.298873	-0.914832	-0.786047
6	-5.924628	-0.312234	-1.754008
6	-4.133238	0.013187	-0.088833
6	-3.767451	-1.485718	-2.008590
6	-5.075343	-1.185333	-2.452833
6	-5.425606	0.289590	-0.585019
1	-5.438268	-1.638779	-3.373499
1	-6.052955	0.995100	-0.044635
6	1.887909	-1.605396	-2.578025
1	0.987693	-1.399822	-1.985346
6	1.563049	-1.198973	-4.039154
1	2.395118	-1.432552	-4.715700
1	1.359861	-0.123407	-4.118237
1	0.679430	-1.744230	-4.397866
6	2.156409	-3.129426	-2.474962
1	3.036651	-3.414246	-3.066619
1	1.295816	-3.697149	-2.853694
1	2.336902	-3.431828	-1.437139
6	4.057727	1.597262	0.925676
1	3.079633	1.503535	1.414654
6	5.114682	1.163706	1.974342
1	6.135597	1.268173	1.585577
1	4.973639	0.119276	2.277822
1	5.034390	1.788438	2.873850
6	4.231285	3.095145	0.559526
1	5.196241	3.271217	0.066402
1	4.195148	3.718893	1.462769
1	3.435568	3.430983	-0.115523
6	6.739568	-0.226550	-2.979132
1	6.562903	-0.836578	-3.877652
6	7.830817	-0.942091	-2.140146
1	8.758818	-1.043854	-2.719010
1	7.501961	-1.944351	-1.837712
1	8.063225	-0.375520	-1.228628
6	7.233433	1.164985	-3.452029
1	8.154917	1.066931	-4.041691
1	7.450948	1.820212	-2.598288
1	6.478154	1.662568	-4.073342
6	0.305113	2.328117	-2.110084
6	-1.045964	2.330570	-2.872490
1	-0.940439	1.813910	-3.836456
1	-1.386510	3.353277	-3.078406
1	-1.831454	1.824114	-2.298044
6	1.427337	2.969512	-2.966987
1	1.510914	2.458891	-3.935849
1	2.397411	2.899559	-2.461060
1	1.219778	4.029493	-3.162435
1	0.583612	1.274123	-1.974570
6	0.547197	2.383712	3.103744
1	0.902172	1.357928	2.961255
6	-0.766058	2.294156	3.925246
1	-1.528480	1.715076	3.390590
1	-1.177044	3.292107	4.128261
1	-0.580599	1.800431	4.888037
6	1.645846	3.120990	3.913193
1	2.586984	3.170219	3.351750
1	1.838044	2.593886	4.856950
1	1.346278	4.148491	4.157074
6	-0.740387	6.539861	0.519131
1	-0.798765	6.854022	1.572070
6	0.312354	7.442155	-0.176387
1	0.407903	7.190186	-1.240886
1	1.300638	7.326380	0.286053
1	0.021026	8.499007	-0.106603
6	-2.143606	6.750920	-0.106849
1	-2.147565	6.479718	-1.170919
1	-2.446502	7.803845	-0.028302
1	-2.898908	6.136052	0.398728
6	-2.923922	-2.420319	-2.890377

1	-1.897061	-2.433275	-2.510024
6	-2.837409	-1.924652	-4.357847
1	-2.154789	-2.565471	-4.932605
1	-2.464363	-0.893451	-4.405508
1	-3.814268	-1.952149	-4.856670
6	-3.444639	-3.880298	-2.829372
1	-2.817423	-4.541022	-3.443160
1	-4.475325	-3.947490	-3.201868
1	-3.434088	-4.259431	-1.799769
6	-3.679462	0.790773	1.156161
1	-2.704886	0.403720	1.481283
6	-4.648782	0.628390	2.355128
1	-5.629460	1.072583	2.140914
1	-4.242160	1.133960	3.240995
1	-4.800591	-0.426827	2.607512
6	-3.486245	2.294270	0.820677
1	-4.429608	2.743714	0.483695
1	-2.740314	2.436091	0.030717
1	-3.143862	2.844606	1.706047
6	-7.333214	-0.012440	-2.269407
1	-7.485540	-0.609599	-3.181034
6	-7.495806	1.480048	-2.659941
1	-8.497922	1.664678	-3.070114
1	-6.755091	1.774344	-3.414146
1	-7.364244	2.133763	-1.787560
6	-8.421766	-0.435786	-1.249160
1	-9.425101	-0.259630	-1.660112
1	-8.335347	0.138072	-0.317056
1	-8.335009	-1.500164	-0.996906

TS-Pd-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.398329	-0.866062	0.303050
6	1.413607	0.562632	0.390718
6	2.373201	-1.659297	-0.644356
6	4.089680	-3.331676	-2.323572
6	2.503857	-1.445702	-2.068289
6	3.184488	-2.733716	-0.099920
6	3.998093	-3.518963	-0.943523
6	3.332534	-2.280644	-2.847787
1	4.581324	-4.319361	-0.495874
1	3.378170	-2.093703	-3.916303
6	2.426461	1.482250	-0.339802
6	4.460430	3.273330	-1.440191
6	3.835605	1.325440	-0.055601
6	2.065998	2.619425	-1.182571
6	3.095646	3.437408	-1.711653
6	4.787197	2.221466	-0.589806
1	2.801741	4.257951	-2.361982
1	5.831508	2.082568	-0.327668
6	0.525391	-1.860407	1.185484
6	-1.091023	-3.905927	2.534579
6	0.518797	-2.010559	2.641534
6	-0.256633	-2.850333	0.459377
6	-1.018431	-3.820456	1.141902
6	-0.317289	-2.982300	3.240632
1	-1.568998	-4.551168	0.554530
1	-0.313264	-3.045841	4.323261
6	3.266780	-3.175714	1.375325
1	2.695463	-2.479555	1.973898
6	2.647531	-4.589749	1.562003
1	1.629367	-4.642154	1.171112
1	2.615768	-4.854153	2.626795
1	3.253173	-5.348269	1.048503

6	4.707884	-3.191221	1.962877
1	5.071335	-2.182884	2.175696
1	5.427034	-3.679020	1.295848
1	4.713979	-3.747981	2.909120
6	1.805500	-0.361385	-2.906470
1	1.219906	0.275683	-2.246719
6	2.869237	0.509045	-3.635905
1	2.395028	1.344097	-4.163449
1	3.409831	-0.080341	-4.387185
1	3.603369	0.919184	-2.938259
6	0.834952	-0.949257	-3.967823
1	0.341448	-0.132097	-4.510775
1	0.054617	-1.569388	-3.516805
1	1.370882	-1.561528	-4.704899
6	4.968965	-4.220751	-3.199286
1	5.445031	-4.963888	-2.541793
6	4.132399	-4.996005	-4.250471
1	3.641509	-4.306886	-4.950588
1	3.351184	-5.596975	-3.768234
1	4.774107	-5.668479	-4.835794
6	6.101181	-3.413140	-3.886032
1	5.689938	-2.659782	-4.571135
1	6.750972	-4.079110	-4.469992
1	6.719273	-2.890251	-3.145354
6	1.415638	-1.335203	3.727786
1	2.084581	-0.614270	3.254818
6	0.571577	-0.587495	4.800805
1	-0.003211	-1.297961	5.408470
1	-0.126372	0.127479	4.366062
1	1.237343	-0.045919	5.487262
6	2.295951	-2.347710	4.526694
1	1.679343	-3.019605	5.136029
1	2.943425	-1.784233	5.213266
1	2.936104	-2.964297	3.898322
6	-0.313724	-3.024656	-1.075134
1	0.174808	-2.175368	-1.543587
6	-1.759657	-3.060769	-1.624807
1	-1.732858	-3.141839	-2.720345
1	-2.294213	-2.146526	-1.354872
1	-2.325282	-3.923013	-1.249617
6	0.413998	-4.320104	-1.534110
1	0.379426	-4.401033	-2.629085
1	-0.076300	-5.211637	-1.118520
1	1.461651	-4.336827	-1.229738
6	0.681324	3.190812	-1.624759
1	0.939536	4.189959	-2.002067
6	0.006749	2.492108	-2.831827
1	-0.797146	3.138839	-3.211198
1	-0.442365	1.530816	-2.548435
1	0.716697	2.333848	-3.649968
6	-0.346277	3.461993	-0.515998
1	-1.152851	4.090668	-0.918575
1	0.101263	3.998141	0.324809
1	-0.798944	2.536396	-0.141187
6	4.490340	0.240423	0.820439
1	3.739670	-0.489385	1.117453
6	5.597124	-0.493343	0.006574
1	5.217030	-0.847034	-0.956417
1	5.981896	-1.355457	0.556849
1	6.449278	0.169382	-0.186476
6	5.105172	0.821881	2.122720
1	4.346614	1.284994	2.759743
1	5.865186	1.582397	1.903502
1	5.593192	0.021191	2.696546
6	5.542410	4.177935	-2.027492
1	6.505061	3.839722	-1.614972
6	5.360175	5.661259	-1.616898
1	5.348991	5.768397	-0.524559
1	4.418985	6.070231	-2.007440

1	6.181940	6.273163	-2.013167
6	5.627486	4.037630	-3.570084
1	4.697109	4.369934	-4.049337
1	5.801284	2.993945	-3.861009
1	6.449546	4.647832	-3.968704
6	-1.875983	-5.032092	3.209572
1	-2.690771	-5.317625	2.525810
6	-0.973034	-6.285504	3.394272
1	-0.546915	-6.613165	2.437885
1	-1.548821	-7.119591	3.818910
1	-0.139633	-6.064953	4.074934
6	-2.516014	-4.632015	4.558902
1	-3.142256	-3.736959	4.457350
1	-1.753093	-4.426692	5.321830
1	-3.143006	-5.449904	4.938622
15	0.885956	1.328779	2.150664
6	-0.775052	2.205801	2.459813
6	-3.132153	3.268544	3.648945
6	-0.877287	3.581872	2.765836
6	-1.884396	1.371634	2.746583
6	-3.045866	1.896481	3.340145
6	-2.045480	4.109864	3.347748
1	-0.037173	4.244514	2.585620
1	-1.817112	0.305545	2.542123
1	-3.868469	1.229683	3.590590
1	-2.093461	5.172373	3.578054
1	-4.022807	3.670808	4.126521
6	2.065706	2.746726	2.656429
6	3.707174	4.737472	3.874064
6	2.585207	3.819775	1.901706
6	2.387275	2.695505	4.037360
6	3.191572	3.677792	4.643529
6	3.399084	4.800375	2.502626
1	2.376612	3.903239	0.844202
1	2.001431	1.882131	4.644531
1	3.417232	3.608976	5.705553
1	3.789604	5.612556	1.893172
1	4.337185	5.495989	4.333742
46	-1.070251	0.243710	-0.456705
15	-3.782738	0.495764	-1.080270
6	-4.621054	2.254756	-1.265490
6	-5.267823	4.468496	-0.162336
6	-4.887533	4.374347	-2.674982
6	-4.785018	5.247703	-1.405355
6	-4.126130	3.034801	-2.508525
6	-4.509715	3.127607	0.006392
1	-6.347893	4.268723	-0.259917
1	-5.949314	4.167334	-2.886984
1	-3.736834	5.552044	-1.257310
1	-3.052032	3.239044	-2.409347
1	-3.453825	3.330390	0.228131
1	-5.686991	2.025814	-1.429572
1	-5.137841	5.078076	0.743287
1	-4.491347	4.917625	-3.545442
1	-5.370940	6.170163	-1.529237
1	-4.255953	2.437587	-3.420225
1	-4.913707	2.599616	0.877996
6	-4.831520	-0.169951	0.427621
6	-6.991751	-0.368910	1.775692
6	-5.117562	-2.055746	2.129048
6	-6.646012	-1.830780	2.137702
6	-4.485720	-1.638885	0.778968
6	-6.368192	0.050544	0.418003
1	-6.614807	0.297995	2.568050
1	-4.659574	-1.468275	2.941155
1	-7.117772	-2.506570	1.406118
1	-4.857844	-2.312112	-0.005168
1	-6.840034	-0.539131	-0.379458
1	-4.425857	0.450740	1.240152

1	-8.082807	-0.232911	1.740083
1	-4.885820	-3.110901	2.333199
1	-7.063847	-2.086626	3.122335
1	-3.397616	-1.767210	0.823945
1	-6.616452	1.101238	0.223902
6	-4.558478	-0.254015	-2.733898
6	-4.059048	-0.751063	-5.207220
6	-5.929974	-1.986668	-4.011335
6	-4.846910	-2.077061	-5.107730
6	-5.317017	-1.602535	-2.639172
6	-3.470233	-0.328199	-3.837891
1	-4.731465	0.039411	-5.578677
1	-6.678484	-1.231355	-4.302783
1	-4.153171	-2.897207	-4.862295
1	-4.637718	-2.404075	-2.319941
1	-2.701688	-1.050176	-3.534153
1	-5.301675	0.499801	-3.040239
1	-3.245784	-0.846513	-5.941431
1	-6.464299	-2.943996	-3.921856
1	-5.302007	-2.323805	-6.078036
1	-6.120693	-1.544563	-1.897365
1	-2.961598	0.639513	-3.937764

		1		
		A		
Frequencies	--	-88.2024		
Red. masses	--	31.3862		
Frc consts	--	0.1439		
IR Inten	--	4.6825		
Atom AN		X	Y	Z
1	6	-0.15	0.00	-0.06
2	6	-0.19	0.04	-0.07
3	6	-0.09	0.01	-0.03
4	6	-0.04	0.02	-0.01
5	6	-0.05	0.01	-0.03
6	6	-0.08	0.02	-0.02
7	6	-0.06	0.02	-0.01
8	6	-0.03	0.02	-0.01
9	1	-0.06	0.03	0.00
10	1	-0.01	0.03	-0.01
11	6	-0.12	0.02	-0.04
12	6	-0.07	0.01	0.00
13	6	-0.12	0.01	-0.02
14	6	-0.08	0.04	-0.03
15	6	-0.06	0.03	-0.02
16	6	-0.10	0.00	0.00
17	1	-0.05	0.04	-0.01
18	1	-0.11	-0.02	0.01
19	6	-0.08	-0.02	-0.02
20	6	-0.03	-0.04	0.01
21	6	-0.06	-0.01	-0.01
22	6	-0.06	-0.05	0.00
23	6	-0.04	-0.05	0.00
24	6	-0.04	-0.02	0.00
25	1	-0.03	-0.07	0.01
26	1	-0.03	-0.02	0.00
27	6	-0.07	0.02	-0.02
28	1	-0.08	0.01	-0.01
29	6	-0.05	0.01	-0.01
30	1	-0.05	-0.01	-0.02
31	1	-0.04	0.01	-0.01
32	1	-0.03	0.01	-0.01
33	6	-0.07	0.03	-0.02
34	1	-0.08	0.03	0.00
35	1	-0.06	0.05	-0.02
36	1	-0.06	0.01	-0.03
37	6	-0.04	0.01	-0.04
38	1	-0.04	0.01	-0.05

39	6	-0.04	0.01	-0.04
40	1	-0.04	0.01	-0.03
41	1	-0.03	0.01	-0.04
42	1	-0.04	0.01	-0.03
43	6	-0.04	0.00	-0.03
44	1	-0.04	-0.01	-0.04
45	1	-0.04	0.00	-0.02
46	1	-0.04	-0.01	-0.03
47	6	-0.02	0.02	0.01
48	1	-0.03	0.02	0.02
49	6	-0.01	0.01	0.01
50	1	-0.01	0.00	0.00
51	1	-0.01	0.01	0.00
52	1	0.00	0.01	0.02
53	6	-0.02	0.01	0.01
54	1	-0.01	0.01	0.01
55	1	-0.01	0.01	0.02
56	1	-0.03	0.02	0.02
57	6	-0.05	0.00	-0.02
58	1	-0.06	0.00	-0.03
59	6	-0.04	0.00	-0.02
60	1	-0.04	0.00	-0.02
61	1	-0.04	0.00	-0.02
62	1	-0.04	0.00	-0.02
63	6	-0.04	0.01	-0.02
64	1	-0.03	0.01	0.00
65	1	-0.03	0.01	-0.04
66	1	-0.05	0.00	-0.02
67	6	-0.06	-0.04	0.00
68	1	-0.05	-0.04	0.00
69	6	-0.06	-0.01	0.00
70	1	-0.07	-0.04	0.00
71	1	-0.05	0.00	-0.03
72	1	-0.08	0.01	0.02
73	6	-0.07	-0.04	-0.01
74	1	-0.06	-0.03	-0.01
75	1	-0.07	-0.04	-0.02
76	1	-0.07	-0.04	-0.01
77	6	-0.07	0.04	-0.04
78	1	-0.07	0.03	-0.07
79	6	-0.07	0.01	-0.02
80	1	-0.10	-0.03	-0.02
81	1	-0.03	-0.01	0.01
82	1	-0.08	0.01	-0.02
83	6	-0.06	0.08	-0.04
84	1	-0.08	0.05	-0.05
85	1	-0.05	0.13	-0.07
86	1	-0.02	0.09	0.03
87	6	-0.12	0.00	-0.02
88	1	-0.12	0.00	-0.02
89	6	-0.12	0.00	-0.02
90	1	-0.11	0.03	-0.04
91	1	-0.13	-0.01	-0.04
92	1	-0.11	0.00	0.00
93	6	-0.11	-0.01	-0.02
94	1	-0.10	-0.02	0.00
95	1	-0.11	-0.01	-0.02
96	1	-0.09	-0.01	-0.04
97	6	-0.04	-0.01	0.01
98	1	-0.06	-0.03	0.03
99	6	-0.02	-0.01	0.01
100	1	-0.03	-0.01	0.01
101	1	-0.01	0.01	-0.01
102	1	0.00	-0.03	0.01
103	6	-0.02	-0.02	0.01
104	1	-0.01	0.00	0.00
105	1	-0.04	-0.02	0.02
106	1	0.00	-0.03	0.03
107	6	-0.02	-0.04	0.02

108	1	-0.02	-0.05	0.03
109	6	-0.01	-0.03	0.02
110	1	-0.01	-0.03	0.02
111	1	0.00	-0.03	0.03
112	1	0.00	-0.02	0.02
113	6	-0.01	-0.03	0.02
114	1	-0.02	-0.03	0.02
115	1	-0.01	-0.02	0.01
116	1	0.00	-0.03	0.03
117	15	-0.04	0.01	-0.01
118	6	-0.03	0.02	0.01
119	6	-0.03	0.03	0.01
120	6	-0.02	0.02	0.01
121	6	-0.04	0.03	0.00
122	6	-0.03	0.03	0.00
123	6	-0.02	0.03	0.01
124	1	-0.02	0.02	0.02
125	1	-0.04	0.03	-0.01
126	1	-0.04	0.03	-0.01
127	1	-0.02	0.03	0.01
128	1	-0.03	0.03	0.00
129	6	-0.03	0.01	-0.01
130	6	-0.01	-0.01	-0.01
131	6	-0.02	0.00	-0.01
132	6	-0.03	0.00	-0.01
133	6	-0.02	-0.01	-0.01
134	6	-0.01	0.00	-0.01
135	1	-0.02	0.01	-0.01
136	1	-0.03	0.00	-0.01
137	1	-0.01	-0.01	-0.01
138	1	0.00	-0.01	-0.01
139	1	0.00	-0.02	-0.01
140	46	0.49	-0.04	0.11
141	15	-0.07	0.01	-0.03
142	6	-0.06	0.01	-0.02
143	6	-0.02	0.02	0.00
144	6	-0.02	0.02	0.00
145	6	-0.01	0.01	0.00
146	6	-0.05	0.01	-0.01
147	6	-0.04	0.00	-0.01
148	1	-0.02	0.03	0.00
149	1	-0.03	0.04	-0.01
150	1	0.00	0.00	0.00
151	1	-0.04	-0.01	-0.01
152	1	-0.04	-0.01	-0.01
153	1	-0.07	0.03	-0.01
154	1	-0.01	0.01	0.00
155	1	-0.02	0.02	0.00
156	1	0.00	0.02	0.01
157	1	-0.05	0.02	-0.02
158	1	-0.04	0.01	-0.01
159	6	-0.04	0.01	-0.01
160	6	-0.02	-0.01	0.01
161	6	0.01	0.01	-0.01
162	6	0.00	-0.01	0.01
163	6	-0.01	0.01	-0.02
164	6	-0.04	-0.01	0.00
165	1	-0.01	-0.01	0.01
166	1	0.01	0.01	-0.01
167	1	0.00	-0.01	0.02
168	1	-0.01	0.00	-0.01
169	1	-0.04	-0.02	0.01
170	1	-0.04	0.01	-0.02
171	1	-0.02	-0.02	0.03
172	1	0.02	0.01	-0.01
173	1	0.02	-0.01	0.01
174	1	-0.01	0.02	-0.02
175	1	-0.05	-0.01	0.00
176	6	-0.06	0.01	-0.02

177	6	-0.01	-0.01	-0.01
178	6	-0.02	-0.01	-0.03
179	6	-0.01	-0.02	-0.01
180	6	-0.05	0.00	-0.02
181	6	-0.04	0.00	-0.01
182	1	-0.01	-0.02	-0.03
183	1	-0.03	-0.02	-0.05
184	1	0.00	-0.01	0.01
185	1	-0.05	0.01	0.00
186	1	-0.04	0.01	0.01
187	1	-0.06	0.00	-0.04
188	1	0.00	-0.02	0.00
189	1	-0.02	-0.02	-0.03
190	1	0.01	-0.03	-0.01
191	1	-0.06	0.01	-0.03
192	1	-0.04	0.01	-0.01

TS-Pd-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-1.101062	1.333678	0.516042
14	-1.455168	-0.890163	0.532715
6	-2.215464	2.419935	-0.621645
6	-3.961064	4.142029	-2.125159
6	-2.326533	2.292606	-2.042876
6	-3.004203	3.427166	0.032642
6	-3.849185	4.261259	-0.730752
6	-3.187383	3.153087	-2.754270
1	-4.439691	5.021906	-0.222683
1	-3.250692	3.044279	-3.834331
6	-2.954199	-1.640311	-0.469722
6	-5.132323	-2.945822	-1.876182
6	-4.316948	-1.188856	-0.334941
6	-2.715660	-2.768495	-1.340971
6	-3.802663	-3.379675	-2.007892
6	-5.355990	-1.855656	-1.028544
1	-3.587155	-4.220902	-2.663976
1	-6.377286	-1.501152	-0.906385
6	0.207780	2.451847	1.396263
6	1.761190	4.491375	2.719770
6	0.398396	2.440622	2.819067
6	0.882992	3.474236	0.646599
6	1.623121	4.465837	1.325329
6	1.159596	3.448983	3.441615
1	2.108818	5.244983	0.742187
1	1.273364	3.415742	4.522512
6	-2.965851	3.676065	1.551835
1	-2.315090	2.923997	2.013114
6	-2.354376	5.062908	1.884719
1	-1.350723	5.166555	1.459972
1	-2.277764	5.193250	2.972416
1	-2.980107	5.874815	1.490306
6	-4.349209	3.520407	2.234480
1	-4.739943	2.504551	2.117316
1	-5.089575	4.219639	1.825064
1	-4.257959	3.724704	3.310136
6	-1.546357	1.268186	-2.879850
1	-0.923867	0.663958	-2.206648
6	-2.504030	0.309116	-3.634275
1	-1.926778	-0.379160	-4.262506
1	-3.182471	0.868088	-4.291253
1	-3.108719	-0.283179	-2.941256
6	-0.597391	1.946342	-3.906537
1	0.005175	1.183179	-4.416799
1	0.085999	2.655919	-3.430640

1	-1.168025	2.490187	-4.671126
6	-4.906155	5.037562	-2.925895
1	-5.380647	5.736624	-2.220968
6	-4.149666	5.882532	-3.983876
1	-3.671912	5.240107	-4.735476
1	-3.366406	6.493064	-3.517275
1	-4.842811	6.553207	-4.509622
6	-6.036115	4.208573	-3.593018
1	-5.626117	3.507066	-4.331791
1	-6.745422	4.866906	-4.112661
1	-6.590045	3.623652	-2.847937
6	-0.176215	1.364063	3.739674
1	-0.729465	0.639890	3.137565
6	0.961019	0.584201	4.450785
1	1.495825	1.222294	5.167057
1	1.694122	0.210750	3.725246
1	0.551310	-0.275281	4.994722
6	-1.172728	1.928526	4.784888
1	-0.679336	2.617245	5.483643
1	-1.602965	1.105751	5.371959
1	-1.997249	2.469943	4.304489
6	0.885134	3.573364	-0.884819
1	0.380938	2.691740	-1.290835
6	2.331027	3.556736	-1.447648
1	2.306367	3.531404	-2.545691
1	2.882354	2.679455	-1.091972
1	2.884989	4.457466	-1.152002
6	0.142611	4.840112	-1.387025
1	0.175249	4.894862	-2.483251
1	0.616188	5.749211	-0.992781
1	-0.907043	4.841738	-1.080134
6	-1.356838	-3.408774	-1.716764
1	-1.632255	-4.373701	-2.166152
6	-0.626366	-2.618341	-2.833030
1	0.225353	-3.205533	-3.203149
1	-0.230134	-1.664582	-2.457536
1	-1.299223	-2.416525	-3.674435
6	-0.377159	-3.760672	-0.578532
1	0.376814	-4.463593	-0.959007
1	-0.879765	-4.238120	0.268013
1	0.170544	-2.884553	-0.207034
6	-4.787208	0.000280	0.522243
1	-3.907147	0.532779	0.896318
6	-5.624514	1.009691	-0.313368
1	-5.082722	1.340385	-1.205732
1	-5.859489	1.897244	0.285441
1	-6.579869	0.573393	-0.633887
6	-5.610132	-0.466457	1.754737
1	-5.029092	-1.131366	2.401006
1	-6.516714	-1.004244	1.445943
1	-5.926973	0.401532	2.350621
6	-6.282253	-3.609928	-2.636873
1	-7.212251	-3.102537	-2.338470
6	-6.435036	-5.110464	-2.276895
1	-6.588576	-5.245412	-1.198672
1	-5.541882	-5.680588	-2.564807
1	-7.294818	-5.547500	-2.803321
6	-6.128894	-3.429529	-4.171207
1	-5.223291	-3.929998	-4.538924
1	-6.058436	-2.367924	-4.439570
1	-6.990057	-3.861757	-4.699205
6	2.523164	5.618823	3.413077
1	2.924518	6.278041	2.628840
6	1.573970	6.471229	4.296785
1	0.737679	6.868039	3.707412
1	2.115197	7.316749	4.742218
1	1.153068	5.871248	5.114538
6	3.723301	5.094589	4.241840
1	4.420750	4.526393	3.613150

1	3.387663	4.434732	5.052537
1	4.271786	5.931069	4.695651
15	-1.215982	-1.855654	2.730947
6	0.077147	-3.243466	2.743527
6	2.135252	-5.169493	3.109992
6	-0.234664	-4.612501	2.898091
6	1.438375	-2.855462	2.764144
6	2.456616	-3.807259	2.948957
6	0.785336	-5.567169	3.076662
1	-1.269685	-4.940777	2.894892
1	1.704833	-1.807856	2.647615
1	3.495121	-3.483633	2.982048
1	0.521635	-6.616596	3.192133
1	2.921470	-5.905142	3.264977
6	-2.814889	-2.803288	3.104106
6	-5.159514	-4.168994	3.946192
6	-3.480198	-3.695850	2.234843
6	-3.344864	-2.604239	4.402112
6	-4.505404	-3.282599	4.823028
6	-4.643477	-4.371460	2.651662
1	-3.106909	-3.857534	1.229456
1	-2.845620	-1.920646	5.084896
1	-4.894239	-3.117855	5.825630
1	-5.144201	-5.048644	1.963795
1	-6.059121	-4.690604	4.265820
46	1.769361	-0.760550	-0.741175
15	4.161912	-0.950582	-1.237692
6	4.774301	-2.764342	-1.567676
6	4.898186	-5.146364	-0.590854
6	4.381969	-4.831954	-3.058875
6	4.127089	-5.701285	-1.808057
6	4.028547	-3.347778	-2.796439
6	4.554910	-3.659999	-0.323499
1	5.980898	-5.251528	-0.769299
1	5.441063	-4.917344	-3.351727
1	3.048656	-5.704920	-1.581906
1	2.946540	-3.259288	-2.614148
1	3.501350	-3.581292	-0.016680
1	5.853161	-2.713161	-1.794504
1	4.663608	-5.737663	0.306447
1	3.786944	-5.202395	-3.906746
1	4.417471	-6.744519	-2.001342
1	4.248197	-2.757289	-3.697509
1	5.160458	-3.300599	0.519996
6	5.160836	-0.457341	0.354916
6	7.154051	-0.499840	1.921385
6	5.305451	1.235294	2.253138
6	6.810739	0.923814	2.421818
6	4.830833	0.988125	0.802182
6	6.684071	-0.726107	0.456473
1	6.660259	-1.238510	2.573860
1	4.720866	0.595603	2.933442
1	7.400041	1.659911	1.851488
1	5.325674	1.709588	0.135601
1	7.243617	-0.046913	-0.201936
1	4.673301	-1.126712	1.081633
1	8.236491	-0.677469	2.004718
1	5.094617	2.275520	2.540366
1	7.101943	1.033924	3.476867
1	3.748916	1.158066	0.723748
1	6.932217	-1.751091	0.147386
6	4.884079	-0.062582	-2.836437
6	4.106219	1.103376	-5.006096
6	6.377092	1.655120	-4.004971
6	5.172969	2.202661	-4.802803
6	5.934231	1.061543	-2.640154
6	3.681250	0.462818	-3.664225
1	4.509430	0.327608	-5.676652
1	6.879077	0.874319	-4.599277

1	4.727895	3.046765	-4.251663
1	5.509166	1.872312	-2.031733
1	3.144021	1.204220	-3.057130
1	5.376971	-0.868169	-3.404793
1	3.219218	1.522892	-5.503512
1	7.117168	2.452252	-3.838911
1	5.504443	2.596477	-5.774814
1	6.816074	0.682907	-2.108600
1	2.968124	-0.352855	-3.842304

1
A

Frequencies -- -54.4186
 Red. masses -- 10.3586
 Frc consts -- 0.0181
 IR Inten -- 1.1251

Atom	AN	X	Y	Z
1	14	-0.08	0.01	0.04
2	14	-0.16	0.04	0.09
3	6	-0.06	0.01	0.02
4	6	-0.03	0.02	0.00
5	6	-0.04	0.01	0.02
6	6	-0.05	0.02	0.01
7	6	-0.04	0.02	0.00
8	6	-0.03	0.01	0.01
9	1	-0.03	0.03	0.00
10	1	-0.02	0.01	0.01
11	6	-0.10	0.02	0.04
12	6	-0.05	0.00	0.00
13	6	-0.10	0.01	0.02
14	6	-0.06	0.03	0.04
15	6	-0.05	0.02	0.02
16	6	-0.08	0.00	0.00
17	1	-0.03	0.02	0.02
18	1	-0.09	-0.01	-0.02
19	6	-0.04	-0.01	0.02
20	6	-0.02	-0.02	0.00
21	6	-0.03	-0.01	0.02
22	6	-0.04	-0.03	0.01
23	6	-0.02	-0.03	0.00
24	6	-0.02	-0.01	0.01
25	1	-0.02	-0.04	-0.01
26	1	-0.01	-0.01	0.01
27	6	-0.05	0.02	0.01
28	1	-0.05	0.02	0.01
29	6	-0.04	0.02	0.01
30	1	-0.04	0.01	0.01
31	1	-0.04	0.02	0.01
32	1	-0.03	0.02	0.00
33	6	-0.05	0.03	0.01
34	1	-0.06	0.03	0.00
35	1	-0.05	0.03	0.01
36	1	-0.05	0.02	0.01
37	6	-0.05	0.00	0.03
38	1	-0.06	-0.01	0.03
39	6	-0.05	0.01	0.02
40	1	-0.06	0.00	0.02
41	1	-0.05	0.01	0.03
42	1	-0.06	0.01	0.02
43	6	-0.04	-0.02	0.03
44	1	-0.04	-0.02	0.03
45	1	-0.03	-0.02	0.02
46	1	-0.03	-0.01	0.02
47	6	-0.02	0.02	-0.01
48	1	-0.02	0.03	-0.01
49	6	-0.01	0.01	0.00
50	1	0.00	0.01	0.00
51	1	0.00	0.01	0.00

52	1	0.00	0.01	-0.01
53	6	-0.02	0.02	-0.01
54	1	-0.02	0.02	0.00
55	1	-0.01	0.03	-0.02
56	1	-0.03	0.03	-0.01
57	6	-0.03	0.00	0.03
58	1	-0.03	0.00	0.03
59	6	-0.03	0.00	0.03
60	1	-0.03	0.00	0.02
61	1	-0.03	-0.01	0.03
62	1	-0.03	0.00	0.03
63	6	-0.02	0.01	0.02
64	1	-0.02	0.01	0.02
65	1	-0.02	0.01	0.03
66	1	-0.02	0.01	0.02
67	6	-0.04	-0.03	0.01
68	1	-0.06	-0.03	0.01
69	6	-0.04	-0.06	0.00
70	1	-0.05	-0.06	0.00
71	1	-0.06	-0.07	0.00
72	1	-0.02	-0.07	0.00
73	6	-0.02	-0.02	0.00
74	1	-0.03	-0.03	0.00
75	1	0.00	-0.03	0.00
76	1	-0.02	-0.01	0.01
77	6	-0.05	0.05	0.04
78	1	-0.03	0.03	0.08
79	6	-0.10	0.04	0.00
80	1	-0.08	0.06	0.01
81	1	-0.14	0.07	-0.05
82	1	-0.12	-0.03	0.00
83	6	0.00	0.13	0.02
84	1	0.01	0.15	0.02
85	1	0.05	0.14	0.06
86	1	-0.02	0.16	-0.02
87	6	-0.11	0.00	0.02
88	1	-0.12	0.01	0.02
89	6	-0.11	0.00	0.02
90	1	-0.10	0.01	0.02
91	1	-0.12	0.00	0.02
92	1	-0.10	0.00	0.00
93	6	-0.11	-0.01	0.01
94	1	-0.10	-0.01	0.01
95	1	-0.11	-0.01	0.01
96	1	-0.11	-0.01	0.02
97	6	-0.03	-0.01	-0.02
98	1	-0.04	-0.02	-0.03
99	6	-0.02	-0.01	-0.02
100	1	-0.04	-0.01	-0.02
101	1	-0.01	0.00	0.00
102	1	-0.01	-0.02	-0.03
103	6	-0.01	-0.01	-0.02
104	1	0.00	0.00	0.00
105	1	-0.02	-0.01	-0.02
106	1	0.00	-0.02	-0.03
107	6	-0.01	-0.02	-0.01
108	1	-0.01	-0.03	-0.02
109	6	0.00	-0.01	-0.01
110	1	0.00	-0.01	-0.01
111	1	0.01	-0.01	-0.02
112	1	0.00	0.00	-0.01
113	6	-0.01	-0.02	-0.01
114	1	-0.01	-0.03	-0.01
115	1	-0.01	-0.01	-0.01
116	1	0.00	-0.02	-0.02
117	15	-0.06	0.01	0.04
118	6	-0.04	0.02	0.01
119	6	-0.02	0.03	-0.03
120	6	-0.03	0.01	0.02

121	6	-0.05	0.03	-0.02
122	6	-0.03	0.04	-0.04
123	6	-0.02	0.02	0.00
124	1	-0.03	0.01	0.05
125	1	-0.06	0.03	-0.04
126	1	-0.04	0.04	-0.07
127	1	-0.01	0.02	0.01
128	1	-0.01	0.04	-0.04
129	6	-0.05	-0.01	0.04
130	6	-0.04	-0.02	0.03
131	6	-0.04	-0.01	0.04
132	6	-0.05	-0.01	0.04
133	6	-0.05	-0.02	0.04
134	6	-0.04	-0.02	0.03
135	1	-0.03	-0.01	0.04
136	1	-0.06	-0.01	0.05
137	1	-0.06	-0.03	0.03
138	1	-0.03	-0.02	0.03
139	1	-0.04	-0.03	0.03
140	46	0.18	-0.02	-0.07
141	15	0.12	-0.03	-0.03
142	6	0.10	-0.03	-0.03
143	6	0.04	-0.03	-0.01
144	6	0.05	-0.03	-0.01
145	6	0.03	-0.01	-0.01
146	6	0.09	-0.02	-0.02
147	6	0.09	-0.02	-0.02
148	1	0.04	-0.06	-0.01
149	1	0.05	-0.06	-0.01
150	1	0.03	0.02	0.00
151	1	0.09	0.01	-0.03
152	1	0.09	0.02	-0.02
153	1	0.11	-0.05	-0.03
154	1	0.03	-0.01	-0.01
155	1	0.04	-0.02	-0.01
156	1	-0.01	-0.02	0.00
157	1	0.11	-0.03	-0.03
158	1	0.10	-0.03	-0.03
159	6	0.09	-0.01	-0.02
160	6	0.06	0.03	0.01
161	6	0.02	-0.01	-0.02
162	6	0.03	0.02	0.01
163	6	0.05	-0.02	-0.03
164	6	0.09	0.02	0.00
165	1	0.06	0.02	0.00
166	1	0.02	-0.02	-0.03
167	1	0.02	0.03	0.02
168	1	0.05	-0.01	-0.02
169	1	0.09	0.02	0.01
170	1	0.09	-0.02	-0.03
171	1	0.06	0.05	0.03
172	1	0.00	-0.01	-0.02
173	1	0.01	0.02	0.01
174	1	0.05	-0.04	-0.05
175	1	0.12	0.02	0.01
176	6	0.10	-0.01	-0.03
177	6	0.07	0.00	-0.01
178	6	0.07	0.02	-0.02
179	6	0.06	0.01	-0.01
180	6	0.09	-0.01	-0.03
181	6	0.09	-0.02	-0.02
182	1	0.07	0.02	-0.03
183	1	0.07	0.03	-0.04
184	1	0.05	0.00	0.01
185	1	0.08	-0.02	-0.01
186	1	0.08	-0.03	0.00
187	1	0.10	-0.01	-0.04
188	1	0.06	0.00	0.00
189	1	0.06	0.02	-0.02

190	1	0.05	0.03	0.00
191	1	0.10	0.00	-0.04
192	1	0.09	-0.02	-0.02

TS-Pd-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-1.203136	1.388671	0.586072
32	-1.309790	-1.014214	0.451036
6	-2.252326	2.484145	-0.705244
6	-3.976376	4.138069	-2.275152
6	-2.320479	2.313514	-2.121313
6	-3.064641	3.486107	-0.086307
6	-3.904088	4.292544	-0.881152
6	-3.175122	3.147743	-2.869497
1	-4.518511	5.054111	-0.404084
1	-3.216251	3.015372	-3.948048
6	-2.930789	-1.745980	-0.533376
6	-5.058938	-3.059481	-1.980455
6	-4.293172	-1.295866	-0.420680
6	-2.660213	-2.865949	-1.399389
6	-3.724980	-3.486701	-2.089118
6	-5.311704	-1.970137	-1.138138
1	-3.489626	-4.324813	-2.742371
1	-6.338532	-1.622976	-1.041459
6	0.224399	2.521524	1.399340
6	1.752092	4.563584	2.704209
6	0.405057	2.508000	2.820736
6	0.900520	3.524451	0.635539
6	1.634730	4.524105	1.306918
6	1.156139	3.525272	3.438687
1	2.125912	5.298176	0.721251
1	1.263965	3.505369	4.520584
6	-3.048693	3.740962	1.431811
1	-2.394737	2.994364	1.908971
6	-2.444534	5.127458	1.771369
1	-1.429984	5.224076	1.370524
1	-2.394902	5.265594	2.859483
1	-3.058080	5.936238	1.353278
6	-4.436470	3.563334	2.096721
1	-4.808796	2.541040	1.970059
1	-5.179760	4.251482	1.675092
1	-4.364816	3.766109	3.173878
6	-1.511315	1.269309	-2.907070
1	-0.904473	0.686155	-2.199551
6	-2.442445	0.282291	-3.660050
1	-1.845574	-0.415610	-4.258897
1	-3.110520	0.818748	-4.346116
1	-3.058003	-0.300420	-2.968070
6	-0.534100	1.919632	-3.925032
1	0.073455	1.142264	-4.406614
1	0.143624	2.631965	-3.446392
1	-1.082094	2.452634	-4.712903
6	-4.912134	5.002422	-3.117321
1	-5.412863	5.709066	-2.438865
6	-4.135045	5.833051	-4.170325
1	-3.633395	5.180034	-4.896925
1	-3.367371	6.455385	-3.693333
1	-4.817812	6.489882	-4.725587
6	-6.012524	4.141758	-3.792678
1	-5.573232	3.426297	-4.500694
1	-6.716480	4.776309	-4.347683
1	-6.577409	3.568406	-3.046712
6	-0.172798	1.420922	3.730916
1	-0.701188	0.684493	3.118090

6	0.956492	0.654425	4.467997
1	1.470023	1.298023	5.194523
1	1.707251	0.283294	3.759387
1	0.539660	-0.206874	5.004060
6	-1.203459	1.970883	4.750322
1	-0.738125	2.674380	5.453557
1	-1.629642	1.143632	5.333335
1	-2.028716	2.492068	4.248378
6	0.906780	3.577314	-0.897080
1	0.386897	2.691190	-1.274531
6	2.352495	3.514062	-1.456213
1	2.328650	3.470632	-2.553798
1	2.879038	2.626678	-1.086973
1	2.929647	4.404279	-1.172919
6	0.180872	4.835901	-1.439840
1	0.216464	4.857656	-2.537117
1	0.660290	5.752298	-1.070949
1	-0.870041	4.853826	-1.136816
6	-1.276958	-3.469580	-1.749685
1	-1.516290	-4.444238	-2.197167
6	-0.559279	-2.655696	-2.859663
1	0.336345	-3.195246	-3.194191
1	-0.232597	-1.674349	-2.491300
1	-1.218087	-2.504868	-3.722422
6	-0.291825	-3.786411	-0.600498
1	0.458332	-4.504514	-0.958436
1	-0.784967	-4.225163	0.272554
1	0.270195	-2.902159	-0.269678
6	-4.784127	-0.103220	0.423043
1	-3.911028	0.433789	0.810877
6	-5.614212	0.900835	-0.427733
1	-5.060959	1.240709	-1.309620
1	-5.873191	1.783810	0.169018
1	-6.558801	0.454910	-0.766997
6	-5.630385	-0.560581	1.644315
1	-5.065256	-1.221998	2.308304
1	-6.532506	-1.097518	1.320313
1	-5.958318	0.313373	2.226181
6	-6.183522	-3.736843	-2.764698
1	-7.126105	-3.238088	-2.492927
6	-6.324832	-5.236266	-2.395925
1	-6.504378	-5.363283	-1.320703
1	-5.414756	-5.794032	-2.653429
1	-7.162488	-5.691687	-2.941497
6	-5.991043	-3.565336	-4.295364
1	-5.070455	-4.058039	-4.634066
1	-5.924046	-2.505300	-4.569602
1	-6.831841	-4.010631	-4.843856
6	2.488849	5.707742	3.394166
1	2.892466	6.363518	2.608531
6	1.509712	6.553108	4.251592
1	0.679512	6.931159	3.641353
1	2.027224	7.410721	4.701371
1	1.080641	5.951944	5.064112
6	3.681261	5.203930	4.245201
1	4.392653	4.637541	3.630557
1	3.340167	4.545777	5.054828
1	4.214400	6.048813	4.700849
15	-1.253973	-1.884869	2.793516
6	0.074702	-3.234074	2.811020
6	2.192209	-5.106069	3.111884
6	-0.197574	-4.609446	2.983752
6	1.426332	-2.812616	2.775168
6	2.473761	-3.737686	2.927999
6	0.852107	-5.537173	3.130785
1	-1.224640	-4.961328	3.015861
1	1.664093	-1.760786	2.633019
1	3.504352	-3.388279	2.914797
1	0.619182	-6.592051	3.261625

1	3.001813	-5.820938	3.242115
6	-2.838927	-2.866071	3.131142
6	-5.190197	-4.257919	3.910562
6	-3.468349	-3.769599	2.246080
6	-3.410481	-2.667512	4.411616
6	-4.573754	-3.359027	4.801949
6	-4.634660	-4.458343	2.632039
1	-3.065671	-3.930485	1.251617
1	-2.939899	-1.973866	5.104685
1	-4.993042	-3.195331	5.792375
1	-5.107244	-5.143814	1.932450
1	-6.091285	-4.790753	4.206573
46	1.991483	-0.822436	-0.754866
15	4.377133	-0.954202	-1.231135
6	5.015810	-2.762739	-1.536638
6	5.108913	-5.136200	-0.527618
6	4.638484	-4.852881	-3.005445
6	4.343823	-5.696023	-1.745896
6	4.296839	-3.360978	-2.775291
6	4.780547	-3.642903	-0.284077
1	6.191562	-5.257991	-0.694370
1	5.702885	-4.956966	-3.270923
1	3.262317	-5.671617	-1.536716
1	3.211221	-3.259855	-2.624324
1	3.725546	-3.549501	0.014512
1	6.097681	-2.701713	-1.744525
1	4.857981	-5.712042	0.375282
1	4.058724	-5.229847	-3.860904
1	4.613443	-6.748450	-1.916579
1	4.547121	-2.787504	-3.679348
1	5.384893	-3.277097	0.557402
6	5.334549	-0.425616	0.376468
6	7.290000	-0.389605	1.991486
6	5.377943	1.289188	2.259849
6	6.886973	1.026058	2.472078
6	4.952284	1.014716	0.799217
6	6.862912	-0.646117	0.517801
1	6.806606	-1.139525	2.638806
1	4.794133	0.638161	2.930051
1	7.468586	1.777250	1.913488
1	5.447447	1.742488	0.139799
1	7.417463	0.042132	-0.135275
1	4.850743	-1.101358	1.100096
1	8.375793	-0.529710	2.100882
1	5.128345	2.325323	2.531503
1	7.145827	1.150904	3.533940
1	3.868661	1.155961	0.688936
1	7.149717	-1.666664	0.227202
6	5.106735	-0.059242	-2.825074
6	4.342485	1.086812	-5.010212
6	6.576697	1.700872	-3.968590
6	5.370380	2.217341	-4.783112
6	6.128742	1.087908	-2.614054
6	3.907090	0.433058	-3.677758
1	4.784340	0.324531	-5.671910
1	7.111091	0.938832	-4.559148
1	4.890305	3.043839	-4.234408
1	5.680057	1.885780	-2.005774
1	3.335915	1.159712	-3.083276
1	5.627248	-0.857310	-3.379228
1	3.454489	1.479643	-5.527195
1	7.290801	2.517797	-3.785438
1	5.705814	2.627903	-5.746788
1	7.013167	0.725835	-2.075259
1	3.221130	-0.402347	-3.871081

		A		
Frequencies	--	-43.1947		
Red. masses	--	11.2729		
Frc consts	--	0.0124		
IR Inten	--	0.3856		
Atom	AN	X	Y	Z
1	32	0.07	-0.01	-0.03
2	32	0.12	-0.03	-0.06
3	6	0.05	0.00	-0.01
4	6	0.02	-0.01	0.00
5	6	0.04	0.00	-0.01
6	6	0.04	-0.01	0.00
7	6	0.03	-0.02	0.00
8	6	0.03	-0.01	-0.01
9	1	0.02	-0.03	0.01
10	1	0.02	-0.01	-0.01
11	6	0.09	-0.01	-0.04
12	6	0.06	0.00	0.00
13	6	0.09	0.00	-0.02
14	6	0.06	-0.02	-0.03
15	6	0.05	-0.01	-0.02
16	6	0.08	0.00	0.00
17	1	0.04	-0.01	-0.02
18	1	0.08	0.01	0.01
19	6	0.03	0.02	-0.01
20	6	0.01	0.03	0.01
21	6	0.02	0.02	-0.01
22	6	0.03	0.03	0.00
23	6	0.02	0.03	0.01
24	6	0.01	0.02	0.00
25	1	0.02	0.04	0.01
26	1	0.01	0.01	0.00
27	6	0.04	-0.02	0.00
28	1	0.04	-0.02	-0.01
29	6	0.03	-0.02	0.00
30	1	0.03	-0.01	0.00
31	1	0.03	-0.02	0.00
32	1	0.03	-0.02	0.01
33	6	0.04	-0.03	0.00
34	1	0.04	-0.03	0.00
35	1	0.04	-0.03	0.00
36	1	0.04	-0.03	0.00
37	6	0.05	0.01	-0.01
38	1	0.05	0.01	-0.02
39	6	0.06	0.00	-0.02
40	1	0.06	0.00	-0.01
41	1	0.06	-0.01	-0.02
42	1	0.06	0.00	-0.02
43	6	0.04	0.02	-0.01
44	1	0.05	0.03	-0.01
45	1	0.03	0.02	-0.01
46	1	0.04	0.01	-0.01
47	6	0.02	-0.02	0.01
48	1	0.01	-0.02	0.01
49	6	0.01	-0.01	0.01
50	1	0.01	0.00	0.00
51	1	0.00	0.00	0.01
52	1	0.00	-0.01	0.01
53	6	0.02	-0.02	0.01
54	1	0.02	-0.01	0.00
55	1	0.01	-0.02	0.01
56	1	0.02	-0.03	0.01
57	6	0.03	0.01	-0.02
58	1	0.03	0.01	-0.02
59	6	0.03	0.01	-0.02
60	1	0.02	0.00	-0.02
61	1	0.03	0.01	-0.02
62	1	0.03	0.00	-0.02
63	6	0.02	0.00	-0.02

64	1	0.02	-0.01	-0.01
65	1	0.02	-0.01	-0.03
66	1	0.02	0.00	-0.01
67	6	0.03	0.04	0.00
68	1	0.04	0.03	-0.01
69	6	0.03	0.06	0.00
70	1	0.04	0.06	0.00
71	1	0.05	0.07	0.01
72	1	0.02	0.07	0.00
73	6	0.02	0.03	0.00
74	1	0.02	0.04	0.00
75	1	0.00	0.04	0.01
76	1	0.02	0.02	0.00
77	6	0.05	-0.04	-0.04
78	1	0.04	-0.02	-0.06
79	6	0.09	-0.03	-0.01
80	1	0.06	-0.06	-0.03
81	1	0.14	-0.06	0.02
82	1	0.09	0.02	0.00
83	6	0.03	-0.09	-0.02
84	1	0.01	-0.11	-0.02
85	1	0.00	-0.08	-0.04
86	1	0.05	-0.11	0.00
87	6	0.10	0.00	-0.02
88	1	0.10	0.00	-0.02
89	6	0.09	0.00	-0.02
90	1	0.09	-0.01	-0.02
91	1	0.10	0.00	-0.02
92	1	0.09	0.00	-0.01
93	6	0.10	0.01	-0.01
94	1	0.10	0.01	-0.01
95	1	0.10	0.01	-0.01
96	1	0.10	0.01	-0.02
97	6	0.04	0.01	0.01
98	1	0.05	0.02	0.03
99	6	0.03	0.01	0.02
100	1	0.04	0.01	0.02
101	1	0.02	0.00	0.01
102	1	0.02	0.02	0.03
103	6	0.02	0.00	0.01
104	1	0.01	-0.01	0.00
105	1	0.03	0.00	0.01
106	1	0.01	0.01	0.02
107	6	0.00	0.02	0.02
108	1	0.00	0.03	0.02
109	6	0.00	0.01	0.02
110	1	0.00	0.01	0.02
111	1	-0.01	0.01	0.03
112	1	0.00	0.01	0.02
113	6	0.00	0.02	0.02
114	1	0.01	0.03	0.01
115	1	0.01	0.02	0.01
116	1	0.00	0.02	0.02
117	15	0.05	0.00	-0.04
118	6	0.04	-0.01	-0.01
119	6	0.02	-0.03	0.02
120	6	0.03	-0.01	-0.01
121	6	0.05	-0.02	0.01
122	6	0.04	-0.03	0.03
123	6	0.02	-0.02	0.00
124	1	0.03	0.00	-0.03
125	1	0.05	-0.02	0.02
126	1	0.04	-0.03	0.05
127	1	0.01	-0.02	0.00
128	1	0.02	-0.03	0.04
129	6	0.05	0.01	-0.04
130	6	0.04	0.02	-0.03
131	6	0.04	0.01	-0.03
132	6	0.05	0.02	-0.04

133	6	0.05	0.02	-0.03
134	6	0.04	0.02	-0.03
135	1	0.04	0.01	-0.03
136	1	0.05	0.02	-0.04
137	1	0.05	0.03	-0.03
138	1	0.03	0.02	-0.03
139	1	0.04	0.03	-0.02
140	46	-0.18	0.00	0.07
141	15	-0.14	0.02	0.03
142	6	-0.12	0.02	0.03
143	6	-0.06	0.02	0.02
144	6	-0.07	0.02	0.02
145	6	-0.05	0.01	0.01
146	6	-0.11	0.01	0.03
147	6	-0.10	0.01	0.02
148	1	-0.06	0.05	0.02
149	1	-0.07	0.06	0.01
150	1	-0.05	-0.03	0.01
151	1	-0.11	-0.02	0.03
152	1	-0.11	-0.02	0.02
153	1	-0.12	0.04	0.03
154	1	-0.05	0.01	0.01
155	1	-0.06	0.01	0.02
156	1	-0.02	0.02	0.00
157	1	-0.13	0.03	0.03
158	1	-0.12	0.02	0.03
159	6	-0.11	0.01	0.02
160	6	-0.08	-0.02	-0.01
161	6	-0.05	0.01	0.02
162	6	-0.05	-0.01	0.00
163	6	-0.08	0.02	0.03
164	6	-0.11	-0.01	0.00
165	1	-0.08	-0.01	0.01
166	1	-0.05	0.02	0.03
167	1	-0.05	-0.02	-0.01
168	1	-0.08	0.01	0.02
169	1	-0.11	-0.02	-0.01
170	1	-0.11	0.02	0.03
171	1	-0.08	-0.03	-0.02
172	1	-0.03	0.02	0.02
173	1	-0.04	-0.01	-0.01
174	1	-0.08	0.03	0.05
175	1	-0.13	-0.02	0.00
176	6	-0.12	0.01	0.03
177	6	-0.09	-0.01	0.01
178	6	-0.09	-0.02	0.02
179	6	-0.08	-0.01	0.01
180	6	-0.11	0.00	0.03
181	6	-0.11	0.01	0.02
182	1	-0.09	-0.02	0.03
183	1	-0.09	-0.03	0.04
184	1	-0.07	0.00	-0.01
185	1	-0.11	0.01	0.01
186	1	-0.10	0.03	0.01
187	1	-0.12	0.00	0.04
188	1	-0.08	0.00	0.00
189	1	-0.08	-0.02	0.02
190	1	-0.07	-0.03	0.01
191	1	-0.12	0.00	0.04
192	1	-0.12	0.02	0.02

TS-Pd-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-1.174137	1.493854	0.668775

S-

S109

50	-1.410524	-1.166691	0.531618
6	-2.152936	2.713328	-0.792852
6	-3.771265	4.428130	-2.375698
6	-2.188691	2.545737	-2.206527
6	-2.943399	3.728975	-0.177360
6	-3.736991	4.571224	-0.978806
6	-2.993902	3.415608	-2.967733
1	-4.339169	5.348631	-0.511589
1	-3.017922	3.295979	-4.048678
6	-3.157225	-1.763329	-0.627816
6	-5.226252	-2.863824	-2.283367
6	-4.488765	-1.226635	-0.585127
6	-2.870765	-2.829355	-1.546141
6	-3.909818	-3.352265	-2.342354
6	-5.488693	-1.801581	-1.406827
1	-3.671288	-4.156201	-3.035971
1	-6.500251	-1.400695	-1.369131
6	0.484049	2.541859	1.504015
6	2.051880	4.476646	2.865542
6	0.642242	2.468331	2.923052
6	1.205221	3.521979	0.762378
6	1.968415	4.477886	1.463673
6	1.417628	3.441647	3.576108
1	2.496800	5.249987	0.907468
1	1.508760	3.398586	4.659063
6	-2.943300	3.947067	1.347021
1	-2.329452	3.157270	1.822317
6	-2.274248	5.284799	1.745761
1	-1.246158	5.334664	1.369583
1	-2.240406	5.383022	2.838849
1	-2.830671	6.139412	1.340763
6	-4.341175	3.784048	1.990546
1	-4.730629	2.772931	1.824206
1	-5.063505	4.499666	1.580181
1	-4.278589	3.948074	3.074777
6	-1.398087	1.462733	-2.960438
1	-0.849469	0.851634	-2.225963
6	-2.338189	0.513883	-3.751925
1	-1.747761	-0.193278	-4.347122
1	-2.972896	1.079180	-4.446212
1	-2.989401	-0.061767	-3.085494
6	-0.342790	2.063241	-3.929237
1	0.238002	1.256875	-4.397085
1	0.355239	2.726968	-3.409763
1	-0.825054	2.638590	-4.730661
6	-4.646269	5.338080	-3.229699
1	-5.138320	6.054418	-2.555404
6	-3.795327	6.148291	-4.239528
1	-3.297478	5.483405	-4.957791
1	-3.016002	6.721128	-3.720617
1	-4.422316	6.848671	-4.806161
6	-5.756518	4.524779	-3.943894
1	-5.322626	3.800173	-4.645628
1	-6.425291	5.186537	-4.509522
1	-6.357287	3.963354	-3.216599
6	-0.002545	1.364758	3.773661
1	-0.516842	0.658793	3.109831
6	1.059387	0.534757	4.538791
1	1.566315	1.135103	5.305051
1	1.823819	0.148387	3.852937
1	0.578739	-0.319707	5.031441
6	-1.077572	1.907166	4.750098
1	-0.638414	2.587875	5.491361
1	-1.549304	1.074422	5.287955
1	-1.865970	2.453729	4.215427
6	1.203049	3.577475	-0.771241
1	0.630542	2.717169	-1.141428
6	2.635126	3.429045	-1.347337
1	2.598145	3.414276	-2.445590

1	3.099635	2.495778	-1.008272
1	3.275320	4.268990	-1.046719
6	0.531300	4.864879	-1.313772
1	0.569782	4.885494	-2.411034
1	1.042985	5.761903	-0.941713
1	-0.520358	4.919511	-1.016443
6	-1.476187	-3.433105	-1.864902
1	-1.701334	-4.376998	-2.378298
6	-0.712117	-2.549903	-2.890907
1	0.214963	-3.048801	-3.202217
1	-0.430019	-1.582277	-2.455664
1	-1.326787	-2.360739	-3.777888
6	-0.518608	-3.827034	-0.708411
1	0.221099	-4.545257	-1.086206
1	-1.026505	-4.288305	0.145846
1	0.077058	-2.979952	-0.341701
6	-4.936860	-0.031340	0.281348
1	-4.041775	0.437534	0.709323
6	-5.672205	1.058347	-0.551863
1	-5.068076	1.404174	-1.398270
1	-5.896050	1.929514	0.077527
1	-6.631141	0.691234	-0.942037
6	-5.839495	-0.462925	1.470602
1	-5.330378	-1.172566	2.131492
1	-6.765860	-0.934225	1.114285
1	-6.124169	0.417374	2.065948
6	-6.322414	-3.471589	-3.155590
1	-7.264264	-2.950776	-2.927089
6	-6.519939	-4.974022	-2.826641
1	-6.758985	-5.113070	-1.764444
1	-5.606309	-5.544390	-3.040144
1	-7.333719	-5.404090	-3.425124
6	-6.025928	-3.266153	-4.664431
1	-5.094288	-3.770081	-4.954151
1	-5.917214	-2.200425	-4.902963
1	-6.836810	-3.677623	-5.280411
6	2.790186	5.586368	3.602142
1	3.234068	6.251780	2.847253
6	1.791509	6.426645	4.441842
1	0.992834	6.831019	3.806232
1	2.299555	7.264913	4.935693
1	1.317881	5.810448	5.217591
6	3.937485	5.023589	4.475638
1	4.642848	4.445225	3.864835
1	3.547697	4.356347	5.255124
1	4.488044	5.834606	4.969082
15	-1.464902	-2.041427	3.026849
6	-0.143641	-3.396146	2.911889
6	1.983146	-5.280160	2.911504
6	-0.409901	-4.780479	2.982095
6	1.204753	-2.969621	2.823148
6	2.257068	-3.900562	2.825422
6	0.645706	-5.714316	2.981656
1	-1.435600	-5.133333	3.044040
1	1.438196	-1.909379	2.754221
1	3.284906	-3.547993	2.767045
1	0.419564	-6.777143	3.035392
1	2.797418	-6.001297	2.925820
6	-3.085498	-2.993316	3.246500
6	-5.569673	-4.266331	3.767304
6	-3.692931	-3.816396	2.271611
6	-3.744955	-2.815850	4.486344
6	-4.976200	-3.447936	4.747441
6	-4.924284	-4.447389	2.528671
1	-3.225602	-3.950062	1.300859
1	-3.293517	-2.180707	5.245049
1	-5.467273	-3.298109	5.706424
1	-5.379915	-5.064976	1.758459
1	-6.523987	-4.749959	3.963177

46	2.287025	-0.820087	-0.910527
15	4.635963	-1.101169	-1.292364
6	5.161657	-2.942044	-1.607871
6	5.051231	-5.328002	-0.626102
6	4.647503	-4.983864	-3.106769
6	4.262292	-5.811715	-1.861564
6	4.423246	-3.471302	-2.866872
6	4.838175	-3.816015	-0.369508
1	6.123118	-5.533190	-0.779449
1	5.704459	-5.172425	-3.354607
1	3.183277	-5.699282	-1.669193
1	3.346282	-3.284066	-2.734716
1	3.788270	-3.643444	-0.086971
1	6.248817	-2.955653	-1.794049
1	4.742606	-5.891940	0.266474
1	4.054581	-5.304651	-3.976049
1	4.446290	-6.881299	-2.039035
1	4.737068	-2.910476	-3.759068
1	5.455742	-3.508069	0.485569
6	5.537315	-0.651156	0.368013
6	7.401923	-0.713318	2.081784
6	5.512671	0.996834	2.308375
6	7.001737	0.692399	2.592314
6	5.164960	0.782828	0.818333
6	7.050294	-0.911504	0.578964
1	6.869373	-1.474714	2.674670
1	4.879536	0.335339	2.921044
1	7.627837	1.450331	2.094573
1	5.711388	1.520442	0.212316
1	7.651774	-0.215303	-0.022397
1	5.002250	-1.336359	1.044895
1	8.476889	-0.880658	2.244014
1	5.268698	2.027625	2.603344
1	7.204408	0.772153	3.670553
1	4.092311	0.950095	0.652751
1	7.329660	-1.928814	0.270652
6	5.441304	-0.201530	-2.843168
6	4.747448	1.043733	-5.003419
6	6.956818	1.590782	-3.879536
6	5.773093	2.155911	-4.695177
6	6.474931	0.920316	-2.564410
6	4.272699	0.335865	-3.713773
1	5.203103	0.310264	-5.687828
1	7.497553	0.852805	-4.494231
1	5.282483	2.955172	-4.116153
1	6.025453	1.695183	-1.927610
1	3.687522	1.039785	-3.104879
1	5.961999	-0.997834	-3.400087
1	3.874764	1.464681	-5.524465
1	7.673055	2.391724	-3.642730
1	6.133089	2.613987	-5.627962
1	7.343716	0.520537	-2.025592
1	3.587453	-0.485499	-3.961159

		1		
		A		
Frequencies	--	-31.2909		
Red. masses	--	10.5264		
Frc consts	--	0.0061		
IR Inten	--	0.3158		
Atom	AN	X	Y	Z
1	50	0.06	-0.01	-0.04
2	50	0.10	-0.01	-0.06
3	6	0.03	0.00	-0.01
4	6	0.01	-0.01	0.01
5	6	0.03	0.00	-0.01
6	6	0.02	-0.02	0.00
7	6	0.01	-0.02	0.01

8	6	0.01	0.00	0.00
9	1	0.00	-0.03	0.02
10	1	0.01	0.00	0.00
11	6	0.07	0.00	-0.03
12	6	0.03	0.00	0.01
13	6	0.07	0.01	-0.02
14	6	0.04	-0.01	-0.03
15	6	0.03	-0.01	-0.01
16	6	0.06	0.01	0.00
17	1	0.01	-0.02	0.00
18	1	0.06	0.01	0.02
19	6	0.03	0.03	-0.01
20	6	0.00	0.03	0.01
21	6	0.01	0.02	-0.01
22	6	0.02	0.03	0.00
23	6	0.01	0.04	0.01
24	6	0.00	0.03	0.00
25	1	0.01	0.04	0.02
26	1	-0.01	0.03	0.00
27	6	0.03	-0.04	0.00
28	1	0.03	-0.04	-0.01
29	6	0.03	-0.04	0.01
30	1	0.03	-0.04	0.01
31	1	0.03	-0.05	0.02
32	1	0.03	-0.04	0.02
33	6	0.03	-0.04	0.01
34	1	0.03	-0.04	0.00
35	1	0.03	-0.04	0.02
36	1	0.04	-0.05	0.01
37	6	0.03	0.01	-0.02
38	1	0.04	0.01	-0.02
39	6	0.05	0.00	-0.02
40	1	0.05	0.01	-0.02
41	1	0.04	0.00	-0.02
42	1	0.05	0.00	-0.02
43	6	0.03	0.03	-0.01
44	1	0.04	0.04	-0.02
45	1	0.02	0.03	-0.01
46	1	0.03	0.03	-0.01
47	6	-0.01	-0.02	0.02
48	1	-0.01	-0.03	0.03
49	6	-0.02	0.00	0.02
50	1	-0.02	0.01	0.01
51	1	-0.02	0.00	0.02
52	1	-0.02	0.00	0.03
53	6	0.00	-0.02	0.02
54	1	0.00	-0.01	0.01
55	1	-0.01	-0.02	0.02
56	1	0.00	-0.03	0.02
57	6	0.01	0.02	-0.02
58	1	0.01	0.02	-0.02
59	6	0.01	0.01	-0.02
60	1	0.01	0.01	-0.02
61	1	0.01	0.01	-0.03
62	1	0.01	0.01	-0.02
63	6	0.01	0.01	-0.01
64	1	0.01	0.00	0.00
65	1	0.01	0.00	-0.02
66	1	0.01	0.01	-0.01
67	6	0.03	0.04	0.00
68	1	0.06	0.03	-0.01
69	6	0.04	0.08	0.01
70	1	0.04	0.07	0.01
71	1	0.07	0.10	0.02
72	1	0.01	0.10	0.00
73	6	0.01	0.03	0.00
74	1	0.01	0.03	0.00
75	1	-0.02	0.04	0.01
76	1	0.00	0.00	0.00

77	6	0.03	-0.03	-0.03
78	1	0.02	-0.02	-0.05
79	6	0.05	-0.03	-0.02
80	1	0.04	-0.04	-0.03
81	1	0.08	-0.04	-0.01
82	1	0.06	0.00	-0.02
83	6	0.01	-0.07	-0.03
84	1	0.00	-0.08	-0.03
85	1	-0.01	-0.07	-0.04
86	1	0.03	-0.09	-0.01
87	6	0.08	0.01	-0.02
88	1	0.09	0.02	-0.04
89	6	0.07	0.01	-0.02
90	1	0.06	0.00	-0.04
91	1	0.08	0.01	-0.03
92	1	0.06	0.00	0.00
93	6	0.10	0.02	-0.01
94	1	0.10	0.03	-0.01
95	1	0.09	0.02	0.01
96	1	0.10	0.03	-0.01
97	6	0.02	0.00	0.03
98	1	0.02	0.01	0.03
99	6	0.01	0.00	0.04
100	1	0.02	0.01	0.04
101	1	0.00	0.00	0.03
102	1	0.00	0.01	0.05
103	6	0.00	-0.01	0.02
104	1	-0.01	-0.02	0.01
105	1	0.00	-0.01	0.01
106	1	-0.01	-0.01	0.03
107	6	-0.01	0.03	0.02
108	1	-0.01	0.04	0.03
109	6	-0.02	0.02	0.03
110	1	-0.02	0.02	0.03
111	1	-0.02	0.02	0.04
112	1	-0.01	0.01	0.02
113	6	-0.01	0.03	0.02
114	1	-0.01	0.04	0.02
115	1	-0.01	0.02	0.01
116	1	-0.01	0.03	0.03
117	15	0.06	0.01	-0.05
118	6	0.05	-0.01	-0.02
119	6	0.03	-0.04	0.02
120	6	0.03	-0.01	-0.03
121	6	0.06	-0.03	0.01
122	6	0.04	-0.04	0.03
123	6	0.02	-0.02	0.00
124	1	0.03	0.00	-0.04
125	1	0.07	-0.03	0.01
126	1	0.05	-0.05	0.05
127	1	0.01	-0.02	-0.01
128	1	0.02	-0.05	0.04
129	6	0.05	0.02	-0.04
130	6	0.05	0.04	-0.03
131	6	0.05	0.02	-0.04
132	6	0.06	0.03	-0.04
133	6	0.05	0.04	-0.04
134	6	0.04	0.03	-0.03
135	1	0.05	0.01	-0.04
136	1	0.06	0.03	-0.05
137	1	0.06	0.05	-0.04
138	1	0.04	0.03	-0.03
139	1	0.04	0.05	-0.03
140	46	-0.14	-0.02	0.08
141	15	-0.13	0.01	0.04
142	6	-0.11	0.01	0.03
143	6	-0.06	0.01	0.02
144	6	-0.08	0.01	0.02
145	6	-0.06	0.00	0.02

146	6	-0.11	0.01	0.03
147	6	-0.09	0.00	0.03
148	1	-0.06	0.03	0.01
149	1	-0.08	0.04	0.01
150	1	-0.06	-0.02	0.02
151	1	-0.11	-0.01	0.04
152	1	-0.09	-0.02	0.03
153	1	-0.11	0.03	0.02
154	1	-0.05	0.00	0.02
155	1	-0.08	0.01	0.02
156	1	-0.04	0.00	0.01
157	1	-0.13	0.02	0.03
158	1	-0.09	0.01	0.03
159	6	-0.10	0.00	0.03
160	6	-0.08	-0.01	0.01
161	6	-0.06	0.01	0.02
162	6	-0.06	0.00	0.01
163	6	-0.08	0.01	0.03
164	6	-0.10	-0.01	0.01
165	1	-0.08	0.00	0.02
166	1	-0.06	0.02	0.03
167	1	-0.06	-0.01	0.00
168	1	-0.08	0.00	0.02
169	1	-0.10	-0.02	0.00
170	1	-0.10	0.01	0.04
171	1	-0.08	-0.02	-0.01
172	1	-0.05	0.02	0.02
173	1	-0.05	0.00	0.00
174	1	-0.08	0.02	0.04
175	1	-0.12	-0.01	0.01
176	6	-0.13	0.01	0.04
177	6	-0.12	0.01	0.04
178	6	-0.11	-0.02	0.02
179	6	-0.10	-0.01	0.02
180	6	-0.11	-0.01	0.03
181	6	-0.13	0.02	0.04
182	1	-0.14	0.00	0.04
183	1	-0.12	-0.04	0.02
184	1	-0.08	0.00	0.02
185	1	-0.10	0.00	0.02
186	1	-0.11	0.03	0.04
187	1	-0.14	0.00	0.03
188	1	-0.12	0.02	0.04
189	1	-0.09	-0.03	0.01
190	1	-0.10	-0.02	0.02
191	1	-0.11	-0.02	0.02
192	1	-0.14	0.03	0.05

TS-Pd-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-1.068607	1.447766	0.665171
82	-1.172278	-1.253628	0.542577
6	-2.106360	2.645833	-0.810378
6	-3.842599	4.291719	-2.301015
6	-2.211461	2.451403	-2.213061
6	-2.886468	3.634889	-0.149550
6	-3.742401	4.449950	-0.909546
6	-3.078599	3.293204	-2.933791
1	-4.338184	5.215742	-0.416779
1	-3.161810	3.164444	-4.010565
6	-3.056566	-1.804698	-0.507827
6	-5.159151	-2.959915	-2.057078
6	-4.388902	-1.281861	-0.416502

6	-2.777806	-2.869602	-1.426114
6	-3.836583	-3.421702	-2.173921
6	-5.410097	-1.887067	-1.188866
1	-3.612360	-4.228188	-2.868953
1	-6.428356	-1.507126	-1.117390
6	0.648805	2.549023	1.367552
6	2.177148	4.546590	2.640451
6	0.840562	2.499029	2.781408
6	1.293010	3.541800	0.582295
6	2.044520	4.532601	1.242642
6	1.602085	3.506868	3.393011
1	2.518398	5.320508	0.660946
1	1.725379	3.488440	4.473256
6	-2.808896	3.859560	1.374910
1	-2.150264	3.097328	1.832491
6	-2.150470	5.213698	1.731383
1	-1.143924	5.281184	1.303790
1	-2.063813	5.319978	2.820826
1	-2.745722	6.051339	1.348350
6	-4.162732	3.662802	2.098237
1	-4.530317	2.638397	1.967201
1	-4.927575	4.350900	1.720560
1	-4.043658	3.843111	3.175268
6	-1.434616	1.374900	-2.993346
1	-0.837641	0.782950	-2.280547
6	-2.389568	0.396856	-3.730611
1	-1.813151	-0.296804	-4.355143
1	-3.075071	0.941368	-4.392039
1	-2.988501	-0.193548	-3.029033
6	-0.440656	1.986722	-4.018747
1	0.131278	1.188622	-4.511528
1	0.269532	2.667950	-3.540228
1	-0.975542	2.546040	-4.797737
6	-4.778188	5.175964	-3.109925
1	-5.247588	5.885529	-2.413078
6	-3.991105	5.993722	-4.162900
1	-3.515518	5.331767	-4.898687
1	-3.196887	6.579667	-3.682128
1	-4.654203	6.681188	-4.702589
6	-5.904073	4.329470	-3.755112
1	-5.489802	3.608895	-4.472651
1	-6.621320	4.967283	-4.286766
1	-6.445495	3.758788	-2.989160
6	0.245699	1.394262	3.671034
1	-0.282603	0.669382	3.041699
6	1.349028	0.588498	4.400811
1	1.882102	1.205943	5.134440
1	2.085344	0.200996	3.685612
1	0.900343	-0.264961	4.924677
6	-0.800202	1.927859	4.684018
1	-0.346035	2.625221	5.399985
1	-1.233781	1.092369	5.249537
1	-1.621474	2.453280	4.177676
6	1.211162	3.580934	-0.949943
1	0.659292	2.693830	-1.285893
6	2.618835	3.494086	-1.592791
1	2.532125	3.464932	-2.687938
1	3.143670	2.589571	-1.265192
1	3.229175	4.367965	-1.329984
6	0.459944	4.834672	-1.467537
1	0.452166	4.853228	-2.565619
1	0.945633	5.754584	-1.117807
1	-0.579752	4.843541	-1.128576
6	-1.377562	-3.444192	-1.794844
1	-1.602969	-4.407908	-2.267492
6	-0.682543	-2.575963	-2.881826
1	0.229889	-3.076222	-3.232121
1	-0.381618	-1.595849	-2.487500
1	-1.346388	-2.410537	-3.736347

6	-0.336485	-3.789376	-0.691308
1	0.399385	-4.492020	-1.100756
1	-0.769418	-4.241045	0.207918
1	0.271758	-2.926265	-0.389571
6	-4.813546	-0.075688	0.449787
1	-3.903682	0.417771	0.815478
6	-5.615543	0.984766	-0.361026
1	-5.064373	1.327639	-1.243991
1	-5.823543	1.863337	0.263987
1	-6.586806	0.593572	-0.693167
6	-5.636751	-0.496910	1.699218
1	-5.073263	-1.178995	2.344952
1	-6.570966	-0.996933	1.408857
1	-5.907770	0.390676	2.290702
6	-6.279571	-3.614809	-2.859034
1	-7.222849	-3.115305	-2.592539
6	-6.414367	-5.113704	-2.485570
1	-6.585367	-5.232461	-1.407751
1	-5.498157	-5.663306	-2.739152
1	-7.249006	-5.581123	-3.023902
6	-6.063360	-3.433082	-4.383691
1	-5.137766	-3.925745	-4.710044
1	-5.984905	-2.369826	-4.644249
1	-6.896090	-3.868919	-4.951463
6	2.913433	5.679896	3.334570
1	3.307172	6.348775	2.555780
6	1.929108	6.498696	4.209618
1	1.093497	6.874495	3.604263
1	2.433557	7.354581	4.675250
1	1.504695	5.875691	5.008112
6	4.108845	5.140794	4.155556
1	4.789982	4.567918	3.512582
1	3.764978	4.470010	4.953410
1	4.671137	5.960735	4.618687
15	-1.152193	-2.030340	3.100883
6	0.181199	-3.357513	2.898468
6	2.328923	-5.216977	2.842997
6	-0.067015	-4.745822	2.959433
6	1.521414	-2.915369	2.759968
6	2.584123	-3.834944	2.739661
6	0.997957	-5.667127	2.934953
1	-1.088020	-5.108210	3.039375
1	1.740739	-1.852960	2.678123
1	3.606578	-3.471253	2.657339
1	0.783799	-6.731942	2.994249
1	3.152004	-5.927883	2.856391
6	-2.745489	-2.999565	3.369901
6	-5.193528	-4.288152	3.991412
6	-3.381611	-3.831256	2.420817
6	-3.362468	-2.811307	4.628102
6	-4.575734	-3.451621	4.940574
6	-4.595529	-4.471777	2.729214
1	-2.954358	-3.961928	1.430991
1	-2.886584	-2.160227	5.357899
1	-5.030465	-3.295074	5.915788
1	-5.074714	-5.098562	1.980960
1	-6.131471	-4.783791	4.229522
46	2.302905	-0.783918	-1.044182
15	4.637416	-1.036241	-1.524154
6	5.176472	-2.872196	-1.842841
6	5.163658	-5.245909	-0.829524
6	4.632970	-4.938957	-3.293967
6	4.335024	-5.765543	-2.024014
6	4.383917	-3.430126	-3.055378
6	4.925049	-3.736350	-0.581269
1	6.232967	-5.426879	-1.025213
1	5.679623	-5.102847	-3.596662
1	3.262940	-5.687484	-1.782070
1	3.311828	-3.267268	-2.864256

1	3.883692	-3.584288	-0.258491
1	6.253310	-2.873749	-2.082230
1	4.906462	-5.805715	0.081745
1	4.003038	-5.282857	-4.127658
1	4.546108	-6.830189	-2.201215
1	4.633057	-2.870571	-3.968383
1	5.568526	-3.403744	0.244851
6	5.603478	-0.548216	0.088035
6	7.539732	-0.560466	1.720553
6	5.644473	1.133125	2.001121
6	7.148486	0.850917	2.221572
6	5.230410	0.887570	0.532785
6	7.127187	-0.787938	0.237380
1	7.038001	-1.314837	2.348458
1	5.048519	0.476549	2.655044
1	7.742325	1.604806	1.680132
1	5.735091	1.623261	-0.110542
1	7.694625	-0.096110	-0.401250
1	5.106948	-1.230150	0.796815
1	8.621670	-0.717229	1.841330
1	5.401774	2.166419	2.287981
1	7.399908	0.954911	3.287413
1	4.148553	1.035990	0.416635
1	7.404026	-1.807634	-0.065226
6	5.336822	-0.138700	-3.124824
6	4.492503	1.069329	-5.252237
6	6.762712	1.654045	-4.272949
6	5.526818	2.193558	-5.026882
6	6.366689	1.002079	-2.920213
6	4.108969	0.374905	-3.925846
1	4.907223	0.329777	-5.955678
1	7.273588	0.909698	-4.905224
1	5.065603	3.000991	-4.435435
1	5.939597	1.781362	-2.273418
1	3.557360	1.081212	-3.289356
1	5.835001	-0.931372	-3.706911
1	3.583941	1.477292	-5.719547
1	7.483028	2.466142	-4.093995
1	5.826400	2.634962	-5.988608
1	7.270065	0.625658	-2.422637
1	3.417640	-0.456242	-4.117012

		1		
		A		
Frequencies	--	-28.9591		
Red. masses	--	8.8231		
Frc consts	--	0.0044		
IR Inten	--	0.2519		
Atom AN		X	Y	Z
1	82	0.04	0.01	-0.02
2	82	0.07	0.01	-0.05
3	6	-0.01	0.01	0.00
4	6	-0.01	0.00	0.02
5	6	0.00	-0.01	0.00
6	6	-0.02	0.03	0.02
7	6	-0.02	0.03	0.02
8	6	0.00	-0.01	0.01
9	1	-0.04	0.04	0.03
10	1	0.01	-0.03	0.01
11	6	0.05	0.00	-0.03
12	6	0.03	0.01	0.00
13	6	0.05	0.00	-0.02
14	6	0.03	0.01	-0.02
15	6	0.02	0.02	-0.01
16	6	0.04	0.01	0.00
17	1	0.01	0.02	0.00
18	1	0.04	0.00	0.01
19	6	-0.01	-0.04	0.01

20	6	-0.01	-0.04	0.01
21	6	-0.02	-0.05	0.01
22	6	0.00	-0.04	0.01
23	6	0.00	-0.04	0.01
24	6	-0.02	-0.05	0.01
25	1	0.01	-0.03	0.01
26	1	-0.03	-0.05	0.01
27	6	-0.03	0.07	0.02
28	1	-0.11	0.13	0.02
29	6	0.07	0.13	0.06
30	1	0.08	0.20	0.07
31	1	0.06	0.14	0.06
32	1	0.14	0.08	0.06
33	6	-0.06	-0.03	0.00
34	1	-0.14	-0.07	-0.02
35	1	0.00	-0.10	0.01
36	1	-0.05	-0.01	0.01
37	6	0.02	-0.02	0.00
38	1	0.02	-0.02	-0.01
39	6	0.02	-0.01	-0.01
40	1	0.03	-0.02	0.00
41	1	0.02	-0.01	-0.01
42	1	0.03	-0.01	-0.01
43	6	0.01	-0.04	0.00
44	1	0.01	-0.04	-0.01
45	1	0.00	-0.04	0.00
46	1	0.00	-0.04	0.00
47	6	-0.01	-0.01	0.03
48	1	-0.01	0.00	0.04
49	6	0.00	-0.03	0.05
50	1	0.01	-0.04	0.04
51	1	-0.01	-0.02	0.06
52	1	0.00	-0.03	0.06
53	6	0.00	-0.02	0.01
54	1	0.01	-0.03	0.00
55	1	0.01	-0.02	0.01
56	1	0.00	0.00	-0.01
57	6	-0.03	-0.06	0.01
58	1	-0.07	-0.08	0.01
59	6	-0.03	-0.02	-0.04
60	1	0.02	0.00	-0.05
61	1	-0.06	-0.01	-0.07
62	1	-0.03	-0.02	-0.03
63	6	0.01	-0.07	0.05
64	1	0.05	-0.03	0.06
65	1	-0.01	-0.07	0.04
66	1	0.02	-0.11	0.08
67	6	0.00	-0.03	0.01
68	1	0.02	-0.02	0.01
69	6	0.01	-0.07	0.01
70	1	0.01	-0.05	0.01
71	1	0.03	-0.08	0.02
72	1	-0.02	-0.09	0.00
73	6	-0.02	-0.02	0.01
74	1	-0.02	-0.03	0.01
75	1	-0.04	-0.03	0.01
76	1	-0.02	0.00	0.00
77	6	0.03	0.02	-0.03
78	1	0.02	0.01	-0.05
79	6	0.04	0.01	-0.01
80	1	0.04	0.02	-0.02
81	1	0.06	0.02	0.01
82	1	0.05	-0.01	-0.01
83	6	0.01	0.06	-0.02
84	1	0.00	0.07	-0.03
85	1	-0.01	0.06	-0.04
86	1	0.02	0.08	0.00
87	6	0.06	-0.01	-0.03
88	1	0.06	-0.02	-0.04

89	6	0.04	0.00	-0.03
90	1	0.03	0.01	-0.04
91	1	0.05	0.00	-0.04
92	1	0.04	0.01	-0.01
93	6	0.07	-0.02	-0.01
94	1	0.08	-0.03	-0.01
95	1	0.07	-0.01	0.00
96	1	0.07	-0.03	-0.02
97	6	0.01	0.01	0.02
98	1	0.02	0.01	0.03
99	6	0.01	0.01	0.03
100	1	0.02	0.01	0.03
101	1	0.01	0.02	0.03
102	1	0.01	0.01	0.04
103	6	0.00	0.02	0.02
104	1	-0.01	0.03	0.01
105	1	0.00	0.03	0.01
106	1	-0.01	0.02	0.03
107	6	0.00	-0.03	0.01
108	1	0.00	-0.03	0.01
109	6	0.02	-0.03	0.03
110	1	0.02	-0.04	0.04
111	1	0.03	-0.02	0.03
112	1	0.02	-0.03	0.03
113	6	0.01	-0.01	-0.01
114	1	0.00	-0.01	-0.02
115	1	0.01	-0.01	-0.01
116	1	0.02	-0.01	0.00
117	15	0.06	-0.02	-0.04
118	6	0.04	0.00	-0.01
119	6	0.01	0.03	0.02
120	6	0.02	0.00	-0.02
121	6	0.05	0.02	0.01
122	6	0.03	0.04	0.03
123	6	0.01	0.01	0.00
124	1	0.01	-0.02	-0.03
125	1	0.06	0.03	0.01
126	1	0.04	0.05	0.04
127	1	-0.01	0.01	0.00
128	1	0.00	0.04	0.04
129	6	0.05	-0.03	-0.03
130	6	0.04	-0.05	-0.01
131	6	0.03	-0.03	-0.02
132	6	0.05	-0.05	-0.03
133	6	0.05	-0.06	-0.02
134	6	0.03	-0.04	-0.01
135	1	0.03	-0.02	-0.02
136	1	0.06	-0.05	-0.03
137	1	0.05	-0.06	-0.02
138	1	0.02	-0.04	-0.01
139	1	0.04	-0.06	0.00
140	46	-0.12	0.03	0.07
141	15	-0.11	0.00	0.03
142	6	-0.09	0.00	0.02
143	6	-0.06	0.00	0.02
144	6	-0.07	0.00	0.02
145	6	-0.05	0.01	0.01
146	6	-0.09	0.00	0.03
147	6	-0.08	0.01	0.02
148	1	-0.05	-0.01	0.01
149	1	-0.07	-0.02	0.01
150	1	-0.05	0.03	0.02
151	1	-0.09	0.02	0.03
152	1	-0.08	0.02	0.02
153	1	-0.09	-0.02	0.02
154	1	-0.05	0.01	0.01
155	1	-0.07	0.00	0.02
156	1	-0.03	0.00	0.01
157	1	-0.10	-0.01	0.03

158	1	-0.08	0.00	0.02
159	6	-0.09	0.00	0.03
160	6	-0.08	0.01	0.01
161	6	-0.06	-0.01	0.02
162	6	-0.06	0.00	0.01
163	6	-0.08	0.00	0.02
164	6	-0.09	0.01	0.01
165	1	-0.08	0.00	0.02
166	1	-0.06	-0.01	0.03
167	1	-0.06	0.01	0.00
168	1	-0.07	0.01	0.02
169	1	-0.09	0.02	0.01
170	1	-0.09	0.00	0.03
171	1	-0.08	0.02	0.00
172	1	-0.05	-0.01	0.02
173	1	-0.05	0.00	0.01
174	1	-0.08	-0.01	0.03
175	1	-0.10	0.01	0.02
176	6	-0.11	0.00	0.03
177	6	-0.10	-0.02	0.04
178	6	-0.08	0.04	0.02
179	6	-0.07	0.01	0.03
180	6	-0.08	0.03	0.02
181	6	-0.11	-0.03	0.05
182	1	-0.13	-0.01	0.04
183	1	-0.10	0.05	0.01
184	1	-0.05	-0.01	0.04
185	1	-0.05	0.02	0.03
186	1	-0.08	-0.04	0.05
187	1	-0.13	0.01	0.02
188	1	-0.10	-0.04	0.05
189	1	-0.06	0.05	0.01
190	1	-0.07	0.01	0.03
191	1	-0.08	0.05	0.01
192	1	-0.13	-0.04	0.05

Pro-Pd-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.368603	-0.056337	-0.274330
6	-0.210122	0.213889	-1.249665
6	-2.600345	0.990374	-0.102059
6	-4.920046	2.748876	0.435637
6	-2.469013	2.408525	0.189883
6	-3.988716	0.534933	-0.181092
6	-5.072296	1.409313	0.081932
6	-3.603517	3.210520	0.473285
1	-6.088181	1.022371	0.018112
1	-3.443195	4.254807	0.728939
6	-0.153361	1.444143	-2.316761
6	-0.260681	3.523835	-4.428146
6	-1.229421	1.560473	-3.274185
6	0.943461	2.411241	-2.542264
6	0.795755	3.433246	-3.523346
6	-1.225288	2.535690	-4.302546
1	1.580852	4.185245	-3.602596
1	-2.038187	2.542163	-5.021130
6	-1.674244	-1.450013	0.621638
6	-2.312600	-3.720318	2.449817
6	-1.844289	-2.837477	0.161350
6	-1.958676	-1.289160	2.047050
6	-2.258055	-2.393964	2.887867
6	-2.103076	-3.895329	1.079766
1	-2.467980	-2.210686	3.941712
1	-2.210749	-4.903315	0.684513

6	-4.473923	-0.885817	-0.534743
1	-3.604665	-1.476036	-0.791892
6	-5.193963	-1.558496	0.665839
1	-4.584028	-1.551421	1.569405
1	-5.429631	-2.603341	0.428284
1	-6.142847	-1.052335	0.891592
6	-5.430062	-0.964397	-1.760145
1	-4.886887	-0.849683	-2.700694
1	-6.228372	-0.213805	-1.728806
1	-5.913750	-1.950044	-1.785197
6	-1.174786	3.236108	0.242442
1	-0.338010	2.615603	-0.073187
6	-1.240381	4.452420	-0.724655
1	-0.250061	4.911653	-0.821209
1	-1.921039	5.230875	-0.352964
1	-1.579506	4.158401	-1.722531
6	-0.873645	3.748980	1.672664
1	0.130601	4.190103	1.709331
1	-0.920939	2.938739	2.405487
1	-1.588334	4.523586	1.981787
6	-6.118641	3.646617	0.740836
1	-7.029807	3.038381	0.634344
6	-6.087714	4.172884	2.196801
1	-5.225025	4.831047	2.363934
1	-6.023197	3.343626	2.911621
1	-6.996410	4.748906	2.417819
6	-6.233546	4.820985	-0.262060
1	-5.375416	5.500840	-0.180022
1	-7.143468	5.405077	-0.068524
1	-6.274178	4.453134	-1.294493
6	-1.943203	-3.351373	-1.296680
1	-1.784871	-2.507174	-1.966872
6	-0.904554	-4.457587	-1.624955
1	-1.121876	-5.381403	-1.072266
1	0.117644	-4.164517	-1.393859
1	-0.955894	-4.709467	-2.692548
6	-3.330757	-3.972943	-1.638174
1	-3.444383	-4.970824	-1.195001
1	-3.407097	-4.088904	-2.728059
1	-4.171192	-3.368187	-1.302195
6	-2.018208	0.052940	2.801204
1	-1.701134	0.841792	2.125949
6	-1.055579	0.095049	4.001133
1	-1.082150	1.089513	4.464434
1	-0.043037	-0.103748	3.659635
1	-1.311953	-0.635708	4.779280
6	-3.439105	0.393902	3.318980
1	-3.431500	1.393032	3.774179
1	-3.763766	-0.318424	4.090982
1	-4.183354	0.395318	2.522451
6	2.383959	2.580453	-1.963909
1	2.906013	3.158371	-2.740413
6	2.464642	3.521453	-0.738939
1	3.516078	3.742379	-0.508166
1	1.987796	3.111594	0.155581
1	1.981132	4.477686	-0.980035
6	3.253558	1.322327	-1.893939
1	4.277877	1.606101	-1.621636
1	3.310742	0.860925	-2.886864
1	2.891419	0.578299	-1.185684
6	-2.515348	0.724075	-3.310732
1	-2.544384	0.066471	-2.444998
6	-3.734785	1.688884	-3.260059
1	-3.603584	2.459847	-2.495035
1	-4.656417	1.148267	-3.046723
1	-3.875960	2.192839	-4.224188
6	-2.627815	-0.173798	-4.568307
1	-1.913957	-0.999158	-4.540030
1	-2.449323	0.389587	-5.492184

1	-3.637653	-0.600716	-4.628577
6	-0.352264	4.606741	-5.498825
1	-1.281101	4.432698	-6.062042
6	0.818518	4.527821	-6.508009
1	0.879681	3.529190	-6.957898
1	1.779568	4.739926	-6.021577
1	0.680965	5.260569	-7.314222
6	-0.450650	6.022383	-4.880598
1	0.468282	6.288036	-4.341614
1	-1.286399	6.083558	-4.173125
1	-0.608406	6.773824	-5.665709
6	-2.696110	-4.855912	3.411753
1	-2.351011	-4.566943	4.417453
6	-4.239498	-5.008508	3.486830
1	-4.717236	-4.070270	3.792338
1	-4.518879	-5.787548	4.209935
1	-4.648528	-5.292275	2.508144
6	-2.053254	-6.226002	3.092492
1	-0.965890	-6.146778	2.983356
1	-2.458943	-6.661216	2.169696
1	-2.262433	-6.937315	3.903865
15	0.520301	-1.445603	-2.114465
6	2.248586	-2.097787	-1.719332
6	4.556270	-3.721168	-1.308679
6	3.366709	-2.010360	-2.580813
6	2.317655	-3.021718	-0.650867
6	3.449411	-3.828140	-0.450532
6	4.510842	-2.802495	-2.370946
1	3.344770	-1.354153	-3.444194
1	1.458124	-3.142177	0.002713
1	3.456758	-4.546695	0.365279
1	5.358336	-2.710058	-3.046296
1	5.433283	-4.344277	-1.153818
6	0.697654	-1.294330	-3.990366
6	0.787405	-1.435488	-6.832982
6	1.195467	-0.222069	-4.753892
6	0.286863	-2.460686	-4.683642
6	0.330023	-2.534284	-6.086520
6	1.230620	-0.286117	-6.158425
1	1.551794	0.676452	-4.269562
1	-0.071651	-3.321378	-4.126883
1	-0.003580	-3.438849	-6.589655
1	1.601782	0.567765	-6.719041
1	0.803154	-1.477107	-7.919018
46	0.807111	0.473508	0.586058
15	2.567287	-0.123809	2.312991
6	4.443642	0.167131	1.812843
6	6.453262	-0.531155	0.403026
6	6.230097	1.885637	1.179727
6	6.774455	0.942985	0.087311
6	4.730225	1.646782	1.475160
6	4.949431	-0.755551	0.684681
1	7.038705	-0.849186	1.279823
1	6.807133	1.735023	2.104929
1	6.333480	1.210672	-0.883734
1	4.135116	1.940386	0.608271
1	4.382216	-0.577466	-0.232856
1	5.001909	-0.078222	2.729616
1	6.763563	-1.167486	-0.437370
1	6.380026	2.932063	0.877345
1	7.860828	1.076898	-0.011207
1	4.429488	2.301996	2.301558
1	4.794372	-1.805725	0.945139
6	2.578969	-2.018724	2.763130
6	3.764435	-4.026584	3.814397
6	1.242235	-4.054736	3.571851
6	2.437584	-4.508011	4.428423
6	1.240872	-2.525594	3.347134
6	3.780797	-2.495542	3.605391

1	3.916984	-4.528928	2.846361
1	1.267916	-4.573265	2.600899
1	2.335023	-4.095126	5.444278
1	1.036481	-2.042479	4.309475
1	3.770304	-2.006625	4.586271
1	2.676036	-2.473243	1.770772
1	4.606024	-4.311298	4.460152
1	0.302235	-4.345499	4.059475
1	2.441341	-5.602535	4.524830
1	0.422807	-2.264554	2.672458
1	4.720318	-2.218947	3.116941
6	2.594267	0.977827	3.950777
6	1.952393	3.280026	4.882205
6	2.308084	1.328367	6.464718
6	1.516858	2.624874	6.207033
6	2.181398	0.326447	5.292976
6	1.826648	2.298991	3.696461
1	2.997189	3.616143	4.970209
1	3.369166	1.577857	6.617226
1	0.440894	2.395466	6.164289
1	1.152225	-0.037898	5.264156
1	0.768725	2.085053	3.519426
1	3.658488	1.231679	4.054789
1	1.343302	4.173416	4.685090
1	1.953168	0.849754	7.388149
1	1.662838	3.325738	7.040019
1	2.819514	-0.537617	5.502501
1	2.198552	2.780035	2.783286

Pro-Pd-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-0.169475	1.330810	0.403605
14	-1.384410	-0.636828	0.578849
6	-1.141245	2.771061	-0.453597
6	-2.549788	5.022472	-1.574411
6	-1.469033	2.819802	-1.847846
6	-1.559010	3.873172	0.371326
6	-2.237895	4.965756	-0.208395
6	-2.158747	3.934206	-2.369922
1	-2.537977	5.796046	0.428224
1	-2.393943	3.948425	-3.431764
6	-3.092510	-0.914835	-0.319851
6	-5.713942	-1.387037	-1.473880
6	-4.221808	-0.086075	0.001515
6	-3.320730	-1.998688	-1.249715
6	-4.610808	-2.194071	-1.793400
6	-5.489423	-0.348465	-0.566944
1	-4.744597	-3.009945	-2.501693
1	-6.325850	0.290655	-0.295941
6	1.353833	2.144328	1.319663
6	3.475341	3.608717	2.632553
6	1.623482	1.982912	2.719396
6	2.212772	3.034038	0.584253
6	3.232698	3.742972	1.258488
6	2.663121	2.707133	3.337625
1	3.856832	4.429276	0.689925
1	2.828330	2.566229	4.403474
6	-1.297297	3.968887	1.887801
1	-0.823467	3.042750	2.221266
6	-0.322789	5.128932	2.226248
1	0.626549	5.023637	1.693632
1	-0.106979	5.140401	3.303108
1	-0.761253	6.100077	1.959575
6	-2.593133	4.122070	2.725297

1	-3.247323	3.253019	2.615857
1	-3.160855	5.016508	2.439596
1	-2.337308	4.218586	3.789435
6	-1.111193	1.719526	-2.859594
1	-0.577477	0.915329	-2.332291
6	-2.384228	1.101459	-3.496140
1	-2.107402	0.322245	-4.217598
1	-2.965734	1.861092	-4.034868
1	-3.031637	0.650371	-2.737316
6	-0.175154	2.244235	-3.981539
1	0.105559	1.421624	-4.652757
1	0.743475	2.681895	-3.573544
1	-0.672105	3.013278	-4.587706
6	-3.298902	6.216135	-2.164415
1	-3.475023	6.932838	-1.348267
6	-2.462204	6.940534	-3.250492
1	-2.269918	6.279324	-4.105933
1	-1.492049	7.262928	-2.851519
1	-2.994391	7.826174	-3.623389
6	-4.683888	5.796931	-2.724241
1	-4.573643	5.091935	-3.558888
1	-5.235234	6.672489	-3.093273
1	-5.289471	5.307546	-1.950965
6	0.826464	1.041105	3.624267
1	0.036737	0.569531	3.033602
6	1.725926	-0.094203	4.176438
1	2.490709	0.300965	4.859080
1	2.242773	-0.616539	3.362178
1	1.118574	-0.826489	4.721563
6	0.133422	1.777094	4.801401
1	0.868265	2.199398	5.500306
1	-0.495174	1.072012	5.361892
1	-0.504954	2.596323	4.449836
6	2.115461	3.299091	-0.928486
1	1.398254	2.595518	-1.363325
6	3.473480	3.065331	-1.639595
1	3.349211	3.146466	-2.727614
1	3.879049	2.075892	-1.407971
1	4.218268	3.813748	-1.340703
6	1.625343	4.738057	-1.240795
1	1.560696	4.890794	-2.326776
1	2.327272	5.481471	-0.838722
1	0.638609	4.932243	-0.813904
6	-2.299333	-3.006696	-1.825796
1	-2.918491	-3.808909	-2.253874
6	-1.520389	-2.399941	-3.021231
1	-0.958064	-3.184800	-3.544575
1	-0.812329	-1.632428	-2.678441
1	-2.208690	-1.940275	-3.739822
6	-1.359993	-3.715940	-0.833099
1	-0.872701	-4.564121	-1.333925
1	-1.907052	-4.111659	0.028582
1	-0.570403	-3.055038	-0.455425
6	-4.182631	1.123386	0.947070
1	-3.139058	1.331037	1.204908
6	-4.756735	2.389564	0.256524
1	-4.249390	2.587802	-0.693466
1	-4.625400	3.267661	0.897167
1	-5.831665	2.286946	0.058494
6	-4.948873	0.840191	2.267100
1	-4.507625	0.005239	2.820109
1	-5.999605	0.591869	2.066498
1	-4.934170	1.727150	2.915690
6	-7.089825	-1.609294	-2.099722
1	-7.774863	-0.870565	-1.657377
6	-7.653401	-3.018019	-1.783591
1	-7.710194	-3.185600	-0.700413
1	-7.018814	-3.804264	-2.213523
1	-8.661964	-3.134257	-2.203093

6	-7.061745	-1.357954	-3.631008
1	-6.406073	-2.079090	-4.137136
1	-6.691188	-0.350481	-3.858549
1	-8.068558	-1.459919	-4.058491
6	4.562851	4.431855	3.322995
1	5.069573	5.026439	2.547878
6	3.950926	5.426223	4.345266
1	3.210559	6.078849	3.865794
1	4.733436	6.057466	4.787999
1	3.447566	4.890739	5.161172
6	5.635646	3.542114	4.001558
1	6.116661	2.876295	3.273652
1	5.193123	2.916720	4.788036
1	6.414495	4.162893	4.464976
15	-1.199041	-1.784948	2.684121
6	-0.371105	-3.489289	2.530755
6	1.049371	-5.953475	2.655081
6	-1.060692	-4.721708	2.578485
6	1.044627	-3.515333	2.543884
6	1.747464	-4.731314	2.608625
6	-0.358097	-5.940956	2.637752
1	-2.146047	-4.737889	2.595923
1	1.597857	-2.579827	2.530695
1	2.835377	-4.723276	2.636475
1	-0.912196	-6.876655	2.677596
1	1.591214	-6.894828	2.715012
6	-2.957170	-2.259764	3.205115
6	-5.515210	-2.919578	4.249529
6	-3.944419	-2.842474	2.379460
6	-3.273369	-2.012665	4.562118
6	-4.539543	-2.340588	5.083529
6	-5.213109	-3.168248	2.896843
1	-3.739913	-3.026362	1.330127
1	-2.523962	-1.561955	5.208548
1	-4.760525	-2.141413	6.129795
1	-5.961667	-3.607202	2.241245
1	-6.496781	-3.168488	4.646914
46	0.684356	-0.708964	-0.688112
15	2.992519	-1.660650	-1.483750
6	3.006563	-3.537214	-1.957664
6	2.735046	-5.954848	-1.185222
6	2.087721	-5.302109	-3.565149
6	1.803999	-6.254197	-2.381157
6	2.031881	-3.818916	-3.127535
6	2.675585	-4.465726	-0.767321
1	3.771048	-6.214411	-1.457527
1	3.085036	-5.521025	-3.979167
1	0.757182	-6.134337	-2.061690
1	1.014983	-3.572527	-2.800432
1	1.671326	-4.234482	-0.388511
1	4.032491	-3.751071	-2.300476
1	2.460851	-6.583950	-0.326961
1	1.362687	-5.475626	-4.373659
1	1.920466	-7.299997	-2.699859
1	2.250604	-3.176096	-3.991303
1	3.367025	-4.300030	0.067081
6	4.232797	-1.619527	0.004507
6	6.291904	-2.441091	1.249708
6	5.219337	-0.218644	1.891357
6	6.536950	-1.020673	1.808539
6	4.479978	-0.184677	0.532111
6	5.567506	-2.394600	-0.120888
1	5.675758	-3.009734	1.965082
1	4.562493	-0.675053	2.647965
1	7.245971	-0.491455	1.151625
1	5.091816	0.377320	-0.187433
1	6.225157	-1.899973	-0.848080
1	3.627206	-2.133374	0.769151
1	7.244082	-2.981787	1.149515

1	5.414280	0.808649	2.226789
1	7.006669	-1.080436	2.800889
1	3.530332	0.351458	0.640058
1	5.400406	-3.417428	-0.481194
6	3.777824	-0.951580	-3.122510
6	3.220318	0.482673	-5.181584
6	5.638990	0.179491	-4.444101
6	4.620797	1.131729	-5.109146
6	5.167236	-0.274988	-3.038912
6	2.743936	-0.011288	-3.795526
1	3.251802	-0.368424	-5.881062
1	5.775939	-0.707705	-5.083643
1	4.563110	2.063939	-4.526120
1	5.129071	0.600900	-2.378550
1	2.564479	0.849102	-3.138227
1	3.897545	-1.837923	-3.764268
1	2.490620	1.198613	-5.586568
1	6.620917	0.667695	-4.361857
1	4.962330	1.407943	-6.116838
1	5.905524	-0.966834	-2.616713
1	1.777385	-0.524223	-3.894330

Pro-Pd-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-0.104645	1.368535	0.414266
32	-1.383417	-0.687362	0.548881
6	-1.036373	2.893039	-0.507399
6	-2.365646	5.168790	-1.651264
6	-1.334813	2.940335	-1.905162
6	-1.435441	4.000974	0.313001
6	-2.078861	5.109034	-0.278926
6	-1.987294	4.070575	-2.441610
1	-2.369782	5.948204	0.350700
1	-2.203857	4.089474	-3.507622
6	-3.161016	-0.896720	-0.393086
6	-5.769015	-1.290751	-1.571799
6	-4.258024	-0.026965	-0.083538
6	-3.399320	-1.972059	-1.323689
6	-4.688134	-2.133645	-1.879954
6	-5.525921	-0.252372	-0.667829
1	-4.837795	-2.946015	-2.589080
1	-6.345510	0.415237	-0.413176
6	1.502041	2.148444	1.353562
6	3.633369	3.538623	2.694749
6	1.742140	1.959314	2.751903
6	2.383262	3.015339	0.627823
6	3.415035	3.691209	1.317296
6	2.789942	2.654692	3.388663
1	4.067582	4.361262	0.760651
1	2.941520	2.502212	4.455215
6	-1.190919	4.079533	1.832907
1	-0.741518	3.139043	2.165766
6	-0.192450	5.210692	2.196233
1	0.770679	5.068808	1.696915
1	-0.012321	5.223341	3.279671
1	-0.588654	6.193726	1.908360
6	-2.497391	4.249779	2.650243
1	-3.171077	3.399501	2.509007
1	-3.036658	5.163585	2.370573
1	-2.260744	4.318696	3.720967
6	-0.982528	1.818742	-2.894075
1	-0.480020	1.009214	-2.343545
6	-2.255818	1.219150	-3.546651
1	-1.982685	0.425635	-4.253922

1	-2.814022	1.983798	-4.102811
1	-2.924543	0.789252	-2.793332
6	-0.004270	2.302851	-3.997505
1	0.278170	1.462450	-4.645701
1	0.911290	2.726779	-3.567885
1	-0.465257	3.072550	-4.630731
6	-3.075635	6.380374	-2.254378
1	-3.247915	7.101574	-1.441356
6	-2.203313	7.084298	-3.325821
1	-2.008480	6.417228	-4.176072
1	-1.234503	7.387564	-2.909028
1	-2.709718	7.979928	-3.710600
6	-4.461031	5.995838	-2.837397
1	-4.354889	5.286618	-3.668940
1	-4.982986	6.884751	-3.217155
1	-5.092312	5.523944	-2.073839
6	0.909041	1.012673	3.620017
1	0.134273	0.556421	2.996543
6	1.775606	-0.141795	4.184668
1	2.527316	0.232458	4.892886
1	2.305279	-0.664503	3.378426
1	1.140262	-0.868603	4.704897
6	0.178474	1.742583	4.776995
1	0.889734	2.176312	5.492920
1	-0.457798	1.032333	5.321695
1	-0.459571	2.552743	4.403762
6	2.297357	3.271261	-0.886118
1	1.540751	2.602869	-1.310952
6	3.636601	2.945163	-1.594732
1	3.520402	3.032701	-2.683422
1	3.967219	1.928595	-1.361112
1	4.431935	3.638379	-1.292439
6	1.880858	4.728769	-1.215643
1	1.829243	4.872715	-2.303551
1	2.613334	5.443719	-0.816821
1	0.900449	4.972615	-0.798062
6	-2.378343	-2.986486	-1.886660
1	-2.994745	-3.761082	-2.366060
6	-1.531835	-2.356914	-3.023964
1	-0.955460	-3.134795	-3.542516
1	-0.828839	-1.612231	-2.623284
1	-2.176139	-1.862967	-3.760869
6	-1.493048	-3.742912	-0.874053
1	-1.012044	-4.594312	-1.375836
1	-2.077002	-4.139347	-0.036033
1	-0.696116	-3.112744	-0.461504
6	-4.178694	1.186005	0.855283
1	-3.129641	1.346158	1.128094
6	-4.680126	2.474394	0.149581
1	-4.131688	2.657817	-0.780621
1	-4.539583	3.345227	0.798786
1	-5.750150	2.412597	-0.088169
6	-4.973880	0.947236	2.166704
1	-4.595236	0.079496	2.715983
1	-6.037835	0.774165	1.956828
1	-4.901798	1.826183	2.822334
6	-7.142325	-1.470515	-2.216503
1	-7.812462	-0.715524	-1.778853
6	-7.749632	-2.864510	-1.918013
1	-7.831806	-3.034770	-0.836898
1	-7.128447	-3.666094	-2.338956
1	-8.752569	-2.951649	-2.357354
6	-7.083170	-1.208904	-3.745239
1	-6.437758	-1.943025	-4.245760
1	-6.682264	-0.209888	-3.958359
1	-8.084925	-1.281069	-4.190107
6	4.739522	4.319735	3.403424
1	5.277330	4.899553	2.638248
6	4.149869	5.329915	4.422954

1	3.443407	6.013880	3.935923
1	4.948487	5.927461	4.883164
1	3.612164	4.808953	5.226223
6	5.769289	3.385483	4.088641
1	6.227005	2.701408	3.362463
1	5.294709	2.777147	4.869738
1	6.569567	3.972003	4.559841
15	-1.285242	-1.816478	2.751912
6	-0.509331	-3.541560	2.581490
6	0.843692	-6.043750	2.649427
6	-1.232620	-4.753966	2.634713
6	0.905450	-3.605208	2.558245
6	1.574895	-4.840931	2.593841
6	-0.562888	-5.992596	2.667575
1	-2.317390	-4.739465	2.675828
1	1.484428	-2.684760	2.535693
1	2.662920	-4.864110	2.592314
1	-1.141531	-6.912964	2.714394
1	1.360381	-7.000200	2.688612
6	-3.074980	-2.237559	3.210362
6	-5.687787	-2.822972	4.158240
6	-4.046177	-2.795436	2.349001
6	-3.436286	-1.972752	4.552634
6	-4.730030	-2.264335	5.026218
6	-5.341694	-3.085040	2.818591
1	-3.808276	-2.988151	1.308148
1	-2.700758	-1.538518	5.225755
1	-4.985571	-2.053933	6.062347
1	-6.076238	-3.506584	2.136313
1	-6.689434	-3.045679	4.519302
46	0.756468	-0.758809	-0.720501
15	3.049022	-1.785910	-1.515349
6	3.007532	-3.665534	-1.986581
6	2.625420	-6.067572	-1.202154
6	2.066878	-5.413631	-3.601733
6	1.709623	-6.338274	-2.416262
6	2.056946	-3.923753	-3.181970
6	2.618001	-4.573469	-0.797267
1	3.655335	-6.372311	-1.449907
1	3.066617	-5.678186	-3.982119
1	0.662177	-6.165707	-2.123806
1	1.039222	-3.635460	-2.891248
1	1.617066	-4.299042	-0.437750
1	4.034138	-3.915419	-2.302213
1	2.307348	-6.677608	-0.345147
1	1.360394	-5.567890	-4.430312
1	1.784637	-7.392030	-2.720866
1	2.328957	-3.301138	-4.045382
1	3.301860	-4.429283	0.047746
6	4.277922	-1.794662	-0.015693
6	6.309331	-2.678378	1.236754
6	5.284964	-0.436623	1.891061
6	6.584120	-1.268638	1.808928
6	4.558826	-0.371156	0.525938
6	5.591900	-2.605687	-0.136539
1	5.678357	-3.239281	1.945077
1	4.611586	-0.887081	2.636771
1	7.308980	-0.750248	1.160735
1	5.191551	0.180421	-0.183398
1	6.266970	-2.127686	-0.858779
1	3.652505	-2.297647	0.740168
1	7.249851	-3.239096	1.135519
1	5.501058	0.582082	2.240328
1	7.046672	-1.348098	2.803275
1	3.621788	0.188643	0.629687
1	5.398534	-3.622393	-0.501434
6	3.888452	-1.104975	-3.141378
6	3.395504	0.290386	-5.242609

6	5.789138	0.015811	-4.417301
6	4.789117	0.949307	-5.135311
6	5.270012	-0.416930	-3.021874
6	2.875914	-0.175305	-3.862135
1	3.455738	-0.575550	-5.921844
1	5.955246	-0.881407	-5.035801
1	4.705600	1.891966	-4.571874
1	5.200471	0.471244	-2.380738
1	2.683739	0.700037	-3.226882
1	4.033232	-2.000518	-3.765521
1	2.676466	0.993401	-5.687985
1	6.764368	0.512393	-4.308409
1	5.163765	1.209171	-6.135633
1	5.998606	-1.093566	-2.560382
1	1.909487	-0.685148	-3.978023

Pro-Pd-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.325023	1.411143	0.555519
50	-1.655210	-0.627334	0.238467
6	0.107596	3.273337	-0.583282
6	-0.356460	5.778717	-1.904778
6	0.012857	3.342403	-2.006626
6	-0.045471	4.479766	0.169543
6	-0.262988	5.702203	-0.505393
6	-0.219647	4.584140	-2.636005
1	-0.367791	6.618284	0.074442
1	-0.294352	4.617858	-3.721269
6	-3.614038	-0.184012	-0.684685
6	-6.307894	0.174344	-1.651726
6	-4.358485	0.996873	-0.379839
6	-4.230841	-1.170140	-1.535448
6	-5.555191	-0.967247	-1.983681
6	-5.680885	1.144973	-0.863139
1	-6.002761	-1.729709	-2.619383
1	-6.234525	2.047561	-0.612028
6	2.224755	1.628686	1.631887
6	4.549157	2.229640	3.208358
6	2.295316	1.252700	3.011459
6	3.363053	2.263080	1.041003
6	4.489314	2.556497	1.843696
6	3.444454	1.563866	3.768529
1	5.347563	3.049826	1.390176
1	3.471643	1.278651	4.818372
6	0.011845	4.527269	1.708005
1	0.126751	3.502287	2.092285
6	1.233792	5.330382	2.225463
1	2.175027	4.881085	1.892587
1	1.238688	5.351316	3.323628
1	1.202670	6.368390	1.868223
6	-1.296743	5.080513	2.328881
1	-2.162793	4.479768	2.030648
1	-1.480772	6.116724	2.017240
1	-1.232187	5.067272	3.425388
6	0.139593	2.101971	-2.903080
1	0.427630	1.241887	-2.274731
6	-1.215524	1.736200	-3.563092
1	-1.110010	0.833729	-4.180220
1	-1.572196	2.550378	-4.208367
1	-1.987145	1.539646	-2.809352
6	1.241037	2.263565	-3.982051
1	1.352672	1.332234	-4.552115
1	2.209901	2.509254	-3.528518
1	0.992139	3.061344	-4.693581

6	-0.599296	7.119557	-2.599477
1	-0.693812	7.885157	-1.814623
6	0.596729	7.523865	-3.501119
1	0.736292	6.802736	-4.317393
1	1.529956	7.563444	-2.925181
1	0.426258	8.511882	-3.950367
6	-1.921594	7.119978	-3.410042
1	-1.885626	6.385987	-4.225859
1	-2.101782	8.108058	-3.855194
1	-2.776985	6.868253	-2.770498
6	1.162868	0.505468	3.725507
1	0.365611	0.294687	3.000593
6	1.630086	-0.868074	4.271255
1	2.385851	-0.753479	5.060209
1	2.066872	-1.479276	3.471025
1	0.775842	-1.414224	4.689783
6	0.521081	1.352421	4.854304
1	1.241497	1.561353	5.656552
1	-0.328814	0.812253	5.291514
1	0.155905	2.314812	4.471916
6	3.467723	2.608251	-0.453331
1	2.542048	2.296833	-0.949965
6	4.625108	1.822090	-1.119817
1	4.628592	1.994372	-2.205072
1	4.518819	0.748235	-0.937397
1	5.601114	2.137569	-0.728461
6	3.638317	4.126453	-0.715858
1	3.755055	4.314227	-1.791919
1	4.529344	4.519690	-0.208322
1	2.767047	4.690971	-0.370656
6	-3.576685	-2.456101	-2.086825
1	-4.370804	-2.950178	-2.664310
6	-2.445416	-2.153851	-3.104577
1	-2.118276	-3.084900	-3.588938
1	-1.571983	-1.698077	-2.621850
1	-2.800698	-1.467284	-3.883737
6	-3.138979	-3.497882	-1.027242
1	-2.917350	-4.455186	-1.519393
1	-3.929739	-3.678253	-0.288544
1	-2.231361	-3.204887	-0.486707
6	-3.808646	2.181956	0.423549
1	-2.784459	1.943154	0.739577
6	-3.730408	3.452721	-0.465427
1	-3.099423	3.285895	-1.345768
1	-3.303638	4.292788	0.095020
1	-4.727981	3.751967	-0.813069
6	-4.632899	2.461887	1.706903
1	-4.685110	1.577735	2.350587
1	-5.660471	2.764175	1.465500
1	-4.174669	3.278482	2.281334
6	-7.744549	0.360478	-2.139717
1	-8.101514	1.326057	-1.750919
6	-8.685780	-0.740265	-1.584536
1	-8.663975	-0.760233	-0.487302
1	-8.388629	-1.733890	-1.945315
1	-9.721149	-0.561678	-1.905304
6	-7.825866	0.424528	-3.687132
1	-7.499344	-0.520603	-4.140842
1	-7.188297	1.225002	-4.083003
1	-8.858239	0.613508	-4.011632
6	5.781633	2.581719	4.042321
1	6.504959	3.070801	3.372488
6	5.439654	3.589853	5.170619
1	4.986854	4.501750	4.761424
1	6.345616	3.872869	5.723878
1	4.730109	3.155265	5.887108
6	6.468228	1.318897	4.624667
1	6.747577	0.617580	3.827725
1	5.801922	0.790027	5.318781

1	7.377958	1.593262	5.175775
15	-2.045445	-1.458218	2.739664
6	-1.974186	-3.351190	2.609392
6	-1.648141	-6.179453	2.635594
6	-3.007932	-4.196097	3.076274
6	-0.772165	-3.949829	2.159111
6	-0.612027	-5.346501	2.168469
6	-2.845315	-5.595386	3.089357
1	-3.936835	-3.767603	3.439853
1	0.041708	-3.321775	1.800511
1	0.321367	-5.782825	1.818571
1	-3.653791	-6.224172	3.456994
1	-1.522756	-7.259768	2.648183
6	-3.871957	-1.154454	3.143610
6	-6.549352	-0.649243	3.948052
6	-4.956806	-1.521508	2.315044
6	-4.151010	-0.524006	4.379012
6	-5.478228	-0.273455	4.780975
6	-6.283313	-1.272469	2.712813
1	-4.771762	-1.994477	1.355494
1	-3.327779	-0.235801	5.028466
1	-5.671035	0.208847	5.736722
1	-7.101966	-1.557403	2.055953
1	-7.575073	-0.456395	4.254820
46	0.680079	-1.043573	-0.809412
15	2.755767	-2.397624	-1.527571
6	2.045181	-4.084472	-2.170056
6	0.666382	-6.170030	-1.632118
6	0.702100	-5.250355	-4.008753
6	-0.129452	-6.001250	-2.945340
6	1.226068	-3.896065	-3.472044
6	1.191926	-4.812691	-1.104374
1	1.518493	-6.846705	-1.807974
1	1.556866	-5.876590	-4.311236
1	-1.049003	-5.433254	-2.737637
1	0.376739	-3.228659	-3.268127
1	0.340735	-4.175204	-0.824169
1	2.921501	-4.709232	-2.409058
1	0.035152	-6.641464	-0.865876
1	0.098803	-5.079467	-4.912111
1	-0.440554	-6.983115	-3.329872
1	1.833673	-3.413159	-4.248478
1	1.774399	-4.983606	-0.189324
6	3.773251	-2.980430	0.017011
6	5.296505	-4.644238	1.207869
6	5.105450	-2.252530	2.067125
6	6.030735	-3.479977	1.910620
6	4.513748	-1.807613	0.707968
6	4.703815	-4.207126	-0.156876
1	4.481828	-5.001572	1.857821
1	4.283092	-2.501906	2.755931
1	6.914887	-3.196843	1.316529
1	5.332278	-1.450366	0.068125
1	5.531394	-3.965622	-0.838187
1	2.959439	-3.280943	0.696780
1	5.980130	-5.492718	1.058985
1	5.652352	-1.414430	2.521152
1	6.399492	-3.805494	2.893831
1	3.828335	-0.964217	0.859408
1	4.161119	-5.051164	-0.601593
6	3.954267	-2.023943	-3.025603
6	4.130646	-0.713099	-5.219498
6	6.239674	-1.479611	-4.013418
6	5.615099	-0.400203	-4.925456
6	5.427203	-1.668354	-2.706584
6	3.325760	-0.918017	-3.914367
1	4.066603	-1.624931	-5.834918
1	6.279627	-2.437044	-4.557327
1	5.687141	0.579651	-4.427541

1	5.474487	-0.738294	-2.126263
1	3.301578	0.022643	-3.347023
1	3.965788	-2.962621	-3.602535
1	3.680645	0.099299	-5.808062
1	7.276861	-1.212095	-3.764512
1	6.181148	-0.322918	-5.864611
1	5.897807	-2.450958	-2.101550
1	2.281856	-1.161064	-4.151615

Pro-Pd-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.302306	1.467407	0.540933
82	-1.537953	-0.988398	0.316389
6	-0.149451	3.376259	-0.596577
6	-0.992397	5.832805	-1.797727
6	-0.453641	3.434505	-1.987286
6	-0.296443	4.556459	0.191768
6	-0.706939	5.760380	-0.422967
6	-0.864558	4.656744	-2.561992
1	-0.812171	6.661638	0.180118
1	-1.091867	4.690468	-3.626385
6	-3.554626	-0.394638	-0.552656
6	-6.159942	0.054209	-1.673375
6	-4.315348	0.757459	-0.191806
6	-4.104997	-1.310350	-1.515044
6	-5.389509	-1.062447	-2.044825
6	-5.602830	0.948180	-0.750286
1	-5.788394	-1.761202	-2.778353
1	-6.178816	1.826173	-0.464097
6	2.362659	1.851713	1.382846
6	4.772339	2.666794	2.690338
6	2.564486	1.579070	2.771740
6	3.404328	2.486422	0.644616
6	4.582878	2.886627	1.314507
6	3.757856	1.995965	3.398122
1	5.372449	3.384399	0.752882
1	3.892188	1.798030	4.460031
6	-0.023297	4.577076	1.707074
1	0.225429	3.555732	2.035013
6	1.205895	5.450352	2.066695
1	2.108026	5.085246	1.565017
1	1.387685	5.426601	3.149605
1	1.045560	6.495506	1.771255
6	-1.259480	5.007507	2.538007
1	-2.105543	4.329820	2.375909
1	-1.584753	6.021964	2.275880
1	-1.018248	4.999080	3.609736
6	-0.362600	2.201044	-2.899397
1	-0.032199	1.341293	-2.291749
6	-1.740692	1.826075	-3.505917
1	-1.650276	0.932951	-4.138647
1	-2.132389	2.640662	-4.129800
1	-2.479697	1.613512	-2.724763
6	0.686694	2.382578	-4.027087
1	0.769891	1.462602	-4.621436
1	1.676162	2.619667	-3.617128
1	0.400522	3.196496	-4.706258
6	-1.435761	7.151437	-2.433158
1	-1.443060	7.913852	-1.639619
6	-0.440602	7.625015	-3.524070
1	-0.399481	6.910468	-4.356869
1	0.573568	7.722643	-3.116331
1	-0.745093	8.598886	-3.931099
6	-2.875743	7.059944	-3.002404

1	-2.933008	6.323025	-3.814394
1	-3.195861	8.030587	-3.405425
1	-3.588095	6.756939	-2.224584
6	1.527604	0.838679	3.632259
1	0.680424	0.546408	2.996670
6	2.095282	-0.479751	4.217351
1	2.918787	-0.288542	4.917980
1	2.477542	-1.127410	3.418231
1	1.306950	-1.023033	4.753405
6	0.946135	1.729016	4.760786
1	1.723271	2.023816	5.478351
1	0.166649	1.182596	5.307907
1	0.499495	2.646935	4.356750
6	3.317683	2.738152	-0.868371
1	2.384409	2.291207	-1.235644
6	4.478557	2.046315	-1.627011
1	4.339977	2.148016	-2.712239
1	4.525065	0.980545	-1.380916
1	5.447157	2.495911	-1.372096
6	3.278092	4.246757	-1.221358
1	3.225227	4.382838	-2.310390
1	4.180187	4.759191	-0.860883
1	2.403161	4.734409	-0.781738
6	-3.400144	-2.543618	-2.126489
1	-4.180956	-3.044681	-2.714727
6	-2.300330	-2.132247	-3.144910
1	-1.930730	-3.016422	-3.683329
1	-1.440437	-1.659100	-2.650639
1	-2.701620	-1.424075	-3.880528
6	-2.883605	-3.625851	-1.139090
1	-2.775529	-4.582255	-1.669491
1	-3.577156	-3.786188	-0.303890
1	-1.891324	-3.397169	-0.727879
6	-3.816463	1.864023	0.751555
1	-2.767933	1.652584	1.009013
6	-3.851723	3.252411	0.055839
1	-3.267287	3.257690	-0.870564
1	-3.437570	4.023934	0.714599
1	-4.881041	3.546581	-0.187000
6	-4.618458	1.916298	2.078680
1	-4.556401	0.970074	2.624715
1	-5.679411	2.127695	1.888633
1	-4.229764	2.714625	2.726753
6	-7.538034	0.298769	-2.285002
1	-7.953462	1.205453	-1.820353
6	-8.511620	-0.870386	-1.988488
1	-8.617643	-1.028057	-0.907546
1	-8.148522	-1.808203	-2.429616
1	-9.505966	-0.665127	-2.407165
6	-7.433433	0.561005	-3.810952
1	-7.019781	-0.312763	-4.332077
1	-6.776763	1.415443	-4.018598
1	-8.422523	0.772726	-4.239104
6	6.038123	3.158135	3.392686
1	6.694902	3.595596	2.625843
6	5.708815	4.276708	4.416666
1	5.187517	5.111921	3.932000
1	6.626635	4.663468	4.879838
1	5.059961	3.897084	5.217106
6	6.817129	2.001917	4.069828
1	7.086935	1.227597	3.340047
1	6.216740	1.526408	4.856462
1	7.740355	2.375720	4.532728
15	-1.754809	-1.560531	2.999559
6	-1.362570	-3.412472	2.842016
6	-0.571343	-6.142284	2.684907
6	-2.320241	-4.449636	2.921621
6	0.001060	-3.768546	2.686372

6	0.392214	-5.117018	2.609350
6	-1.928076	-5.800275	2.842953
1	-3.370466	-4.208901	3.057225
1	0.758451	-2.988785	2.634985
1	1.445732	-5.366177	2.498180
1	-2.682917	-6.581704	2.906012
1	-0.269692	-7.185971	2.629575
6	-3.593999	-1.559321	3.449267
6	-6.299238	-1.417711	4.306437
6	-4.648875	-1.907214	2.575179
6	-3.918440	-1.138960	4.761427
6	-5.258633	-1.069721	5.189114
6	-5.989480	-1.836692	2.998078
1	-4.434640	-2.207167	1.553676
1	-3.119270	-0.864094	5.445945
1	-5.485779	-0.742264	6.201200
1	-6.784585	-2.094516	2.302468
1	-7.335618	-1.355840	4.630630
46	0.777920	-1.220730	-0.889403
15	2.745481	-2.504822	-1.665212
6	2.202485	-4.309113	-2.114110
6	1.195039	-6.510575	-1.285663
6	0.786949	-5.753671	-3.683752
6	0.213027	-6.530106	-2.477623
6	1.192704	-4.312384	-3.290140
6	1.607220	-5.067993	-0.904116
1	2.095412	-7.089669	-1.548025
1	1.669330	-6.286819	-4.072923
1	-0.738522	-6.069819	-2.168754
1	0.298539	-3.748972	-2.988154
1	0.728338	-4.522488	-0.531154
1	3.119513	-4.825840	-2.443071
1	0.740673	-7.001436	-0.413468
1	0.050646	-5.720171	-4.499938
1	-0.013248	-7.566814	-2.765980
1	1.609875	-3.800397	-4.168258
1	2.324591	-5.109445	-0.074836
6	3.945351	-2.811527	-0.178624
6	5.717794	-4.156480	1.052461
6	5.246745	-1.742749	1.731004
6	6.315890	-2.853920	1.632848
6	4.551103	-1.496702	0.370872
6	5.029298	-3.908499	-0.315253
1	4.976602	-4.560418	1.760893
1	4.488989	-2.034040	2.475153
1	7.138019	-2.512406	0.983488
1	5.290361	-1.098666	-0.338347
1	5.792554	-3.600607	-1.042768
1	3.221909	-3.158689	0.576824
1	6.501308	-4.920016	0.941944
1	5.693867	-0.805632	2.089998
1	6.752251	-3.047946	2.623203
1	3.767377	-0.737470	0.486236
1	4.595738	-4.848140	-0.681839
6	3.692521	-2.049333	-3.304500
6	3.480136	-0.625690	-5.431986
6	5.775431	-1.340126	-4.588258
6	4.974754	-0.246870	-5.330404
6	5.179206	-1.636472	-3.188391
6	2.881247	-0.952133	-4.044266
1	3.371747	-1.500919	-6.092631
1	5.767639	-2.264920	-5.187742
1	5.073026	0.705635	-4.786082
1	5.273994	-0.736918	-2.566280
1	2.869938	-0.044416	-3.424146
1	3.658349	-2.969409	-3.909134
1	2.911624	0.193924	-5.894968
1	6.827261	-1.037204	-4.483972
1	5.394249	-0.084664	-6.333493

1	5.763759	-2.428385	-2.705806
1	1.832612	-1.262682	-4.147761

TS-N₂H₄-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.799858	0.333644	0.116294
6	-0.560637	-0.231116	0.484061
6	1.022481	1.851531	0.068133
6	1.611877	4.734982	0.059144
6	0.350729	2.794685	-0.828370
6	2.023595	2.455593	0.941779
6	2.282112	3.844922	0.899397
6	0.648228	4.169309	-0.785704
1	3.050576	4.243542	1.557096
1	0.127509	4.821057	-1.482027
6	-1.948357	0.422043	0.064944
6	-4.754895	1.140945	-0.280484
6	-2.638634	1.319510	0.977927
6	-2.676721	0.062227	-1.138086
6	-4.033965	0.447490	-1.256916
6	-4.013502	1.592641	0.812631
1	-4.544600	0.200054	-2.183937
1	-4.510164	2.215946	1.551749
6	2.063607	-0.541097	0.010948
6	4.667190	-1.859904	-0.401115
6	2.607864	-1.530261	0.964712
6	2.902102	-0.315563	-1.160388
6	4.147068	-0.954188	-1.327673
6	3.864352	-2.121705	0.713146
1	4.724738	-0.739475	-2.223391
1	4.240342	-2.823722	1.450455
6	2.903206	1.720448	1.965386
1	2.579861	0.689562	2.017419
6	4.399648	1.742962	1.545065
1	4.544273	1.294193	0.556683
1	5.005418	1.178487	2.267299
1	4.790595	2.769941	1.513972
6	2.750778	2.309783	3.393101
1	1.703484	2.270342	3.712536
1	3.091854	3.351148	3.454209
1	3.354906	1.729348	4.105057
6	-0.620487	2.449266	-1.977207
1	-0.816627	1.386057	-1.944045
6	-1.976765	3.198083	-1.870562
1	-2.662195	2.840864	-2.650166
1	-1.845746	4.277494	-2.022470
1	-2.458992	3.049391	-0.904420
6	-0.035030	2.782409	-3.381023
1	-0.744942	2.466939	-4.159110
1	0.919744	2.291331	-3.574701
1	0.118713	3.862651	-3.495944
6	1.940355	6.226480	0.038323
1	2.720553	6.403320	0.794096
6	2.514171	6.670140	-1.334016
1	1.774464	6.534267	-2.134332
1	3.405497	6.087354	-1.598279
1	2.791192	7.733141	-1.310987
6	0.714010	7.095283	0.421507
1	-0.100496	6.972190	-0.304816
1	0.986309	8.159461	0.442452
1	0.327055	6.819098	1.410485
6	2.060159	-2.026179	2.335097
1	1.044673	-1.691894	2.468868

6	2.026022	-3.581107	2.428974
1	3.026302	-4.011721	2.566965
1	1.575466	-4.032490	1.540109
1	1.428591	-3.878605	3.303470
6	2.876899	-1.497084	3.549098
1	3.940445	-1.758887	3.470599
1	2.490629	-1.954411	4.472400
1	2.794058	-0.414590	3.656761
6	2.514012	0.573071	-2.351662
1	1.500288	0.923368	-2.191189
6	2.521507	-0.222757	-3.687396
1	2.095357	0.388777	-4.495037
1	1.931500	-1.142834	-3.610561
1	3.538738	-0.500322	-3.990375
6	3.442594	1.810446	-2.474818
1	3.163783	2.418087	-3.346317
1	4.488846	1.504627	-2.606268
1	3.382097	2.444469	-1.584540
6	-2.224080	-0.579320	-2.501463
1	-2.560850	0.186386	-3.218668
6	-0.727284	-0.813206	-2.829290
1	-0.601643	-1.761754	-3.358660
1	-0.087211	-0.842449	-1.949895
1	-0.346051	-0.024963	-3.484466
6	-3.041099	-1.851848	-2.879504
1	-2.878183	-2.075530	-3.942497
1	-4.119316	-1.725780	-2.730831
1	-2.715588	-2.723033	-2.311366
6	-2.008211	2.138885	2.138457
1	-0.931170	1.990065	2.159623
6	-2.192231	3.668115	1.932516
1	-1.672872	4.007088	1.031530
1	-1.757498	4.200756	2.789782
1	-3.246870	3.959604	1.857427
6	-2.601248	1.749211	3.524592
1	-2.589829	0.665843	3.716450
1	-3.649907	2.062481	3.605737
1	-2.047146	2.246235	4.331924
6	-6.239863	1.464763	-0.435751
1	-6.552840	2.011340	0.466556
6	-7.104854	0.180665	-0.527384
1	-6.954842	-0.460331	0.350846
1	-6.849675	-0.403593	-1.421649
1	-8.171236	0.436975	-0.587821
6	-6.505073	2.388860	-1.653875
1	-6.241325	1.889145	-2.595555
1	-5.916305	3.312216	-1.586938
1	-7.567994	2.660769	-1.706542
6	6.026772	-2.528047	-0.591725
1	6.432884	-2.184227	-1.554903
6	7.028524	-2.106257	0.516111
1	7.148128	-1.016089	0.547752
1	8.014316	-2.557468	0.338505
1	6.681783	-2.434517	1.505024
6	5.905837	-4.073293	-0.657959
1	5.219185	-4.383829	-1.455552
1	5.524728	-4.480544	0.287787
1	6.886482	-4.530103	-0.848877
15	-0.561596	-2.387656	0.520643
6	-0.606421	-3.564739	-0.972859
6	-0.346017	-5.567726	-2.979844
6	-1.607710	-4.548608	-1.152685
6	0.545921	-3.625688	-1.796169
6	0.668467	-4.605937	-2.796024
6	-1.477866	-5.540079	-2.144581
1	-2.486835	-4.556986	-0.516467
1	1.353162	-2.911100	-1.652957
1	1.557147	-4.624392	-3.423219
1	-2.262650	-6.284665	-2.261629

1	-0.249849	-6.329064	-3.750728
6	-2.223557	-2.763045	1.368308
6	-4.530880	-3.515883	2.855940
6	-3.519916	-2.577933	0.837166
6	-2.107870	-3.338026	2.658995
6	-3.246710	-3.712565	3.397960
6	-4.661696	-2.946531	1.574602
1	-3.649215	-2.139344	-0.144235
1	-1.117877	-3.503733	3.076815
1	-3.128736	-4.158582	4.382989
1	-5.648960	-2.791962	1.145089
1	-5.414097	-3.805000	3.421109
7	0.168211	0.280045	2.864031
1	-0.228650	0.285746	3.824419
7	-0.690202	-0.346278	2.059068
1	-1.658991	-0.496898	2.374290

		1		
		A		
Frequencies	--	-264.4616		
Red. masses	--	3.5747		
Frc consts	--	0.1473		
IR Inten	--	62.9048		
Atom	AN	X	Y	Z
1	6	0.05	0.04	0.08
2	6	-0.06	0.04	0.23
3	6	0.02	0.01	0.00
4	6	0.00	0.01	0.00
5	6	0.00	0.00	0.01
6	6	0.02	0.01	0.00
7	6	0.01	0.01	0.00
8	6	0.00	0.00	0.00
9	1	0.01	0.02	0.01
10	1	0.00	0.00	0.01
11	6	-0.02	0.01	0.01
12	6	-0.01	0.00	0.00
13	6	-0.02	0.01	0.01
14	6	0.00	0.01	0.01
15	6	0.00	0.01	0.00
16	6	-0.02	0.01	0.00
17	1	0.00	0.00	0.00
18	1	-0.03	0.01	0.00
19	6	-0.01	0.02	0.02
20	6	-0.01	0.00	0.00
21	6	-0.01	-0.01	0.01
22	6	0.00	0.02	0.01
23	6	-0.01	0.01	0.01
24	6	-0.01	0.00	0.00
25	1	-0.01	0.00	0.00
26	1	-0.01	-0.01	0.00
27	6	0.02	0.01	0.00
28	1	0.01	0.01	0.00
29	6	0.01	0.01	0.00
30	1	0.01	0.01	0.00
31	1	0.01	0.00	0.00
32	1	0.02	0.00	0.00
33	6	0.01	0.01	0.00
34	1	0.00	-0.01	-0.01
35	1	0.00	0.01	0.01
36	1	0.01	0.01	0.00
37	6	0.00	0.00	0.01
38	1	0.00	0.00	0.01
39	6	0.00	0.00	0.00
40	1	0.00	0.00	0.00
41	1	0.00	0.00	0.00
42	1	0.00	0.00	0.00
43	6	0.00	0.00	0.00
44	1	0.00	0.00	0.01

45	1	0.00	0.00	0.00
46	1	0.00	0.00	0.00
47	6	0.00	0.00	0.00
48	1	0.00	0.01	0.00
49	6	0.00	0.00	0.00
50	1	0.00	0.00	0.00
51	1	0.00	0.00	0.00
52	1	0.00	0.00	0.00
53	6	0.00	0.00	0.00
54	1	0.00	0.00	0.00
55	1	0.00	0.00	0.00
56	1	0.00	0.00	0.00
57	6	-0.01	0.00	0.01
58	1	-0.01	-0.01	0.00
59	6	0.00	0.00	0.01
60	1	0.00	0.00	0.00
61	1	0.00	0.00	0.01
62	1	0.00	0.00	0.01
63	6	0.00	0.00	0.00
64	1	0.00	-0.01	0.00
65	1	0.00	0.01	0.00
66	1	0.01	0.00	-0.01
67	6	0.00	0.01	0.00
68	1	0.00	0.01	0.00
69	6	0.00	0.00	0.01
70	1	-0.01	0.00	0.01
71	1	0.00	0.00	0.01
72	1	0.00	0.00	0.00
73	6	0.00	0.00	0.00
74	1	0.00	0.00	0.00
75	1	0.00	0.00	0.00
76	1	0.00	0.01	0.00
77	6	0.01	0.00	0.01
78	1	0.02	0.00	0.01
79	6	0.01	0.00	0.05
80	1	0.03	-0.01	0.08
81	1	-0.01	0.01	0.07
82	1	0.03	-0.01	0.04
83	6	0.01	0.00	0.01
84	1	0.02	0.00	0.01
85	1	0.01	0.00	-0.01
86	1	0.00	0.00	0.01
87	6	-0.02	0.01	0.01
88	1	-0.02	-0.01	0.04
89	6	-0.01	0.01	0.01
90	1	-0.01	0.00	0.01
91	1	-0.01	0.00	0.01
92	1	-0.01	0.01	0.01
93	6	-0.01	-0.01	0.00
94	1	0.03	-0.01	-0.01
95	1	-0.01	-0.02	0.02
96	1	0.00	-0.02	0.00
97	6	-0.01	0.00	-0.01
98	1	-0.01	0.00	-0.01
99	6	0.00	0.00	0.00
100	1	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	1	0.00	0.00	0.00
103	6	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	1	0.00	0.00	-0.01
107	6	-0.01	0.00	0.00
108	1	-0.01	0.00	0.00
109	6	0.00	0.00	0.00
110	1	0.00	0.00	0.00
111	1	-0.01	0.00	0.00
112	1	0.00	0.00	0.00

113	6	0.00	0.00	0.00
114	1	0.00	0.00	0.00
115	1	0.00	0.00	0.00
116	1	0.00	0.01	0.00
117	15	-0.01	-0.08	-0.02
118	6	0.00	-0.05	0.01
119	6	0.00	-0.01	-0.02
120	6	-0.01	-0.04	-0.02
121	6	-0.01	-0.03	0.00
122	6	0.00	-0.01	-0.01
123	6	-0.01	-0.02	-0.03
124	1	-0.01	-0.04	-0.01
125	1	-0.01	-0.02	0.01
126	1	0.00	0.00	-0.01
127	1	0.00	-0.02	-0.04
128	1	0.00	-0.01	-0.03
129	6	0.00	-0.03	0.00
130	6	-0.01	0.00	0.01
131	6	0.00	-0.02	0.00
132	6	-0.01	-0.02	0.01
133	6	-0.01	0.00	0.01
134	6	0.00	0.00	0.00
135	1	0.01	-0.02	0.00
136	1	-0.01	-0.04	0.00
137	1	-0.02	0.01	0.02
138	1	0.00	0.00	0.00
139	1	-0.01	0.01	0.01
140	7	0.09	0.07	-0.15
141	1	0.37	-0.76	-0.03
142	7	-0.01	0.14	-0.23
143	1	0.09	-0.16	-0.11

TS-N₂H₄-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	1.082376	0.166304	0.552802
14	-1.099903	-0.278468	0.110523
6	1.971639	1.898114	0.376250
6	3.503992	4.348789	0.097269
6	1.522641	2.978440	-0.462281
6	3.209045	2.101835	1.079543
6	3.937616	3.301952	0.922581
6	2.289315	4.158186	-0.578401
1	4.873151	3.421903	1.465587
1	1.917313	4.952125	-1.221754
6	-2.531462	0.996738	-0.074893
6	-4.784045	2.781004	-0.390605
6	-2.982565	1.837615	1.007173
6	-3.210668	1.119091	-1.338557
6	-4.303904	2.007570	-1.456158
6	-4.099813	2.680711	0.828818
1	-4.788291	2.087034	-2.428102
1	-4.436053	3.292371	1.662701
6	2.333769	-1.221500	-0.040665
6	4.466755	-2.998194	-0.844725
6	2.691631	-2.364787	0.751837
6	3.014533	-1.051703	-1.295517
6	4.061001	-1.929876	-1.656771
6	3.749204	-3.204666	0.345016
1	4.568145	-1.778445	-2.608007
1	4.008398	-4.051504	0.975382
6	3.813647	1.082654	2.054563
1	3.206134	0.174943	2.032681
6	5.250967	0.654813	1.658427

1	5.269494	0.228570	0.648860
1	5.628053	-0.104828	2.356364
1	5.946485	1.503926	1.683892
6	3.789703	1.631351	3.506743
1	2.778978	1.950172	3.796361
1	4.442444	2.507544	3.608208
1	4.139733	0.869653	4.217359
6	0.218670	2.968544	-1.270146
1	-0.266201	1.997816	-1.138601
6	-0.764574	4.048401	-0.750194
1	-1.736845	3.951860	-1.248556
1	-0.378378	5.058940	-0.940330
1	-0.925626	3.946001	0.326628
6	0.450823	3.171115	-2.792101
1	-0.504940	3.101412	-3.328384
1	1.132302	2.420143	-3.207435
1	0.875770	4.160528	-3.004802
6	4.314730	5.639830	-0.036867
1	5.232549	5.515485	0.557554
6	4.745469	5.917674	-1.500912
1	3.873248	6.070838	-2.149984
1	5.327473	5.082782	-1.910828
1	5.362905	6.825089	-1.552541
6	3.548380	6.858259	0.543520
1	2.623914	7.047812	-0.018053
1	4.166898	7.764572	0.487376
1	3.275302	6.692238	1.593095
6	1.965927	-2.757983	2.047277
1	1.039085	-2.183343	2.112653
6	1.539291	-4.249393	2.048751
1	2.402559	-4.926895	2.076060
1	0.938921	-4.482026	1.163413
1	0.927321	-4.458837	2.937278
6	2.823579	-2.464998	3.307468
1	3.750948	-3.053207	3.293595
1	2.270916	-2.734355	4.218854
1	3.108783	-1.408962	3.378774
6	2.635189	0.004417	-2.345506
1	1.811334	0.606426	-1.951302
6	2.114117	-0.668304	-3.645203
1	1.780519	0.094949	-4.361912
1	1.266750	-1.332452	-3.436896
1	2.898433	-1.262397	-4.131547
6	3.804600	0.969950	-2.669832
1	3.489170	1.718059	-3.409512
1	4.662332	0.429005	-3.091463
1	4.142162	1.500681	-1.772770
6	-2.938581	0.369455	-2.668826
1	-3.202968	1.098986	-3.449659
6	-1.507246	-0.084639	-3.019342
1	-1.488292	-0.417218	-4.067289
1	-1.169167	-0.926960	-2.411350
1	-0.778333	0.722091	-2.905487
6	-3.936381	-0.812020	-2.821929
1	-3.795328	-1.308192	-3.791233
1	-4.974241	-0.461420	-2.759621
1	-3.781833	-1.563844	-2.042929
6	-2.318100	1.880694	2.394433
1	-1.311551	1.464002	2.305036
6	-2.167559	3.317264	2.970239
1	-1.676683	3.999096	2.266679
1	-1.564414	3.285678	3.888146
1	-3.137887	3.755704	3.240079
6	-3.104509	1.016313	3.417285
1	-3.179909	-0.025551	3.092613
1	-4.122256	1.411070	3.547659
1	-2.611883	1.041336	4.400770
6	-5.975836	3.721103	-0.561506
1	-6.173084	4.190360	0.414013

6	-7.256153	2.954161	-0.981611
1	-7.506689	2.174202	-0.251414
1	-7.123061	2.469133	-1.957642
1	-8.110486	3.639835	-1.061214
6	-5.657526	4.856810	-1.570050
1	-5.450547	4.449683	-2.568708
1	-4.777013	5.429927	-1.252915
1	-6.506720	5.547845	-1.657611
6	5.620932	-3.911623	-1.260304
1	5.992557	-3.553264	-2.232205
6	6.801079	-3.837128	-0.256238
1	7.165697	-2.807605	-0.149576
1	7.636641	-4.465092	-0.594562
1	6.496383	-4.190599	0.737731
6	5.157329	-5.379461	-1.452335
1	4.346211	-5.445703	-2.188203
1	4.789696	-5.805340	-0.509434
1	5.990603	-6.005081	-1.800436
15	-1.453723	-2.590286	0.400266
6	-2.057194	-3.454855	-1.191501
6	-2.740742	-4.934501	-3.528940
6	-3.314603	-4.092354	-1.306696
6	-1.137843	-3.597114	-2.259586
6	-1.477461	-4.319512	-3.418295
6	-3.652275	-4.824083	-2.462941
1	-4.036368	-4.026925	-0.498697
1	-0.145890	-3.155433	-2.181347
1	-0.755948	-4.409357	-4.227795
1	-4.627589	-5.302842	-2.528209
1	-3.004563	-5.494620	-4.423724
6	-2.984577	-2.718772	1.510850
6	-5.171901	-3.070324	3.288314
6	-4.215947	-2.066281	1.275952
6	-2.865943	-3.548403	2.650106
6	-3.949429	-3.724067	3.533781
6	-5.301400	-2.242537	2.155595
1	-4.331351	-1.415325	0.413852
1	-1.926492	-4.061946	2.839200
1	-3.838886	-4.368226	4.403702
1	-6.241187	-1.731858	1.958165
1	-6.010166	-3.202990	3.969008
7	0.642171	0.209379	2.887870
1	1.266882	0.434980	3.698503
7	-0.293972	-0.683318	3.119493
1	-0.435653	-0.884638	4.139986

		1		
		A		
Frequencies	--	-286.5110		
Red. masses	--	6.5117		
Frc consts	--	0.3149		
IR Inten	--	79.9462		
Atom AN		X	Y	Z
1	14	0.02	0.00	0.22
2	14	-0.06	-0.02	0.07
3	6	0.00	0.01	0.04
4	6	0.00	0.00	0.00
5	6	0.00	-0.01	0.01
6	6	0.01	0.01	0.01
7	6	0.01	0.00	0.00
8	6	0.00	-0.01	0.00
9	1	0.02	0.01	-0.01
10	1	0.00	-0.02	-0.01
11	6	-0.01	0.00	-0.01
12	6	0.00	0.00	0.00
13	6	0.00	0.01	0.00

14	6	-0.01	0.00	0.00
15	6	0.00	0.00	-0.01
16	6	0.00	0.00	0.00
17	1	0.00	0.01	0.00
18	1	0.00	0.00	0.00
19	6	-0.01	0.01	0.03
20	6	-0.01	0.00	0.00
21	6	-0.01	0.00	0.01
22	6	-0.02	0.01	0.02
23	6	-0.02	0.01	0.01
24	6	-0.01	0.00	0.00
25	1	-0.03	0.01	0.01
26	1	-0.01	0.00	0.00
27	6	0.02	0.01	0.01
28	1	0.03	0.00	0.01
29	6	0.01	0.01	0.00
30	1	0.01	0.01	0.00
31	1	0.01	0.01	0.00
32	1	0.02	0.01	0.00
33	6	0.02	0.01	0.01
34	1	0.02	0.01	0.01
35	1	0.02	0.00	0.01
36	1	0.01	0.00	0.01
37	6	0.00	-0.01	0.01
38	1	-0.01	-0.01	0.01
39	6	0.00	-0.01	0.00
40	1	0.00	-0.01	0.00
41	1	0.01	-0.01	0.00
42	1	0.00	0.00	0.00
43	6	0.00	-0.01	0.01
44	1	0.00	-0.01	0.01
45	1	0.00	-0.01	0.00
46	1	0.00	-0.01	0.01
47	6	0.00	0.00	0.00
48	1	0.00	0.00	0.00
49	6	0.00	0.00	0.00
50	1	0.00	0.00	0.00
51	1	0.00	0.00	0.00
52	1	0.00	0.00	0.00
53	6	0.00	0.00	0.00
54	1	0.00	0.00	0.00
55	1	0.00	0.00	0.00
56	1	0.00	0.00	0.00
57	6	0.00	-0.01	0.01
58	1	-0.01	-0.03	0.05
59	6	0.00	-0.01	0.00
60	1	0.00	-0.01	0.00
61	1	0.00	-0.01	0.00
62	1	0.00	-0.01	0.00
63	6	0.01	-0.01	0.01
64	1	0.00	-0.02	0.01
65	1	0.00	0.00	0.01
66	1	0.01	-0.01	0.00
67	6	-0.02	0.01	0.02
68	1	-0.01	0.02	0.02
69	6	-0.01	0.01	0.01
70	1	-0.01	0.00	0.01
71	1	0.00	0.00	0.01
72	1	0.00	0.01	0.02
73	6	-0.01	0.00	0.01
74	1	-0.01	0.00	0.01
75	1	-0.02	-0.01	0.01
76	1	0.00	0.00	0.01
77	6	0.00	0.00	0.00
78	1	0.01	-0.01	-0.01
79	6	0.01	0.00	0.03
80	1	0.03	-0.03	0.04
81	1	0.01	0.02	0.05

82	1	0.00	0.01	0.01
83	6	0.00	0.00	0.00
84	1	0.01	0.00	0.00
85	1	0.00	0.00	-0.01
86	1	0.00	0.00	0.00
87	6	0.00	0.00	0.00
88	1	0.00	0.00	0.02
89	6	0.00	0.00	0.00
90	1	0.00	0.01	0.00
91	1	0.00	0.00	0.00
92	1	0.00	0.01	0.00
93	6	-0.01	0.01	0.00
94	1	0.00	0.01	0.00
95	1	-0.01	0.01	0.00
96	1	0.00	0.00	-0.01
97	6	0.00	0.00	0.00
98	1	0.00	0.00	0.00
99	6	0.00	0.00	0.00
100	1	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	1	0.00	0.00	0.00
103	6	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	1	0.00	0.00	0.00
107	6	-0.01	0.01	0.00
108	1	-0.01	0.01	0.00
109	6	0.00	0.00	0.00
110	1	0.00	0.00	0.00
111	1	-0.01	0.00	0.00
112	1	0.00	0.00	0.00
113	6	0.00	0.00	0.00
114	1	0.00	0.00	0.00
115	1	0.00	0.00	0.00
116	1	0.00	0.01	0.00
117	15	0.00	-0.01	0.00
118	6	0.00	-0.01	0.00
119	6	0.00	0.00	0.00
120	6	0.00	0.00	0.00
121	6	0.00	0.00	0.00
122	6	0.00	0.00	0.00
123	6	0.00	0.00	0.00
124	1	0.00	0.00	0.00
125	1	0.00	-0.01	0.00
126	1	0.00	0.00	0.00
127	1	0.00	0.00	-0.01
128	1	0.00	0.00	0.00
129	6	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	6	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	6	0.00	0.00	0.00
134	6	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	1	0.01	0.01	0.01
137	1	0.01	0.01	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00
140	7	0.09	0.03	-0.47
141	1	0.23	0.05	-0.61
142	7	0.04	-0.02	-0.25
143	1	0.03	0.40	-0.18

TS-N₂H₄-Ge

S-

S144

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.095201	0.170231	0.634331
32	-1.118530	-0.309430	-0.259020
6	2.046116	1.947875	0.396724
6	3.580350	4.372751	0.099969
6	1.581963	3.021247	-0.436255
6	3.290872	2.131259	1.080734
6	4.026832	3.324641	0.917156
6	2.354233	4.195263	-0.559889
1	4.973708	3.437484	1.441878
1	1.980496	4.993790	-1.196356
6	-2.626877	1.020515	-0.171623
6	-4.830387	2.863040	-0.330833
6	-3.007031	1.817447	0.963043
6	-3.344579	1.202248	-1.406569
6	-4.414931	2.122469	-1.447383
6	-4.108710	2.696564	0.860040
1	-4.939514	2.250311	-2.392870
1	-4.402692	3.280894	1.729560
6	2.393691	-1.256319	-0.059701
6	4.464800	-3.044661	-0.949806
6	2.743444	-2.417869	0.702459
6	3.031033	-1.071064	-1.329631
6	4.053189	-1.958507	-1.735445
6	3.776806	-3.267050	0.255504
1	4.535142	-1.800920	-2.698754
1	4.036557	-4.133058	0.859380
6	3.895522	1.084379	2.027041
1	3.265241	0.188974	2.009764
6	5.300746	0.611635	1.574500
1	5.262742	0.186956	0.565077
1	5.680370	-0.162079	2.255436
1	6.020996	1.439616	1.572637
6	3.937471	1.608921	3.487797
1	2.951264	1.963809	3.818710
1	4.626065	2.457744	3.579753
1	4.283123	0.824267	4.175578
6	0.268273	3.009688	-1.232501
1	-0.217872	2.037725	-1.102714
6	-0.717046	4.087530	-0.712309
1	-1.690164	3.985847	-1.208442
1	-0.335114	5.098705	-0.907300
1	-0.876713	3.988699	0.364357
6	0.486810	3.208355	-2.756912
1	-0.477350	3.161558	-3.280131
1	1.144971	2.441858	-3.180744
1	0.930161	4.188621	-2.973295
6	4.393122	5.657997	-0.051217
1	5.323342	5.530396	0.522542
6	4.788768	5.926082	-1.526374
1	3.901051	6.082974	-2.153189
1	5.350372	5.081918	-1.946033
1	5.413391	6.826546	-1.599988
6	3.639774	6.875331	0.546503
1	2.703732	7.064677	0.004373
1	4.256105	7.782096	0.481292
1	3.387001	6.704504	1.600510
6	2.023191	-2.817565	1.999681
1	1.103702	-2.229959	2.073858
6	1.569676	-4.300442	1.987412
1	2.421178	-4.992943	1.988499
1	0.949335	-4.507960	1.109687
1	0.967700	-4.513010	2.881832
6	2.895007	-2.549350	3.255698
1	3.809579	-3.156046	3.229998
1	2.345977	-2.812773	4.171208
1	3.207502	-1.500021	3.328165

6	2.624889	0.006895	-2.346889
1	1.818080	0.607533	-1.915796
6	2.053634	-0.637568	-3.639907
1	1.710323	0.141624	-4.334638
1	1.202303	-1.291970	-3.416191
1	2.813622	-1.235576	-4.159011
6	3.789574	0.970104	-2.692039
1	3.458309	1.728097	-3.414461
1	4.632608	0.429413	-3.142220
1	4.152799	1.489151	-1.798135
6	-3.159138	0.465686	-2.762697
1	-3.539523	1.180620	-3.507301
6	-1.749481	0.080244	-3.275659
1	-1.815204	-0.125698	-4.355011
1	-1.362044	-0.826974	-2.801646
1	-1.013738	0.876992	-3.127577
6	-4.097038	-0.772074	-2.823452
1	-4.024511	-1.256679	-3.806382
1	-5.142416	-0.483249	-2.654037
1	-3.819396	-1.517183	-2.070198
6	-2.285853	1.775325	2.321753
1	-1.309586	1.303108	2.178725
6	-2.037024	3.180859	2.938808
1	-1.540441	3.865538	2.242936
1	-1.401545	3.084737	3.829751
1	-2.973998	3.654586	3.262521
6	-3.067237	0.919018	3.353936
1	-3.172489	-0.116593	3.022361
1	-4.070305	1.337511	3.519708
1	-2.539935	0.915281	4.318210
6	-6.008751	3.829572	-0.428106
1	-6.162222	4.274894	0.566210
6	-7.314179	3.090621	-0.821871
1	-7.549930	2.296765	-0.101698
1	-7.219087	2.625587	-1.812075
1	-8.161676	3.788146	-0.858169
6	-5.707120	4.984769	-1.419184
1	-5.536823	4.598123	-2.432853
1	-4.808431	5.537617	-1.117217
1	-6.548489	5.689181	-1.464415
6	5.598218	-3.961514	-1.409717
1	5.949252	-3.589637	-2.384131
6	6.800953	-3.909965	-0.431775
1	7.172984	-2.883747	-0.318131
1	7.625333	-4.537108	-0.797332
1	6.515330	-4.275739	0.563403
6	5.116090	-5.421034	-1.615191
1	4.288144	-5.466355	-2.333791
1	4.764688	-5.859154	-0.671738
1	5.934771	-6.048836	-1.992395
15	-1.499174	-2.631033	0.461882
6	-2.096816	-3.487556	-1.129203
6	-2.800458	-4.876700	-3.511830
6	-3.355475	-4.116925	-1.255408
6	-1.187375	-3.582512	-2.211816
6	-1.536262	-4.264189	-3.391613
6	-3.703891	-4.803701	-2.435735
1	-4.069296	-4.073599	-0.438619
1	-0.201143	-3.128220	-2.129309
1	-0.823362	-4.320714	-4.211861
1	-4.681773	-5.275224	-2.511235
1	-3.072280	-5.403751	-4.423914
6	-3.027971	-2.729821	1.566968
6	-5.209072	-3.044992	3.353424
6	-4.249088	-2.058610	1.334731
6	-2.913155	-3.554483	2.710252
6	-3.994764	-3.714712	3.597233
6	-5.331845	-2.215912	2.220800
1	-4.353434	-1.402939	0.474458

1	-1.977350	-4.075650	2.897466
1	-3.888476	-4.358551	4.467717
1	-6.263042	-1.687564	2.030029
1	-6.046085	-3.165386	4.037537
7	0.804890	0.187985	2.903753
1	1.633924	0.333960	3.520610
7	-0.116136	-0.638748	3.344069
1	0.076107	-0.987786	4.310879

1				
A				
Frequencies	--	-132.9363		
Red. masses	--	7.1778		
Frc consts	--	0.0747		
IR Inten	--	11.4267		
Atom	AN	X	Y	Z
1	32	0.00	0.01	0.08
2	32	-0.02	-0.01	-0.01
3	6	-0.01	0.00	0.05
4	6	0.00	0.00	0.01
5	6	0.00	-0.01	0.03
6	6	0.01	0.00	0.02
7	6	0.01	0.00	0.01
8	6	0.00	-0.01	0.01
9	1	0.02	0.00	-0.01
10	1	0.00	-0.02	0.00
11	6	0.00	0.01	0.00
12	6	-0.01	0.01	-0.01
13	6	-0.01	0.02	0.00
14	6	0.00	0.01	0.00
15	6	-0.01	0.01	0.00
16	6	-0.01	0.01	-0.01
17	1	-0.01	0.00	0.00
18	1	-0.01	0.01	-0.01
19	6	0.00	0.00	0.06
20	6	-0.01	0.01	0.01
21	6	0.00	-0.01	0.03
22	6	-0.02	0.01	0.04
23	6	-0.02	0.01	0.03
24	6	0.00	-0.01	0.01
25	1	-0.04	0.02	0.02
26	1	0.00	-0.01	0.00
27	6	0.04	0.00	0.00
28	1	0.08	-0.03	-0.02
29	6	0.05	0.04	0.00
30	1	0.06	0.06	-0.01
31	1	0.06	0.03	-0.02
32	1	0.04	0.05	0.01
33	6	0.03	-0.02	0.01
34	1	0.02	-0.06	0.03
35	1	0.00	0.00	0.02
36	1	0.06	-0.02	0.00
37	6	0.00	-0.02	0.02
38	1	0.00	-0.01	0.02
39	6	0.00	-0.01	0.01
40	1	0.00	-0.01	0.01
41	1	0.00	-0.01	0.01
42	1	-0.01	-0.01	0.01
43	6	0.00	-0.01	0.02
44	1	0.00	-0.01	0.02
45	1	0.00	-0.01	0.02
46	1	0.00	-0.01	0.02
47	6	0.00	0.00	0.00
48	1	0.00	0.00	0.00
49	6	-0.01	-0.01	0.00
50	1	-0.01	-0.01	0.00
51	1	-0.01	-0.01	0.00
52	1	-0.01	-0.01	-0.01

53	6	0.00	0.00	0.00
54	1	-0.01	-0.01	0.00
55	1	-0.01	0.00	-0.01
56	1	0.00	0.00	0.00
57	6	0.01	-0.04	0.03
58	1	0.00	-0.06	0.05
59	6	0.02	-0.04	0.01
60	1	0.02	-0.04	0.00
61	1	0.02	-0.03	0.01
62	1	0.02	-0.05	0.01
63	6	0.01	-0.04	0.03
64	1	0.01	-0.03	0.02
65	1	0.01	-0.04	0.02
66	1	0.00	-0.03	0.03
67	6	-0.03	0.01	0.04
68	1	-0.03	0.01	0.04
69	6	-0.02	0.01	0.04
70	1	-0.03	0.00	0.04
71	1	-0.01	0.00	0.04
72	1	-0.01	0.01	0.04
73	6	-0.03	0.01	0.03
74	1	-0.03	0.00	0.03
75	1	-0.03	0.00	0.04
76	1	-0.02	0.01	0.03
77	6	0.00	0.01	0.00
78	1	-0.02	0.00	0.00
79	6	-0.01	0.02	-0.03
80	1	-0.02	0.04	-0.03
81	1	0.00	0.02	-0.04
82	1	-0.01	0.03	-0.02
83	6	0.01	0.00	0.01
84	1	0.00	0.00	0.01
85	1	0.01	-0.01	0.01
86	1	0.02	0.00	0.00
87	6	-0.01	0.03	-0.01
88	1	0.00	0.05	-0.01
89	6	-0.03	0.03	0.00
90	1	-0.05	0.04	0.01
91	1	-0.02	0.03	0.00
92	1	-0.04	0.01	0.01
93	6	0.02	0.00	-0.01
94	1	0.05	0.00	-0.01
95	1	0.01	-0.03	-0.01
96	1	0.02	0.01	-0.01
97	6	-0.01	0.00	-0.01
98	1	-0.01	0.00	-0.01
99	6	-0.01	0.00	-0.01
100	1	-0.01	0.00	-0.01
101	1	-0.01	0.00	-0.01
102	1	-0.01	0.00	-0.01
103	6	-0.01	0.00	-0.01
104	1	-0.01	0.00	-0.01
105	1	-0.01	0.00	0.00
106	1	-0.01	0.00	-0.01
107	6	-0.01	0.01	0.00
108	1	-0.02	0.02	0.00
109	6	-0.01	0.01	-0.01
110	1	-0.01	0.01	0.00
111	1	-0.01	0.01	-0.01
112	1	0.00	0.00	-0.01
113	6	-0.01	0.01	0.00
114	1	-0.01	0.01	0.00
115	1	0.00	0.01	0.00
116	1	-0.01	0.02	-0.01
117	15	0.00	0.00	0.00
118	6	0.00	-0.01	0.01
119	6	0.00	0.00	0.00
120	6	0.00	-0.01	0.01
121	6	0.00	0.00	0.00

122	6	0.00	0.00	0.00
123	6	0.00	-0.01	0.00
124	1	0.00	-0.02	0.01
125	1	-0.01	0.00	0.00
126	1	0.00	0.00	0.00
127	1	0.00	-0.01	0.00
128	1	0.00	0.00	0.00
129	6	0.00	-0.01	0.00
130	6	0.00	0.00	0.00
131	6	0.00	-0.01	0.00
132	6	0.00	0.00	0.01
133	6	0.00	0.00	0.01
134	6	0.00	0.00	0.00
135	1	0.00	-0.01	-0.01
136	1	0.00	0.01	0.01
137	1	0.00	0.01	0.01
138	1	0.00	-0.01	0.00
139	1	0.00	0.00	0.00
140	7	0.17	-0.03	-0.47
141	1	0.10	0.11	-0.45
142	7	0.07	0.03	-0.37
143	1	-0.04	0.43	-0.21

TS-N₂H₄-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	1.182808	0.170067	0.751458
50	-1.224731	-0.382775	-0.260500
6	2.191499	2.032093	0.384644
6	3.775814	4.376484	0.025481
6	1.736107	3.083736	-0.471436
6	3.446852	2.170908	1.043994
6	4.218008	3.333501	0.852766
6	2.538583	4.230658	-0.626018
1	5.176607	3.429163	1.358958
1	2.184268	5.030359	-1.272381
6	-2.719309	1.145385	-0.177727
6	-4.796251	3.083724	-0.362550
6	-3.036842	1.970307	0.951723
6	-3.389396	1.361671	-1.425445
6	-4.407981	2.332614	-1.482913
6	-4.089472	2.903996	0.835873
1	-4.916806	2.486795	-2.432471
1	-4.359688	3.513732	1.695614
6	2.469176	-1.368154	-0.107695
6	4.434258	-3.218260	-1.023010
6	2.765461	-2.540381	0.649379
6	3.075440	-1.197221	-1.389675
6	4.055575	-2.121728	-1.812676
6	3.753520	-3.430629	0.189773
1	4.532466	-1.985605	-2.782187
1	3.988934	-4.308779	0.785960
6	3.994814	1.089758	1.985006
1	3.319572	0.221357	1.956361
6	5.371811	0.541712	1.537721
1	5.310320	0.117529	0.528820
1	5.706140	-0.252394	2.218690
1	6.135165	1.329550	1.534941
6	4.020763	1.581136	3.453985
1	3.030752	1.942645	3.764696
1	4.722916	2.413933	3.578256
1	4.331260	0.772038	4.129776
6	0.407184	3.061240	-1.246242
1	-0.077248	2.090143	-1.086680

6	-0.573293	4.146044	-0.731335
1	-1.548786	4.045053	-1.223786
1	-0.187552	5.153986	-0.934663
1	-0.730771	4.054676	0.346621
6	0.594878	3.225821	-2.779092
1	-0.381313	3.184906	-3.281018
1	1.230910	2.440118	-3.202436
1	1.047628	4.194741	-3.024999
6	4.607944	5.641822	-0.142258
1	5.540319	5.502271	0.424500
6	4.989575	5.882520	-1.624071
1	4.096642	6.048511	-2.241000
1	5.522961	5.016232	-2.036105
1	5.634921	6.765183	-1.720738
6	3.869364	6.864445	0.460684
1	2.931770	7.060618	-0.076284
1	4.491302	7.766820	0.399719
1	3.617483	6.686470	1.514090
6	2.019355	-2.878760	1.950603
1	1.120002	-2.250768	2.011157
6	1.500320	-4.338287	1.969191
1	2.321215	-5.066474	1.983152
1	0.869388	-4.534110	1.096322
1	0.887666	-4.504405	2.865862
6	2.882490	-2.601413	3.208606
1	3.787201	-3.222480	3.203798
1	2.316382	-2.834362	4.121638
1	3.204077	-1.553175	3.261094
6	2.670819	-0.095961	-2.385632
1	1.886780	0.517655	-1.926269
6	2.055440	-0.706613	-3.675874
1	1.725723	0.090547	-4.357420
1	1.187666	-1.337580	-3.446402
1	2.787146	-1.322379	-4.214588
6	3.842364	0.852379	-2.746635
1	3.511071	1.614932	-3.464861
1	4.672154	0.300555	-3.207275
1	4.221917	1.367844	-1.857447
6	-3.193997	0.601536	-2.769806
1	-3.550849	1.312516	-3.528152
6	-1.782783	0.185111	-3.271213
1	-1.837542	0.000445	-4.354648
1	-1.430520	-0.751172	-2.822009
1	-1.017105	0.947869	-3.096069
6	-4.140473	-0.628767	-2.830404
1	-4.055999	-1.127634	-3.804831
1	-5.184343	-0.327998	-2.679703
1	-3.882577	-1.369561	-2.064461
6	-2.292997	1.905457	2.301412
1	-1.329699	1.405454	2.144461
6	-1.988584	3.303844	2.911207
1	-1.479198	3.970508	2.206877
1	-1.343361	3.188530	3.792918
1	-2.904365	3.809024	3.247204
6	-3.069187	1.070317	3.353865
1	-3.200546	0.033815	3.031805
1	-4.059278	1.509902	3.539883
1	-2.518427	1.060675	4.304974
6	-5.946493	4.076055	-0.470023
1	-6.092365	4.535331	0.518638
6	-7.259795	3.348336	-0.856761
1	-7.501944	2.566604	-0.125073
1	-7.164434	2.864872	-1.837978
1	-8.101046	4.051432	-0.906043
6	-5.604491	5.205631	-1.474932
1	-5.435168	4.796328	-2.479682
1	-4.689241	5.730402	-1.171904
1	-6.420575	5.936509	-1.539664
6	5.540884	-4.163822	-1.477488

1	5.902687	-3.809702	-2.454311
6	6.736600	-4.123527	-0.491012
1	7.124015	-3.101440	-0.388938
1	7.553213	-4.770838	-0.836753
1	6.432165	-4.465312	0.507102
6	5.011270	-5.607621	-1.665778
1	4.180119	-5.627934	-2.382160
1	4.642363	-6.018832	-0.716999
1	5.804608	-6.270246	-2.035655
15	-1.632414	-2.817164	0.476185
6	-2.257464	-3.557337	-1.152240
6	-3.007432	-4.804783	-3.590903
6	-3.546431	-4.105815	-1.312212
6	-1.345351	-3.639122	-2.234345
6	-1.717670	-4.253741	-3.442714
6	-3.917795	-4.726502	-2.520940
1	-4.260402	-4.050923	-0.495923
1	-0.340803	-3.229512	-2.131333
1	-1.002867	-4.309153	-4.261522
1	-4.916516	-5.145911	-2.619836
1	-3.293409	-5.290739	-4.520868
6	-3.155600	-2.788071	1.579873
6	-5.308048	-2.878463	3.416644
6	-4.327987	-2.035277	1.345600
6	-3.065706	-3.564761	2.756052
6	-4.134720	-3.614518	3.668686
6	-5.398790	-2.083161	2.256620
1	-4.403131	-1.397202	0.468373
1	-2.155420	-4.127811	2.946951
1	-4.048970	-4.226334	4.563517
1	-6.293265	-1.495167	2.064989
1	-6.138576	-2.920515	4.116984
7	0.759270	0.193665	3.050515
1	1.508243	0.361063	3.753618
7	-0.171748	-0.700521	3.388586
1	-0.085310	-1.005612	4.380778

		1		
		A		
Frequencies	--	-111.0865		
Red. masses	--	6.3891		
Frc consts	--	0.0465		
IR Inten	--	14.0696		
Atom AN		X	Y	Z
1	50	0.01	0.00	0.02
2	50	-0.02	-0.02	0.04
3	6	-0.01	0.01	0.04
4	6	0.00	-0.01	0.01
5	6	-0.01	-0.01	0.02
6	6	0.00	0.00	0.02
7	6	0.00	0.00	0.01
8	6	0.00	-0.01	0.01
9	1	0.01	0.00	0.00
10	1	0.00	-0.02	0.00
11	6	0.01	0.02	0.00
12	6	0.00	0.00	-0.01
13	6	0.00	0.02	0.00
14	6	0.01	0.01	0.00
15	6	0.00	0.00	-0.01
16	6	0.00	0.01	-0.01
17	1	0.00	0.00	-0.01
18	1	-0.01	0.01	-0.01
19	6	0.00	0.00	0.04
20	6	-0.01	0.00	0.01
21	6	0.00	0.00	0.03
22	6	-0.01	0.01	0.03
23	6	-0.02	0.01	0.02
24	6	0.00	0.00	0.01

25	1	-0.02	0.01	0.01
26	1	0.00	-0.01	0.01
27	6	0.01	0.00	0.02
28	1	0.03	-0.01	0.02
29	6	0.01	0.01	0.00
30	1	0.01	0.02	0.00
31	1	0.02	0.01	-0.01
32	1	0.01	0.02	0.00
33	6	0.03	0.00	0.02
34	1	0.03	0.00	0.03
35	1	0.03	0.00	0.01
36	1	0.03	0.00	0.01
37	6	0.00	-0.01	0.02
38	1	-0.01	0.00	0.02
39	6	0.00	0.00	0.01
40	1	0.00	0.00	0.01
41	1	0.00	-0.01	0.01
42	1	-0.01	0.00	0.01
43	6	0.00	-0.01	0.02
44	1	0.00	-0.01	0.02
45	1	0.00	-0.01	0.02
46	1	0.00	-0.01	0.02
47	6	0.00	-0.01	0.00
48	1	0.00	-0.01	0.00
49	6	-0.01	-0.01	0.00
50	1	-0.01	-0.01	0.00
51	1	-0.01	-0.01	0.00
52	1	-0.01	-0.01	0.00
53	6	0.00	-0.01	0.00
54	1	0.00	-0.01	0.00
55	1	0.00	-0.01	0.00
56	1	0.00	0.00	0.00
57	6	0.00	-0.01	0.02
58	1	0.00	-0.02	0.06
59	6	0.01	-0.01	0.01
60	1	0.00	-0.02	0.00
61	1	0.00	-0.01	0.01
62	1	0.01	-0.02	0.01
63	6	0.01	-0.03	0.02
64	1	0.02	-0.02	0.01
65	1	0.01	-0.03	0.02
66	1	0.00	-0.02	0.03
67	6	-0.02	0.01	0.03
68	1	-0.02	0.01	0.03
69	6	-0.01	0.01	0.03
70	1	-0.02	0.01	0.03
71	1	-0.01	0.00	0.03
72	1	-0.01	0.01	0.03
73	6	-0.02	0.01	0.03
74	1	-0.02	0.01	0.02
75	1	-0.02	0.01	0.03
76	1	-0.01	0.01	0.02
77	6	0.01	0.01	0.00
78	1	0.01	0.01	0.00
79	6	0.02	0.02	0.00
80	1	0.02	0.01	0.00
81	1	0.02	0.03	0.01
82	1	0.01	0.03	-0.01
83	6	0.02	0.00	0.00
84	1	0.02	0.01	0.00
85	1	0.02	0.00	0.00
86	1	0.02	0.00	0.00
87	6	0.01	0.03	-0.01
88	1	0.01	0.05	-0.01
89	6	-0.02	0.04	0.00
90	1	-0.04	0.05	0.00
91	1	-0.02	0.05	0.00
92	1	-0.03	0.01	0.01
93	6	0.03	0.01	-0.01

94	1	0.07	0.00	-0.01
95	1	0.01	-0.03	-0.02
96	1	0.01	0.04	0.00
97	6	-0.01	0.00	-0.01
98	1	-0.01	0.00	-0.01
99	6	0.00	0.00	-0.01
100	1	0.00	0.00	-0.01
101	1	0.00	0.00	-0.01
102	1	0.00	0.00	-0.01
103	6	-0.01	0.00	-0.01
104	1	0.00	0.00	-0.01
105	1	-0.01	0.00	-0.01
106	1	-0.01	0.00	-0.01
107	6	-0.01	0.01	0.00
108	1	-0.01	0.01	0.00
109	6	-0.01	0.01	0.00
110	1	-0.01	0.01	0.00
111	1	-0.01	0.01	-0.01
112	1	0.00	0.00	0.00
113	6	-0.01	0.01	0.00
114	1	-0.01	0.01	0.00
115	1	0.00	0.00	0.00
116	1	-0.01	0.01	0.00
117	15	0.01	-0.02	-0.01
118	6	-0.01	-0.01	-0.01
119	6	-0.01	0.00	-0.01
120	6	-0.01	-0.01	-0.01
121	6	-0.01	0.00	-0.01
122	6	-0.01	0.00	-0.01
123	6	-0.01	-0.01	-0.01
124	1	-0.01	-0.01	0.00
125	1	-0.01	0.00	-0.01
126	1	-0.01	0.00	-0.01
127	1	-0.01	-0.01	-0.01
128	1	-0.01	0.00	-0.01
129	6	0.01	-0.01	-0.01
130	6	0.01	0.00	0.00
131	6	0.00	-0.01	-0.01
132	6	0.01	0.00	0.00
133	6	0.01	0.01	0.00
134	6	0.01	0.00	-0.01
135	1	0.00	-0.02	-0.01
136	1	0.01	0.01	0.01
137	1	0.01	0.02	0.01
138	1	0.00	-0.01	-0.01
139	1	0.01	0.01	0.00
140	7	0.13	0.02	-0.38
141	1	-0.09	0.27	-0.23
142	7	0.07	-0.04	-0.44
143	1	-0.33	0.50	-0.24

TS-N₂H₄-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-1.292581	0.175966	-0.676803
82	1.315559	-0.390749	0.110272
6	-2.388558	2.038775	-0.320560
6	-4.032832	4.311171	0.016760
6	-1.954569	3.095593	0.526358
6	-3.628884	2.121331	-1.005931
6	-4.438254	3.258918	-0.820369
6	-2.792142	4.216891	0.674897
1	-5.395649	3.326664	-1.333637
1	-2.469023	5.031687	1.319055

6	2.754995	1.300627	0.168661
6	4.686700	3.365854	0.431883
6	3.024969	2.168851	-0.933198
6	3.369922	1.536882	1.438328
6	4.320351	2.574972	1.533507
6	4.010777	3.168614	-0.782184
1	4.794483	2.751005	2.497670
1	4.250808	3.813461	-1.625087
6	-2.484862	-1.511607	0.174415
6	-4.339967	-3.449925	1.072467
6	-2.707072	-2.684927	-0.600912
6	-3.090927	-1.368583	1.452069
6	-4.022584	-2.341343	1.873942
6	-3.648648	-3.625712	-0.142179
1	-4.509613	-2.234196	2.842065
1	-3.841209	-4.513017	-0.740632
6	-4.107964	1.012033	-1.954845
1	-3.390402	0.179213	-1.919887
6	-5.458030	0.391074	-1.523014
1	-5.381233	-0.033394	-0.514853
1	-5.739946	-0.419359	-2.208480
1	-6.264154	1.134792	-1.524474
6	-4.125512	1.487200	-3.429239
1	-3.138656	1.866245	-3.726870
1	-4.852278	2.294496	-3.579616
1	-4.395637	0.657323	-4.097139
6	-0.614676	3.089010	1.282413
1	-0.112218	2.129820	1.093587
6	0.341017	4.198332	0.771853
1	1.319264	4.117347	1.263338
1	-0.066920	5.196237	0.980356
1	0.500149	4.115535	-0.307197
6	-0.789618	3.222118	2.818662
1	0.191276	3.208559	3.312967
1	-1.395158	2.408053	3.233700
1	-1.275118	4.170382	3.081206
6	-4.911161	5.542351	0.192676
1	-5.837936	5.373532	-0.374942
6	-5.298346	5.749776	1.677960
1	-4.410619	5.943209	2.294554
1	-5.792725	4.855507	2.079208
1	-5.979632	6.602856	1.789488
6	-4.214121	6.792728	-0.401430
1	-3.283581	7.015434	0.137479
1	-4.864508	7.674319	-0.337777
1	-3.954558	6.626452	-1.454969
6	-1.939510	-2.968696	-1.904313
1	-1.071457	-2.297233	-1.964798
6	-1.350393	-4.401983	-1.939039
1	-2.132988	-5.171163	-1.967961
1	-0.712622	-4.581384	-1.067070
1	-0.725933	-4.524275	-2.834775
6	-2.806166	-2.718039	-3.166497
1	-3.678131	-3.384986	-3.184703
1	-2.216071	-2.905589	-4.074788
1	-3.174754	-1.684956	-3.207896
6	-2.724460	-0.237536	2.428103
1	-1.972518	0.405743	1.951456
6	-2.061702	-0.802905	3.713988
1	-1.759054	0.015607	4.382442
1	-1.169204	-1.395414	3.474180
1	-2.754899	-1.448517	4.267743
6	-3.927746	0.670050	2.784997
1	-3.623423	1.449636	3.496755
1	-4.737125	0.091267	3.247648
1	-4.323797	1.166027	1.891825
6	3.169907	0.757685	2.767240
1	3.465153	1.476122	3.545252

6	1.751361	0.289461	3.188598
1	1.754182	0.079386	4.268113
1	1.450646	-0.650339	2.706644
1	0.978218	1.040529	2.994900
6	4.162245	-0.432012	2.867435
1	4.075213	-0.921649	3.846663
1	5.196354	-0.090329	2.739556
1	3.955343	-1.192722	2.105965
6	2.284535	2.071279	-2.278721
1	1.345221	1.530188	-2.121492
6	1.902668	3.451121	-2.879604
1	1.361327	4.079996	-2.163709
1	1.253172	3.300969	-3.752399
1	2.784094	4.010623	-3.220209
6	3.094725	1.266225	-3.327626
1	3.277050	0.239753	-2.993662
1	4.063447	1.746682	-3.522817
1	2.539434	1.221137	-4.275073
6	5.787379	4.410964	0.568226
1	5.922124	4.888806	-0.413196
6	7.129256	3.737255	0.956716
1	7.408094	2.972039	0.220654
1	7.050454	3.243131	1.934146
1	7.939658	4.475189	1.014675
6	5.390194	5.513490	1.582364
1	5.234504	5.088669	2.582897
1	4.455238	6.001834	1.278895
1	6.173612	6.278566	1.657866
6	-5.404263	-4.447797	1.512968
1	-5.788123	-4.117285	2.489550
6	-6.592178	-4.449083	0.516383
1	-7.017851	-3.441846	0.418111
1	-7.385776	-5.130541	0.849357
1	-6.264929	-4.769585	-0.481499
6	-4.809314	-5.866302	1.694240
1	-3.981654	-5.851118	2.415013
1	-4.415610	-6.252488	0.744971
1	-5.571845	-6.568400	2.055511
15	1.845369	-2.930246	-0.489975
6	2.480971	-3.532361	1.183058
6	3.230882	-4.644258	3.687038
6	3.794782	-3.999493	1.398749
6	1.546088	-3.619754	2.247429
6	1.919096	-4.166261	3.488235
6	4.165121	-4.556099	2.637815
1	4.523989	-3.939699	0.596163
1	0.521058	-3.277617	2.104364
1	1.187443	-4.230862	4.291362
1	5.179750	-4.922489	2.776194
1	3.515781	-5.085215	4.639519
6	3.377333	-2.779240	-1.565588
6	5.507086	-2.609121	-3.422824
6	4.490571	-1.947608	-1.304359
6	3.333735	-3.502229	-2.778564
6	4.392584	-3.422822	-3.700881
6	5.548987	-1.865077	-2.225843
1	4.523899	-1.342214	-0.400914
1	2.466274	-4.122536	-2.991675
1	4.343277	-3.994518	-4.624359
1	6.393123	-1.212663	-2.015661
1	6.329001	-2.549875	-4.131748
7	-0.622368	0.207219	-2.851896
1	-1.227146	0.204583	-3.701439
7	0.379653	-0.756763	-2.855428
1	0.645142	-0.987633	-3.835530

1
A

Frequencies -- -220.8238
 Red. masses -- 4.9054
 Frc consts -- 0.1409
 IR Inten -- 118.7647

Atom	AN	X	Y	Z
1	82	0.01	0.00	0.00
2	82	0.00	0.00	0.05
3	6	-0.03	-0.01	0.02
4	6	-0.01	0.01	0.00
5	6	-0.01	0.00	0.01
6	6	-0.02	0.01	0.01
7	6	-0.01	0.01	0.00
8	6	-0.01	0.01	0.00
9	1	-0.01	0.02	-0.01
10	1	0.00	0.01	-0.01
11	6	0.01	0.00	-0.02
12	6	0.00	0.01	-0.01
13	6	0.01	0.01	-0.01
14	6	0.00	0.00	-0.01
15	6	0.00	0.00	-0.01
16	6	0.01	0.01	-0.01
17	1	0.00	0.00	-0.01
18	1	0.01	0.02	-0.01
19	6	-0.01	0.00	0.02
20	6	-0.01	-0.01	0.01
21	6	-0.01	0.00	0.01
22	6	-0.01	-0.01	0.01
23	6	-0.01	-0.01	0.01
24	6	-0.01	0.00	0.01
25	1	-0.02	-0.01	0.01
26	1	0.00	-0.01	0.01
27	6	-0.01	0.00	0.01
28	1	0.00	0.01	0.02
29	6	0.00	0.00	0.00
30	1	0.00	0.00	0.00
31	1	0.00	0.00	0.00
32	1	-0.01	-0.01	0.00
33	6	0.00	0.00	0.00
34	1	-0.01	0.01	0.01
35	1	-0.01	-0.01	0.00
36	1	0.01	0.00	0.00
37	6	-0.01	0.00	0.00
38	1	-0.01	0.00	0.00
39	6	-0.01	0.00	0.00
40	1	0.00	-0.01	0.00
41	1	0.00	0.00	0.00
42	1	-0.01	0.00	0.00
43	6	0.00	0.00	0.00
44	1	0.00	0.00	0.00
45	1	0.00	0.00	0.00
46	1	0.00	0.00	0.00
47	6	0.00	0.01	0.00
48	1	0.00	0.01	0.00
49	6	0.00	0.01	0.00
50	1	0.00	0.00	0.00
51	1	0.00	0.00	0.00
52	1	0.00	0.01	0.00
53	6	0.00	0.01	0.00
54	1	0.00	0.01	0.00
55	1	0.00	0.01	0.00
56	1	0.00	0.01	0.00
57	6	0.00	0.00	0.01
58	1	0.00	0.00	0.05
59	6	0.00	0.00	0.01
60	1	-0.01	0.00	0.01
61	1	0.00	0.00	0.00
62	1	-0.01	-0.01	0.00
63	6	0.01	0.01	0.01
64	1	0.00	0.03	0.01

65	1	0.00	-0.01	0.00
66	1	0.02	0.02	0.00
67	6	-0.01	0.00	0.01
68	1	-0.01	-0.01	0.00
69	6	0.00	0.00	0.00
70	1	0.00	0.00	0.00
71	1	0.00	0.00	0.00
72	1	0.00	0.00	0.01
73	6	-0.01	0.00	0.01
74	1	0.00	0.00	0.01
75	1	-0.01	0.00	0.01
76	1	0.00	0.00	0.01
77	6	0.01	0.01	-0.01
78	1	0.02	0.01	-0.02
79	6	0.01	0.02	0.03
80	1	0.03	0.05	0.04
81	1	0.00	0.01	0.06
82	1	0.01	0.01	0.02
83	6	0.00	0.00	-0.01
84	1	0.01	0.01	0.00
85	1	0.00	-0.01	-0.02
86	1	-0.01	0.00	0.00
87	6	0.00	0.00	0.00
88	1	0.00	0.01	0.03
89	6	0.00	0.00	-0.01
90	1	0.00	0.00	-0.01
91	1	0.00	0.00	-0.01
92	1	0.00	0.00	-0.01
93	6	-0.01	-0.01	0.00
94	1	-0.02	-0.01	0.00
95	1	-0.01	-0.02	0.00
96	1	-0.01	-0.01	0.00
97	6	0.00	0.01	0.00
98	1	0.01	0.01	0.00
99	6	0.00	0.00	0.00
100	1	0.00	0.00	0.00
101	1	0.00	0.00	0.00
102	1	0.00	0.00	0.00
103	6	0.00	0.00	0.00
104	1	0.00	0.00	0.00
105	1	0.00	0.00	0.00
106	1	0.00	0.00	0.01
107	6	-0.01	-0.01	0.00
108	1	-0.01	-0.01	0.00
109	6	0.00	0.00	0.00
110	1	0.00	0.00	0.00
111	1	-0.01	0.00	0.00
112	1	0.00	0.00	0.00
113	6	0.00	-0.01	0.00
114	1	0.00	0.00	0.00
115	1	0.00	0.00	0.00
116	1	0.00	-0.01	0.00
117	15	0.01	-0.02	-0.03
118	6	-0.01	0.00	-0.01
119	6	-0.01	0.01	-0.01
120	6	-0.01	0.00	-0.01
121	6	-0.01	0.01	-0.01
122	6	0.00	0.01	-0.01
123	6	-0.01	0.01	-0.01
124	1	-0.01	0.00	-0.01
125	1	-0.01	0.01	-0.01
126	1	0.00	0.01	-0.01
127	1	-0.01	0.01	-0.01
128	1	-0.01	0.01	-0.01
129	6	0.01	-0.02	-0.01
130	6	0.01	0.01	-0.01
131	6	0.00	-0.01	-0.01
132	6	0.02	-0.01	-0.02

133	6	0.02	0.00	-0.02
134	6	0.00	0.00	-0.01
135	1	0.00	-0.01	-0.01
136	1	0.03	-0.03	-0.01
137	1	0.02	0.00	-0.02
138	1	0.00	0.00	0.00
139	1	0.01	0.01	-0.01
140	7	0.05	-0.06	-0.28
141	1	0.03	0.12	-0.27
142	7	-0.05	0.06	-0.39
143	1	-0.50	-0.48	-0.38

Pro-N₂H₄-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.912050	0.332207	0.487055
6	-0.750373	-0.245192	0.468421
6	1.360133	1.829453	0.104270
6	2.244556	4.604953	-0.065603
6	0.750976	2.767135	-0.807684
6	2.478460	2.331643	0.875007
6	2.878543	3.678466	0.767333
6	1.198794	4.108752	-0.846116
1	3.719389	4.018131	1.366926
1	0.702628	4.785379	-1.535486
6	-2.014868	0.579257	0.077330
6	-4.698937	1.669918	-0.184332
6	-2.554264	1.536658	1.035065
6	-2.802039	0.359538	-1.116104
6	-4.100506	0.914114	-1.197399
6	-3.881381	1.994795	0.900845
1	-4.662016	0.748681	-2.113744
1	-4.278192	2.659545	1.663883
6	2.030160	-0.756688	0.129165
6	4.394276	-2.386314	-0.403093
6	2.478220	-1.790302	1.062914
6	2.764009	-0.669212	-1.106244
6	3.909218	-1.467024	-1.331046
6	3.641711	-2.530805	0.769013
1	4.445266	-1.349590	-2.268951
1	3.968678	-3.265709	1.497498
6	3.360374	1.532083	1.860064
1	3.063521	0.488757	1.870585
6	4.848078	1.509120	1.413014
1	4.948786	1.080063	0.409327
1	5.435307	0.892278	2.107155
1	5.291333	2.512611	1.401978
6	3.234533	2.075519	3.308843
1	2.189204	2.068692	3.639401
1	3.603775	3.105637	3.384978
1	3.827732	1.462044	4.001575
6	-0.336291	2.493375	-1.870107
1	-0.656674	1.462183	-1.780693
6	-1.591258	3.394408	-1.715038
1	-2.336787	3.120553	-2.472424
1	-1.343805	4.452546	-1.869037
1	-2.058526	3.293809	-0.736350
6	0.187927	2.716257	-3.320513
1	-0.597999	2.448685	-4.040634
1	1.077332	2.129721	-3.555160
1	0.436556	3.771630	-3.487085
6	2.694255	6.063882	-0.124157
1	3.519374	6.182222	0.594492
6	3.241194	6.443855	-1.525124

1	2.457496	6.363666	-2.290217
1	4.067041	5.784086	-1.819736
1	3.608847	7.479091	-1.528696
6	1.562305	7.033345	0.304676
1	0.709821	6.976551	-0.385244
1	1.922711	8.071094	0.308104
1	1.196017	6.792385	1.310577
6	1.856989	-2.242253	2.422772
1	0.844591	-1.854677	2.518416
6	1.689932	-3.787617	2.501594
1	2.645821	-4.311958	2.623804
1	1.190735	-4.175474	1.608897
1	1.072822	-4.039344	3.376113
6	2.706398	-1.792595	3.648821
1	3.723044	-2.203339	3.593498
1	2.245791	-2.162106	4.575155
1	2.805099	-0.704384	3.741772
6	2.431326	0.243092	-2.298715
1	1.480908	0.730133	-2.109557
6	2.278360	-0.568863	-3.616788
1	1.889735	0.079012	-4.414240
1	1.590476	-1.412376	-3.499690
1	3.240800	-0.965113	-3.962437
6	3.511115	1.340961	-2.502014
1	3.274534	1.958652	-3.378467
1	4.496703	0.889462	-2.673813
1	3.583573	1.999784	-1.632226
6	-2.444608	-0.318183	-2.481462
1	-2.715380	0.469027	-3.203229
6	-0.979819	-0.692240	-2.816169
1	-0.952643	-1.618677	-3.396248
1	-0.358874	-0.849179	-1.935786
1	-0.506968	0.082964	-3.423381
6	-3.391411	-1.506025	-2.828459
1	-3.264542	-1.771467	-3.886675
1	-4.447109	-1.257172	-2.672727
1	-3.157417	-2.392809	-2.240441
6	-1.801372	2.233681	2.207532
1	-0.752656	1.938126	2.226029
6	-1.764397	3.778575	2.027640
1	-1.193064	4.060077	1.137787
1	-1.265130	4.228374	2.897078
1	-2.765628	4.220907	1.951417
6	-2.433998	1.910556	3.594048
1	-2.553482	0.833301	3.777135
1	-3.432058	2.357625	3.690767
1	-1.806814	2.321085	4.396475
6	-6.137942	2.172398	-0.280686
1	-6.344290	2.754358	0.630025
6	-7.148603	0.996266	-0.321914
1	-7.032072	0.346348	0.554827
1	-7.000906	0.382189	-1.220366
1	-8.180433	1.372472	-0.337169
6	-6.344786	3.117118	-1.493264
1	-6.180218	2.588142	-2.441433
1	-5.650322	3.965887	-1.456504
1	-7.370042	3.510993	-1.504252
6	5.660607	-3.199011	-0.665231
1	6.045326	-2.898786	-1.651575
6	6.764997	-2.890229	0.379161
1	7.004841	-1.819550	0.396921
1	7.683553	-3.445381	0.145575
1	6.445508	-3.179994	1.389012
6	5.367966	-4.721133	-0.722672
1	4.611167	-4.950516	-1.483353
1	4.994839	-5.089667	0.241923
1	6.281523	-5.280691	-0.965383
15	-0.823992	-2.356747	0.421168
6	-1.137633	-3.507586	-1.072480

6	-1.169675	-5.584695	-3.023641
6	-2.241297	-4.385635	-1.183030
6	-0.034944	-3.716166	-1.939498
6	-0.054061	-4.729572	-2.912535
6	-2.256068	-5.414140	-2.146329
1	-3.086580	-4.286793	-0.509453
1	0.854874	-3.098392	-1.836093
1	0.803621	-4.862816	-3.568609
1	-3.115425	-6.078870	-2.206174
1	-1.182922	-6.377099	-3.768681
6	-2.441629	-2.553109	1.402780
6	-4.726631	-2.993379	3.039569
6	-3.736934	-2.230603	0.940412
6	-2.313090	-3.097429	2.702370
6	-3.442189	-3.320075	3.514241
6	-4.868433	-2.445565	1.750543
1	-3.873767	-1.798692	-0.043570
1	-1.325057	-3.347494	3.077880
1	-3.317777	-3.743592	4.508486
1	-5.854741	-2.184541	1.373052
1	-5.601441	-3.162095	3.663882
7	0.657911	0.434693	1.992207
1	1.351517	-0.039012	2.567732
7	-0.582629	-0.333807	1.949111
1	-1.325723	0.064968	2.515790

Pro-N₂H₄-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	1.200988	0.185044	0.549717
14	-1.199048	-0.280707	0.456506
6	2.178434	1.842078	0.306669
6	3.783818	4.224156	0.062283
6	1.766728	2.930004	-0.526020
6	3.396503	1.996407	1.046035
6	4.168494	3.168940	0.902659
6	2.571747	4.083482	-0.632453
1	5.092726	3.262833	1.469790
1	2.233990	4.894729	-1.273604
6	-2.518746	1.088556	0.052368
6	-4.638012	3.004733	-0.432586
6	-2.946089	2.018596	1.073237
6	-3.128675	1.217129	-1.245372
6	-4.155493	2.168432	-1.447632
6	-4.000853	2.917963	0.812314
1	-4.587813	2.243589	-2.444325
1	-4.321937	3.589115	1.604245
6	2.324373	-1.307425	-0.000160
6	4.345950	-3.225983	-0.741400
6	2.594890	-2.455721	0.826090
6	3.015098	-1.217018	-1.252016
6	4.008730	-2.161188	-1.588443
6	3.606368	-3.362766	0.445707
1	4.531460	-2.063628	-2.538021
1	3.810767	-4.209900	1.095432
6	3.909020	0.958568	2.054626
1	3.269174	0.072698	2.010085
6	5.340228	0.462081	1.727622
1	5.380256	0.018608	0.725585
1	5.651084	-0.303104	2.451520
1	6.071944	1.279036	1.770494
6	3.822679	1.510641	3.503037
1	2.798936	1.825387	3.740838
1	4.481571	2.378448	3.634992

1	4.130918	0.743758	4.227557
6	0.448733	2.947627	-1.310586
1	-0.065607	1.996344	-1.145651
6	-0.495929	4.060733	-0.786793
1	-1.473672	3.998203	-1.280948
1	-0.077018	5.057314	-0.979219
1	-0.654422	3.962961	0.291875
6	0.661424	3.114096	-2.838478
1	-0.302724	3.070886	-3.363029
1	1.311040	2.331938	-3.248232
1	1.121198	4.083002	-3.071663
6	4.646047	5.480342	-0.065240
1	5.548224	5.323873	0.545000
6	5.108295	5.720412	-1.525663
1	4.251245	5.901247	-2.187748
1	5.655966	4.852939	-1.915107
1	5.766754	6.597792	-1.582594
6	3.919050	6.731386	0.494257
1	3.009569	6.950573	-0.080865
1	4.571650	7.613463	0.440759
1	3.625618	6.582622	1.541001
6	1.829654	-2.796987	2.120244
1	0.925244	-2.186604	2.170246
6	1.336905	-4.269330	2.135342
1	2.165673	-4.987410	2.187050
1	0.736695	-4.488642	1.246413
1	0.703816	-4.433661	3.018670
6	2.685143	-2.535477	3.391053
1	3.573341	-3.181965	3.404900
1	2.099693	-2.751507	4.295731
1	3.038172	-1.498764	3.453310
6	2.693827	-0.157701	-2.317744
1	1.902056	0.496579	-1.937681
6	2.140031	-0.820618	-3.608063
1	1.844440	-0.052766	-4.336352
1	1.262848	-1.442062	-3.390085
1	2.895000	-1.459314	-4.083125
6	3.911091	0.743416	-2.647619
1	3.640229	1.496248	-3.399924
1	4.742878	0.152066	-3.052085
1	4.266207	1.268371	-1.754318
6	-2.823624	0.429928	-2.543850
1	-2.957774	1.168444	-3.349382
6	-1.402256	-0.125987	-2.747716
1	-1.323857	-0.545565	-3.759246
1	-1.155327	-0.940099	-2.061105
1	-0.644786	0.656656	-2.652738
6	-3.900700	-0.663092	-2.787638
1	-3.738056	-1.153473	-3.756587
1	-4.906959	-0.226006	-2.788790
1	-3.866533	-1.438406	-2.019126
6	-2.321311	2.118924	2.479372
1	-1.311778	1.705728	2.448657
6	-2.147000	3.575263	2.987372
1	-1.619270	4.198710	2.256037
1	-1.552793	3.564107	3.910899
1	-3.103128	4.060273	3.221919
6	-3.171286	1.319777	3.507707
1	-3.357104	0.288193	3.183616
1	-4.153424	1.794404	3.638206
1	-2.677176	1.298208	4.489578
6	-5.775112	3.996978	-0.671999
1	-5.975640	4.504801	0.283249
6	-7.081332	3.282044	-1.104396
1	-7.386462	2.532639	-0.363123
1	-6.952121	2.769679	-2.066901
1	-7.898697	4.006980	-1.217392
6	-5.377430	5.086725	-1.702401
1	-5.172388	4.644790	-2.686546

1	-4.476687	5.624694	-1.380876
1	-6.189289	5.816395	-1.824484
6	5.452860	-4.210716	-1.118554
1	5.858180	-3.893839	-2.091394
6	6.619304	-4.178238	-0.096731
1	7.034800	-3.166873	-0.003083
1	7.426267	-4.854730	-0.409737
1	6.281344	-4.495889	0.898498
6	4.910618	-5.653895	-1.288219
1	4.106824	-5.689334	-2.034337
1	4.507017	-6.039173	-0.342615
1	5.712031	-6.331739	-1.612266
15	-1.654210	-2.664851	0.369191
6	-2.313307	-3.436629	-1.229686
6	-3.026029	-4.879592	-3.575546
6	-3.601534	-4.001368	-1.368485
6	-1.379925	-3.629826	-2.278273
6	-1.733992	-4.332174	-3.443352
6	-3.953060	-4.717963	-2.528955
1	-4.330313	-3.896500	-0.570495
1	-0.363580	-3.252881	-2.173567
1	-1.000552	-4.465480	-4.235762
1	-4.948651	-5.149024	-2.611308
1	-3.299150	-5.432305	-4.471592
6	-3.183074	-2.656213	1.498144
6	-5.373300	-2.766116	3.302903
6	-4.366610	-1.924765	1.243025
6	-3.112108	-3.436609	2.675476
6	-4.197980	-3.493343	3.571597
6	-5.453704	-1.980873	2.136269
1	-4.443678	-1.303620	0.354861
1	-2.206465	-3.999336	2.886771
1	-4.124812	-4.101203	4.470642
1	-6.354269	-1.409466	1.923368
1	-6.212806	-2.808518	3.993286
7	0.621962	0.193993	2.271757
1	1.172682	-0.203978	3.035789
7	-0.714671	-0.484729	2.183388
1	-1.293284	-0.286185	2.995141

Pro-N₂H₄-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.263965	0.171863	0.513181
32	-1.246518	-0.286807	0.420549
6	2.296457	1.881315	0.288188
6	3.910756	4.246694	0.056958
6	1.887313	2.968832	-0.541734
6	3.511121	2.016189	1.029319
6	4.290853	3.185133	0.892995
6	2.698336	4.118590	-0.642000
1	5.215939	3.271508	1.460300
1	2.367142	4.935542	-1.279716
6	-2.610022	1.152674	-0.005858
6	-4.676264	3.109903	-0.502288
6	-3.026893	2.077729	1.017627
6	-3.198171	1.292880	-1.309776
6	-4.203492	2.266789	-1.517537
6	-4.057069	3.003658	0.750926
1	-4.625104	2.355442	-2.517947
1	-4.372314	3.677575	1.542990
6	2.416011	-1.387726	-0.057724
6	4.367587	-3.353204	-0.825130
6	2.653414	-2.543419	0.761537

6	3.100257	-1.297314	-1.310002
6	4.062172	-2.269267	-1.661380
6	3.633715	-3.478599	0.367790
1	4.583129	-2.179585	-2.612992
1	3.817658	-4.336718	1.009254
6	4.005023	0.959385	2.026277
1	3.348995	0.084125	1.966142
6	5.430151	0.446788	1.698386
1	5.468606	0.014804	0.691157
1	5.728291	-0.331075	2.413946
1	6.172132	1.253724	1.753695
6	3.918490	1.492374	3.481492
1	2.896345	1.811745	3.719478
1	4.584479	2.352747	3.626791
1	4.217348	0.713101	4.196517
6	0.568629	2.982215	-1.325090
1	0.059206	2.026189	-1.160968
6	-0.382764	4.088524	-0.798435
1	-1.358988	4.024683	-1.295608
1	0.032835	5.087761	-0.984322
1	-0.544144	3.984933	0.279914
6	0.782514	3.145207	-2.852802
1	-0.180640	3.102561	-3.379215
1	1.431228	2.359407	-3.258070
1	1.245297	4.112274	-3.087782
6	4.780673	5.498610	-0.063532
1	5.680869	5.334014	0.547513
6	5.247153	5.742371	-1.522027
1	4.392535	5.931446	-2.184958
1	5.790323	4.873317	-1.914279
1	5.911052	6.615964	-1.573718
6	4.060462	6.751566	0.500355
1	3.153305	6.978993	-0.075246
1	4.718633	7.629772	0.451802
1	3.764425	6.599910	1.545952
6	1.883602	-2.850471	2.060025
1	0.994825	-2.215127	2.108777
6	1.352496	-4.308419	2.096447
1	2.163200	-5.047366	2.143187
1	0.734079	-4.520786	1.218140
1	0.727197	-4.447598	2.989173
6	2.752421	-2.588729	3.321538
1	3.622591	-3.259120	3.343395
1	2.166051	-2.769825	4.233125
1	3.132578	-1.560379	3.359106
6	2.802745	-0.210043	-2.353921
1	2.042569	0.469008	-1.950683
6	2.202298	-0.829785	-3.644595
1	1.929784	-0.040363	-4.358730
1	1.301811	-1.415632	-3.421130
1	2.921828	-1.494853	-4.138422
6	4.046168	0.653559	-2.685716
1	3.791412	1.429285	-3.420221
1	4.852003	0.041756	-3.111758
1	4.430386	1.150165	-1.787866
6	-2.890467	0.499269	-2.602845
1	-3.014547	1.234810	-3.412413
6	-1.470624	-0.068286	-2.791216
1	-1.372593	-0.456144	-3.813840
1	-1.255770	-0.911164	-2.127287
1	-0.703207	0.699327	-2.651443
6	-3.969121	-0.591751	-2.847937
1	-3.810190	-1.078696	-3.819265
1	-4.975041	-0.153972	-2.843589
1	-3.932380	-1.370435	-2.081964
6	-2.410069	2.136492	2.427478
1	-1.407582	1.704934	2.389380
6	-2.214053	3.578465	2.965245
1	-1.674890	4.207139	2.246493

1	-1.623684	3.541138	3.890321
1	-3.164567	4.072393	3.204739
6	-3.271397	1.323082	3.433756
1	-3.442623	0.293348	3.096596
1	-4.258052	1.790815	3.554671
1	-2.791161	1.293689	4.422187
6	-5.789465	4.127480	-0.749402
1	-5.980486	4.644199	0.202991
6	-7.110734	3.439439	-1.180350
1	-7.433020	2.700372	-0.435949
1	-6.991267	2.919625	-2.140148
1	-7.911914	4.181521	-1.297995
6	-5.365894	5.202939	-1.784187
1	-5.170266	4.752266	-2.766285
1	-4.453210	5.721246	-1.464122
1	-6.160479	5.950726	-1.910380
6	5.439956	-4.369751	-1.218829
1	5.843134	-4.061940	-2.195463
6	6.619032	-4.374404	-0.210907
1	7.064028	-3.375523	-0.118840
1	7.402642	-5.072284	-0.536011
1	6.284017	-4.685938	0.787207
6	4.853411	-5.795646	-1.386084
1	4.041570	-5.805390	-2.124235
1	4.447948	-6.171285	-0.437433
1	5.630968	-6.496264	-1.719697
15	-1.763965	-2.727545	0.373046
6	-2.454696	-3.440899	-1.238670
6	-3.223423	-4.788146	-3.623637
6	-3.755716	-3.974890	-1.380793
6	-1.537887	-3.615539	-2.305142
6	-1.919185	-4.271005	-3.488657
6	-4.134896	-4.644014	-2.560889
1	-4.472717	-3.884078	-0.570564
1	-0.513496	-3.260392	-2.201476
1	-1.198024	-4.391024	-4.294319
1	-5.139877	-5.052266	-2.645694
1	-3.518076	-5.304116	-4.534648
6	-3.288758	-2.663544	1.505201
6	-5.470116	-2.683476	3.323560
6	-4.464805	-1.926397	1.230990
6	-3.219871	-3.402061	2.709398
6	-4.301519	-3.413715	3.612247
6	-5.547827	-1.938443	2.130463
1	-4.538117	-1.333876	0.322678
1	-2.319322	-3.966532	2.936788
1	-4.230293	-3.989568	4.532242
1	-6.442312	-1.363326	1.902414
1	-6.306292	-2.691754	4.019194
7	0.632169	0.195130	2.310406
1	1.191024	-0.233034	3.056066
7	-0.699946	-0.511890	2.231708
1	-1.281310	-0.248402	3.027885

Pro-N₂H₄-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-1.449100	0.126752	-0.430631
50	1.364810	-0.327439	-0.353789
6	-2.554155	1.981310	-0.205660
6	-4.064698	4.409881	-0.040990
6	-2.209348	2.989782	0.742631
6	-3.657990	2.211465	-1.079874
6	-4.388670	3.415898	-0.979325

6	-2.967922	4.177322	0.808874
1	-5.227909	3.586261	-1.651367
1	-2.691082	4.937853	1.536180
6	2.824482	1.275015	0.060420
6	4.839904	3.300912	0.443680
6	3.175166	2.183995	-0.995194
6	3.454025	1.452998	1.336993
6	4.436454	2.459550	1.491915
6	4.182459	3.151168	-0.786210
1	4.893774	2.578646	2.473517
1	4.450542	3.818129	-1.602476
6	-2.708335	-1.576138	0.116379
6	-4.571347	-3.649920	0.792264
6	-2.861868	-2.722894	-0.728866
6	-3.449853	-1.523985	1.335181
6	-4.366556	-2.553486	1.644694
6	-3.797728	-3.719731	-0.380758
1	-4.932058	-2.501068	2.573803
1	-3.917672	-4.576289	-1.040066
6	-4.064816	1.215365	-2.174289
1	-3.507664	0.278995	-2.021238
6	-5.563940	0.829350	-2.115342
1	-5.827693	0.418626	-1.133043
1	-5.790070	0.069227	-2.874911
1	-6.211626	1.694143	-2.308415
6	-3.674477	1.749644	-3.578497
1	-2.598673	1.956334	-3.628272
1	-4.212770	2.679069	-3.806037
1	-3.927111	1.015104	-4.355977
6	-1.004267	2.860204	1.683358
1	-0.591824	1.846838	1.568706
6	0.119643	3.853254	1.286152
1	1.010010	3.707576	1.911571
1	-0.218253	4.890970	1.407086
1	0.416709	3.715236	0.240128
6	-1.379714	3.030872	3.177525
1	-0.501646	2.856594	3.814334
1	-2.166644	2.327885	3.476439
1	-1.741277	4.045988	3.385328
6	-4.880660	5.701179	0.039653
1	-5.672829	5.638059	-0.721362
6	-5.573438	5.858710	1.418384
1	-4.833783	5.940013	2.225962
1	-6.217060	4.997539	1.638116
1	-6.192789	6.765743	1.437787
6	-4.019182	6.948228	-0.289007
1	-3.215491	7.079676	0.447591
1	-4.635900	7.857182	-0.278537
1	-3.554940	6.858288	-1.279115
6	-2.051111	-2.928650	-2.018984
1	-1.221990	-2.213967	-2.040495
6	-1.393141	-4.330755	-2.093236
1	-2.136928	-5.136975	-2.141112
1	-0.743998	-4.505255	-1.227852
1	-0.770819	-4.397462	-2.995661
6	-2.927081	-2.682407	-3.277886
1	-3.742515	-3.416006	-3.338481
1	-2.322061	-2.773762	-4.190534
1	-3.383758	-1.683913	-3.266492
6	-3.270358	-0.408564	2.375088
1	-2.526585	0.307216	1.999430
6	-2.706079	-0.968257	3.708192
1	-2.516537	-0.152924	4.419711
1	-1.763788	-1.506815	3.542092
1	-3.411540	-1.665886	4.176909
6	-4.575304	0.392239	2.613138
1	-4.411224	1.191263	3.348790
1	-5.374685	-0.255942	2.994724

1	-4.924915	0.855461	1.683160
6	3.208646	0.660545	2.642115
1	3.372029	1.393008	3.447036
6	1.794586	0.095903	2.886330
1	1.701538	-0.205211	3.938454
1	1.594462	-0.811406	2.303004
1	1.014503	0.837930	2.679376
6	4.284679	-0.442469	2.833852
1	4.165621	-0.934193	3.808450
1	5.294237	-0.016377	2.783629
1	4.201689	-1.216998	2.065747
6	2.505294	2.170552	-2.378898
1	1.550188	1.643613	-2.301945
6	2.151945	3.585217	-2.905599
1	1.567422	4.149372	-2.167941
1	1.547952	3.494988	-3.817895
1	3.043112	4.174346	-3.157745
6	3.386479	1.416154	-3.411364
1	3.613306	0.393229	-3.084359
1	4.344522	1.934607	-3.552998
1	2.883054	1.365498	-4.387053
6	5.922849	4.362968	0.632999
1	6.058455	4.870358	-0.333823
6	7.285171	3.733471	1.023894
1	7.607672	2.994495	0.279490
1	7.222680	3.226434	1.995863
1	8.060782	4.507648	1.098768
6	5.497160	5.439206	1.666078
1	5.358914	4.998791	2.662509
1	4.551836	5.913872	1.374463
1	6.264744	6.220676	1.748033
6	-5.591649	-4.733795	1.143971
1	-6.036517	-4.466310	2.114352
6	-6.743413	-4.790342	0.106116
1	-7.244648	-3.818072	0.018486
1	-7.491618	-5.539028	0.400071
1	-6.365819	-5.064051	-0.887917
6	-4.927775	-6.125895	1.305212
1	-4.136882	-6.101310	2.065408
1	-4.475920	-6.461734	0.362658
1	-5.672172	-6.875605	1.606228
15	2.086087	-2.881750	-0.348518
6	2.809646	-3.460765	1.300064
6	3.652026	-4.597949	3.768105
6	4.130355	-3.936938	1.463333
6	1.912699	-3.581168	2.391020
6	2.329479	-4.135157	3.613771
6	4.545790	-4.501782	2.685182
1	4.834192	-3.881737	0.638262
1	0.876868	-3.262748	2.278041
1	1.622617	-4.217015	4.436734
1	5.565611	-4.867171	2.786361
1	3.974805	-5.034191	4.710626
6	3.608555	-2.731228	-1.476666
6	5.778078	-2.611628	-3.305294
6	4.737613	-1.921945	-1.206957
6	3.580380	-3.471247	-2.681669
6	4.656184	-3.412968	-3.589879
6	5.815000	-1.864953	-2.110895
1	4.776983	-1.327324	-0.297647
1	2.716400	-4.091867	-2.904961
1	4.616605	-3.990535	-4.510688
1	6.672288	-1.234523	-1.886310
1	6.609504	-2.565821	-4.005136
7	-0.673885	0.180353	-2.345992
1	-1.212795	-0.221235	-3.123386
7	0.653486	-0.557375	-2.279673
1	1.205619	-0.306318	-3.105054

Pro-N₂H₄-Pb

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-2.564313	-0.198849	0.866572
82	2.483986	0.303704	0.955120
6	-2.572266	2.026210	0.275494
6	-2.608652	4.840829	-0.307335
6	-2.400966	2.996909	1.314137
6	-2.759012	2.493755	-1.062551
6	-2.773525	3.884648	-1.323539
6	-2.422966	4.374893	1.007514
1	-2.921585	4.232227	-2.345092
1	-2.296322	5.096867	1.812197
6	4.172169	0.876263	-0.513792
6	6.354777	1.653093	-2.226611
6	4.090550	0.717513	-1.929442
6	5.378211	1.434798	0.034330
6	6.435224	1.800301	-0.828123
6	5.172704	1.113657	-2.752170
1	7.342501	2.213911	-0.389627
1	5.090985	0.991775	-3.831267
6	-4.261935	-1.175382	-0.320148
6	-6.506213	-2.468599	-1.531345
6	-4.068082	-2.136541	-1.357516
6	-5.584119	-0.893355	0.124172
6	-6.681017	-1.536871	-0.495104
6	-5.190208	-2.757636	-1.945449
1	-7.692633	-1.310866	-0.160479
1	-5.035487	-3.484033	-2.739888
6	-2.969755	1.549272	-2.255788
1	-2.870441	0.518078	-1.901073
6	-4.400809	1.685434	-2.838703
1	-5.156944	1.462317	-2.077431
1	-4.543790	0.983690	-3.671342
1	-4.581534	2.701297	-3.214763
6	-1.910612	1.757394	-3.368801
1	-0.890824	1.645222	-2.981103
1	-1.988537	2.755837	-3.817976
1	-2.051509	1.020122	-4.170982
6	-2.211306	2.607865	2.790156
1	-2.157246	1.510653	2.856718
6	-0.882699	3.147812	3.379630
1	-0.755780	2.806994	4.416164
1	-0.861631	4.245143	3.383484
1	-0.020016	2.797185	2.798160
6	-3.419411	3.051778	3.656809
1	-3.293560	2.718649	4.696053
1	-4.358528	2.632825	3.271988
1	-3.521741	4.144722	3.662788
6	-2.631854	6.335989	-0.630450
1	-2.802012	6.436701	-1.712874
6	-3.794827	7.065235	0.091569
1	-3.675663	7.018613	1.182202
1	-4.762499	6.613294	-0.160189
1	-3.823806	8.124668	-0.197331
6	-1.274401	7.014688	-0.309117
1	-1.049060	6.959944	0.764214
1	-1.296018	8.075319	-0.594121
1	-0.451643	6.530201	-0.850039
6	-2.663724	-2.555794	-1.812838
1	-1.977133	-1.732359	-1.572739
6	-2.187866	-3.809270	-1.025540
1	-2.823194	-4.673002	-1.262975
1	-2.241092	-3.647442	0.058801

1	-1.150787	-4.063932	-1.283074
6	-2.535220	-2.799071	-3.336053
1	-3.095696	-3.686163	-3.658096
1	-1.482747	-2.966187	-3.601366
1	-2.902065	-1.938968	-3.910850
6	-5.879438	0.074600	1.281107
1	-4.934745	0.543242	1.603819
6	-6.452513	-0.673400	2.514247
1	-6.606981	0.020550	3.351815
1	-5.774948	-1.470457	2.846077
1	-7.419165	-1.135741	2.276994
6	-6.809243	1.241312	0.860506
1	-6.962526	1.932158	1.700516
1	-7.794078	0.872097	0.547133
1	-6.377210	1.807175	0.026891
6	5.644545	1.691503	1.533776
1	6.681065	2.054168	1.586732
6	4.776798	2.834172	2.128170
1	5.112192	3.075610	3.146430
1	3.713418	2.568273	2.190917
1	4.857862	3.739718	1.514423
6	5.614920	0.419429	2.421431
1	5.981669	0.655144	3.429820
1	6.253397	-0.368292	2.002430
1	4.608319	-0.003708	2.551997
6	2.854073	0.152411	-2.640339
1	2.153609	-0.208889	-1.879177
6	2.124483	1.261337	-3.444444
1	1.837402	2.100961	-2.797320
1	1.217897	0.863314	-3.919531
1	2.771484	1.660581	-4.236606
6	3.185722	-1.053818	-3.556616
1	3.696064	-1.845796	-2.997381
1	3.830297	-0.760196	-4.395253
1	2.262256	-1.472359	-3.980147
6	7.510922	2.055765	-3.142965
1	7.191022	1.867078	-4.178859
6	8.773678	1.192485	-2.883300
1	8.553850	0.124800	-3.009672
1	9.149572	1.339884	-1.862062
1	9.578038	1.464075	-3.580502
6	7.844988	3.565688	-3.027707
1	8.192894	3.818872	-2.017418
1	6.963907	4.183043	-3.243794
1	8.639960	3.840050	-3.734555
6	-7.712869	-3.154437	-2.174898
1	-8.616147	-2.759764	-1.685740
6	-7.824058	-2.828055	-3.686971
1	-7.878645	-1.745031	-3.854865
1	-8.723697	-3.289437	-4.116561
1	-6.955020	-3.210163	-4.238693
6	-7.693779	-4.688390	-1.944471
1	-7.650662	-4.927193	-0.874364
1	-6.821824	-5.150074	-2.426507
1	-8.595502	-5.153669	-2.365479
15	2.124035	-2.434203	0.625490
6	2.320830	-3.043930	2.402705
6	2.468934	-3.940188	5.100940
6	3.376995	-3.882085	2.830373
6	1.336938	-2.667138	3.351964
6	1.411811	-3.105503	4.685693
6	3.446945	-4.327020	4.165103
1	4.141999	-4.192163	2.124043
1	0.501308	-2.037766	3.047675
1	0.643976	-2.803159	5.394796
1	4.266370	-4.974809	4.470323
1	2.525457	-4.284866	6.130885
6	3.535450	-3.301256	-0.282214
6	5.552020	-4.707666	-1.707981

6	4.861144	-2.812717	-0.330042
6	3.235657	-4.504226	-0.966151
6	4.234564	-5.204441	-1.670525
6	5.861248	-3.508769	-1.037440
1	5.113965	-1.881525	0.168357
1	2.219955	-4.891951	-0.943292
1	3.983748	-6.128299	-2.187200
1	6.873139	-3.111129	-1.066719
1	6.324069	-5.244452	-2.254862
7	-0.521176	-0.496962	-0.174663
1	-0.070250	-1.428697	-0.031281
7	0.410982	0.424366	-0.262469
1	-0.020848	1.349693	-0.433556

