Supporting Information

Mechanisms of the Reaction of Water, Butadiene, and Palladium Complex to 1,2-dimetallacyclohexene ($R_2M{=}MR_2$, M = C, Si, Ge, Sn, Pb). A Theoretical Study.

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(All geometries were calculated B3LYP/LANL2DZ)

Rea-C=C-Singlet

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.691092	0.326852	0.002397
6	-0.691047	0.326925	-0.002446
6	-1.576336	-0.945683	-0.005742
6	-0.668561	-2.164546	0.384082
6	0.668274	-2.164850	-0.382834
6	1.576235	-0.945836	0.006164
1	-0.452242	-2.131392	1.460748
1	-1.192674	-3.109755	0.205153
1	1.192258	-3.110017	-0.203307
1	0.451919	-2.132379	-1.459504
6	-1.410990	1.656822	0.089728
6	-2.199752	2.178974	-0.959919
6	-1.315246	2.420766	1.277997
6	-2.863596	3.412821	-0.831623
1	-2.280350	1.641702	-1.898323
6	-1.978655	3.651737	1.414989
1	-0.706204	2.048451	2.097201
6	-2.761153	4.156054	0.358679
1	-3.454823	3.793550	-1.661797
1	-1.880950	4.216034	2.339746
1	-3.274754	5.109363	0.458998
6	1.411108	1.656630	-0.090094
6	2.200425	2.178577	0.959189
6	1.315497	2.420227	-1.278548
6	2.864656	3.412167	0.830505
1	2.281172	1.641384	1.897617
6	1.979305	3.650933	-1.415974
1	0.706283	2.047849	-2.097600
6	2.762158	4.155232	-0.359917
1	3.456268	3.792808	1.660444
1	1.881658	4.215055	-2.340850
1	3.276100	5.108333	-0.460537
14	3.018245	-0.926889	-1.346712
14	2.357016	-1.328481	1.800130
14	-2.356983	-1.329297	-1.799514

14	-3.018690	-0.925822	1.346714
6	4.348515	0.426956	-1.226443
1	3.961614	1.406356	-1.525943
1	4.784690	0.529783	-0.229999
1	5.160860	0.160670	-1.919769
6	3.925507	-2.606532	-1.274149
1	3.238434	-3.456656	-1.371666
1	4.633246	-2.659791	-2.113904
1	4.504847	-2.742823	-0.352571
6	2.311090	-0.794835	-3.110253
1	3.151236	-0.699013	-3.813306
1	1.738219	-1.682705	-3.404464
1	1.670707	0.084382	-3.239782
6	4.149413	-0.732061	2.068415
1	4.444720	-1.021080	3.087727
1	4.862374	-1.197366	1.378351
1	4.258564	0.354602	1.986595
6	2.411003	-3.212675	2.098372
1	3.018331	-3.741307	1.353929
1	2.862212	-3.396801	3.084188
1	1.411202	-3.664262	2.104644
6	1.337827	-0.593067	3.235412
1	0.872298	0.367333	2.989553
1	0.536007	-1.274892	3.539000
1	1.990177	-0.440236	4.106807
6	-1.337672	-0.594706	-3.235118
1	-0.872994	0.366296	-2.990017
1	-0.535214	-1.276245	-3.537654
1	-1.989764	-0.443235	-4.106941
6	-2.411210	-3.213654	-2.096654
1	-3.018416	-3.741795	-1.351749
1	-2.862687	-3.398282	-3.082256
1	-1.411477	-3.665385	-2.102912
6	-4.149375	-0.732993	-2.068069
1	-4.444654	-1.022505	-3.087249
1	-4.862299	-1.198022	-1.377750
1	-4.258568	0.353704	-1.986721
6	-2.312142	-0.793672	3.110493
1	-1.739626	-1.681613	3.405157
1	-1.671573	0.085417	3.240001

1	-3.152521	-0.697417	3.813209
6	-3.926662	-2.605035	1.273920
1	-4.635380	-2.657659	2.112888
1	-4.505014	-2.741443	0.351727
1	-3.240021	-3.455384	1.372542
6	-4.348272	0.428631	1.225601
1	-4.783884	0.531626	0.228921
1	-5.161110	0.162803	1.918530
1	-3.961021	1.407852	1.525279

Rea-C=C-Triplet

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.788889	0.340384	-0.013169
6	-0.788674	0.340545	0.013285
6	-1.603039	-0.940603	-0.023433
6	-0.669449	-2.143788	0.379440
6	0.669069	-2.144900	-0.374700
6	1.602987	-0.940903	0.025024
1	-0.458835	-2.099836	1.457589
1	-1.185083	-3.094849	0.205549
1	1.184498	-3.095589	-0.198296
1	0.458470	-2.103832	-1.452971
6	-1.441614	1.663393	0.147564
6	-2.354022	2.152937	-0.828309
6	-1.171300	2.510139	1.262850
6	-2.975507	3.405626	-0.693315
1	-2.544865	1.569307	-1.723046
6	-1.813031	3.747723	1.413714
1	-0.469295	2.178574	2.024320
6	-2.721279	4.209195	0.435083
1	-3.650515	3.755719	-1.472899
1	-1.605249	4.356050	2.292316
1	-3.208015	5.175185	0.545782
6	1.442156	1.662911	-0.148509
6	2.355651	2.152597	0.826345

6	1.171219	2.509399	-1.263884
6	2.977447	3.405011	0.690324
1	2.547055	1.569433	1.721225
6	1.813213	3.746702	-1.415751
1	0.468495	2.177812	-2.024657
6	2.722486	4.208273	-0.438124
1	3.653246	3.755146	1.469201
1	1.604833	4.354767	-2.294381
1	3.209421	5.174075	-0.549583
14	3.028102	-0.940351	-1.362472
14	2.411974	-1.365470	1.807581
14	-2.410605	-1.368292	-1.805860
14	-3.029953	-0.937846	1.362144
6	4.358342	0.413891	-1.285126
1	3.955140	1.391901	-1.568031
1	4.832832	0.517176	-0.306371
1	5.142691	0.151828	-2.011688
6	3.919560	-2.628960	-1.328588
1	3.219944	-3.470026	-1.415574
1	4.601964	-2.681681	-2.189202
1	4.523136	-2.781085	-0.425380
6	2.253393	-0.783826	-3.095212
1	3.064557	-0.672865	-3.829392
1	1.669738	-1.666115	-3.384586
1	1.609362	0.098672	-3.179279
6	4.220036	-0.794189	2.020156
1	4.543777	-1.087778	3.029450
1	4.904157	-1.268546	1.307314
1	4.344226	0.290594	1.935311
6	2.447744	-3.251682	2.091816
1	3.028843	-3.777169	1.323912
1	2.924732	-3.453933	3.061944
1	1.443182	-3.691643	2.118667
6	1.433416	-0.588822	3.246804
1	1.023990	0.397436	2.996953
1	0.595092	-1.226525	3.549367
1	2.091328	-0.468570	4.119277
6	-1.431501	-0.594279	-3.246042
1	-1.020980	0.391813	-2.997365
1	-0.593955	-1.233160	-3.548106

1	-2.089479	-0.474317	-4.118481
6	-2.446182	-3.255068	-2.086454
1	-3.027749	-3.779109	-1.317934
1	-2.922365	-3.459351	-3.056545
1	-1.441542	-3.694950	-2.111652
6	-4.218179	-0.796470	-2.020913
1	-4.541286	-1.092074	-3.029818
1	-4.903334	-1.268484	-1.307561
1	-4.341386	0.288638	-1.938713
6	-2.257331	-0.782128	3.095923
1	-1.675478	-1.665330	3.386240
1	-1.612004	0.099379	3.180725
1	-3.069333	-0.669761	3.828977
6	-3.923986	-2.625131	1.327421
1	-4.607513	-2.676597	2.187216
1	-4.526789	-2.776344	0.423552
1	-3.225878	-3.467365	1.415269
6	-4.358372	0.418065	1.281998
1	-4.829769	0.522633	0.301874
1	-5.145278	0.156514	2.005974
1	-3.954836	1.395414	1.566694

Rea-Si=Si-Singlet

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.077082	0.650205	0.060523
14	-1.077190	0.650157	-0.060864
6	-1.844094	-1.105327	0.094549
6	-0.630481	-2.071395	0.465553
6	0.630565	-2.071931	-0.464315
6	1.844079	-1.105614	-0.094337
1	-0.301018	-1.845775	1.486957
1	-1.016116	-3.099521	0.489808
1	1.016430	-3.100017	-0.487368
1	0.301334	-1.847394	-1.485975
6	-2.106783	2.228988	-0.084860

6	-3.268200	2.360304	-0.890469
6	-1.706587	3.359974	0.676753
6	-4.000940	3.560450	-0.930450
1	-3.605921	1.525924	-1.499727
6	-2.433823	4.563796	0.634263
1	-0.824459	3.299198	1.310207
6	-3.587070	4.669624	-0.167892
1	-4.887867	3.629263	-1.556710
1	-2.103408	5.412054	1.229896
1	-4.152680	5.598206	-0.197305
6	2.106774	2.229381	0.084022
6	3.268059	2.361501	0.890405
6	1.706531	3.360347	-0.678070
6	4.000414	3.562092	0.930143
1	3.605730	1.527350	1.500370
6	2.433495	4.564357	-0.635512
1	0.824744	3.299155	-1.311934
6	3.586364	4.670778	0.166998
1	4.887051	3.631462	1.556801
1	2.103073	5.412280	-1.231541
1	4.151659	5.599522	0.196299
14	3.049401	-1.214489	-1.636010
14	2.698061	-1.717782	1.561901
14	-2.697682	-1.718719	-1.561581
14	-3.049571	-1.213374	1.636138
6	4.491886	0.022660	-1.617902
1	4.136713	1.058946	-1.652567
1	5.143654	-0.080862	-0.745116
1	5.106923	-0.148926	-2.513471
6	3.766038	-2.978907	-1.770969
1	2.973985	-3.736853	-1.831501
1	4.365257	-3.057417	-2.689304
1	4.419413	-3.238720	-0.929046
6	2.091064	-0.885415	-3.249928
1	2.809382	-0.720701	-4.065703
1	1.454057	-1.730144	-3.541710
1	1.460049	0.009482	-3.176263
6	4.577856	-1.395999	1.630258
1	4.947773	-1.743868	2.605528
1	5.134528	-1.936729	0.855961

1	4.830546	-0.332362	1.544986
6	2.460893	-3.598334	1.765184
1	2.871197	-4.162435	0.918176
1	2.984691	-3.934019	2.671606
1	1.404283	-3.872266	1.875520
6	1.991241	-0.873644	3.116540
1	2.128693	0.215724	3.093081
1	0.920401	-1.061068	3.251352
1	2.514160	-1.256115	4.005580
6	-1.991486	-0.874619	-3.116514
1	-2.129483	0.214558	-3.093328
1	-0.920613	-1.061442	-3.251503
1	-2.514296	-1.257481	-4.005431
6	-2.459196	-3.599246	-1.763700
1	-2.868752	-4.162979	-0.916137
1	-2.983042	-3.936089	-2.669640
1	-1.402426	-3.872443	-1.874183
6	-4.577657	-1.398322	-1.630144
1	-4.947150	-1.746723	-2.605362
1	-5.133960	-1.939380	-0.855896
1	-4.831295	-0.335013	-1.545179
6	-2.091794	-0.881542	3.249773
1	-1.453746	-1.725231	3.542422
1	-1.461855	0.014013	3.175553
1	-2.810436	-0.716963	4.065277
6	-3.764805	-2.978240	1.773158
1	-4.363760	-3.056296	2.691682
1	-4.418096	-3.239519	0.931687
1	-2.972144	-3.735479	1.834339
6	-4.492913	0.022706	1.616185
1	-5.144086	-0.081956	0.743199
1	-5.108395	-0.148697	2.511474
1	-4.138719	1.059229	1.650311

Rea-Si=Si-Triplet

Atomic Number	Coordinates (Angstroms) X	Y	Z

14	1.121902	0.650723	0.398540
14	-1.121968	0.650539	-0.399033
6	-1.857643	-1.093474	0.029720
6	-0.633066	-2.023926	0.458457
6	0.633184	-2.024131	-0.457719
6	1.857728	-1.093383	-0.029540
1	-0.317250	-1.755109	1.473935
1	-1.001316	-3.056600	0.525030
1	1.001479	-3.056827	-0.523783
1	0.317331	-1.755841	-1.473321
6	-2.133113	2.222733	-0.136174
6	-3.355065	2.422138	-0.839356
6	-1.658562	3.300494	0.661812
6	-4.072810	3.625537	-0.742461
1	-3.743991	1.632492	-1.479799
6	-2.375179	4.509503	0.759706
1	-0.728267	3.198828	1.216879
6	-3.584047	4.679193	0.057920
1	-5.002840	3.745113	-1.294413
1	-1.987580	5.315237	1.379721
1	-4.133590	5.615578	0.127135
6	2.132927	2.222978	0.135612
6	3.354626	2.422734	0.839135
6	1.658443	3.300506	-0.662731
6	4.072186	3.626246	0.742247
1	3.743471	1.633306	1.479888
6	2.374873	4.509628	-0.760618
1	0.728338	3.198569	-1.218068
6	3.583485	4.679669	-0.058478
1	5.002008	3.746101	1.294490
1	1.987322	5.315180	-1.380899
1	4.132874	5.616148	-0.127674
14	3.031629	-1.106565	-1.598635
14	2.740005	-1.830867	1.561511
14	-2.739614	-1.831813	-1.561110
14	-3.031703	-1.105980	1.598695
6	4.502960	0.095144	-1.577799
1	4.174559	1.139822	-1.598414
1	5.164641	-0.034960	-0.716020

1	5.100259	-0.085354	-2.483994
6	3.720991	-2.871448	-1.854614
1	2.921364	-3.622277	-1.900156
1	4.263519	-2.912896	-2.810242
1	4.422898	-3.172162	-1.066587
6	2.032014	-0.687906	-3.169351
1	2.731207	-0.465250	-3.988391
1	1.402390	-1.524396	-3.499800
1	1.388217	0.191803	-3.036243
6	4.615615	-1.488893	1.601911
1	5.017900	-1.866227	2.553005
1	5.162114	-1.985144	0.791456
1	4.841946	-0.416203	1.553596
6	2.493121	-3.718541	1.652607
1	2.873436	-4.236841	0.763530
1	3.034925	-4.112600	2.524554
1	1.435552	-3.985612	1.775742
6	2.076783	-1.095824	3.191424
1	2.300182	-0.023425	3.275173
1	0.992515	-1.211786	3.303564
1	2.559244	-1.604254	4.040199
6	-2.076792	-1.096906	-3.191247
1	-2.300728	-0.024641	-3.275259
1	-0.992477	-1.212367	-3.303402
1	-2.559044	-1.605787	-4.039866
6	-2.491863	-3.719408	-1.651580
1	-2.872095	-4.237555	-0.762373
1	-3.033353	-4.114001	-2.523476
1	-1.434153	-3.986048	-1.774432
6	-4.615390	-1.490777	-1.601624
1	-5.017515	-1.868851	-2.552491
1	-5.161610	-1.986837	-0.790862
1	-4.842240	-0.418163	-1.553925
6	-2.032476	-0.685304	3.169107
1	-1.401999	-1.520914	3.500130
1	-1.389564	0.194957	3.035362
1	-2.731880	-0.462768	3.987998
6	-3.720025	-2.871058	1.856071
1	-4.262680	-2.912025	2.811647
1	-4.421628	-3.172858	1.068189

1	-2.919964	-3.621376	1.902372
6	-4.503763	0.094839	1.576842
1	-5.165352	-0.036199	0.715130
1	-5.101004	-0.085390	2.483130
1	-4.175951	1.139714	1.596794

Rea-Ge=Ge-Singlet

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	1.106886	0.622846	0.389046
32	-1.106984	0.622537	-0.390222
6	-1.876229	-1.192607	0.082433
6	-0.620680	-2.086049	0.481921
6	0.621015	-2.085948	-0.482004
6	1.876472	-1.192264	-0.082455
1	-0.274891	-1.777096	1.476172
1	-0.961320	-3.125303	0.587728
1	0.961722	-3.125158	-0.587949
1	0.275080	-1.776970	-1.476236
6	-2.269147	2.207123	-0.183067
6	-3.397375	2.381845	-1.026048
6	-1.949196	3.255994	0.718293
6	-4.185648	3.545758	-0.960836
1	-3.667359	1.610688	-1.746019
6	-2.735035	4.423154	0.784095
1	-1.089083	3.162908	1.377938
6	-3.857818	4.571808	-0.053070
1	-5.047625	3.651776	-1.616154
1	-2.471191	5.209816	1.487788
1	-4.465811	5.472162	-0.000468
6	2.268881	2.207411	0.182530
6	3.397566	2.381593	1.024811
6	1.948177	3.256864	-0.717797
6	4.185608	3.545618	0.960039
1	3.668224	1.609916	1.743876
6	2.733791	4.424186	-0.783278

1	1.087637	3.164163	-1.376976
6	3.857088	4.572365	0.053308
1	5.048003	3.651215	1.614858
1	2.469375	5.211355	-1.486224
1	4.464930	5.472847	0.001017
14	3.006738	-1.135907	-1.677400
14	2.786976	-1.977029	1.461883
14	-2.787229	-1.977950	-1.461303
14	-3.005960	-1.135504	1.677660
6	4.472449	0.071652	-1.607915
1	4.135660	1.113682	-1.590645
1	5.129605	-0.083048	-0.746892
1	5.076937	-0.069827	-2.516063
6	3.700811	-2.880798	-2.031654
1	2.906008	-3.636737	-2.078142
1	4.207232	-2.876687	-3.007492
1	4.434361	-3.205324	-1.282966
6	1.980712	-0.646738	-3.207797
1	2.665210	-0.348562	-4.014652
1	1.373074	-1.479125	-3.585654
1	1.309962	0.198564	-3.009214
6	4.651267	-1.584249	1.522014
1	5.066421	-2.010743	2.446396
1	5.206480	-2.016621	0.681259
1	4.851753	-0.505514	1.538566
6	2.599651	-3.873920	1.439376
1	2.969519	-4.319814	0.507900
1	3.177416	-4.306651	2.268566
1	1.554496	-4.182439	1.571819
6	2.100480	-1.371043	3.135343
1	2.218549	-0.286980	3.266557
1	1.037132	-1.600777	3.267558
1	2.652561	-1.864284	3.949039
6	-2.101945	-1.372018	-3.135287
1	-2.220605	-0.287972	-3.266598
1	-1.038523	-1.601240	-3.268032
1	-2.654266	-1.865674	-3.948584
6	-2.599162	-3.874760	-1.438594
1	-2.968483	-4.320617	-0.506874
1	-3.177125	-4.307825	-2.267482

1	-1.553934	-4.182900	-1.571419
6	-4.651717	-1.585899	-1.520519
1	-5.067181	-2.012531	-2.444715
1	-5.206346	-2.018476	-0.679464
1	-4.852579	-0.507190	-1.536956
6	-1.979341	-0.645804	3.207482
1	-1.371346	-1.477966	3.585211
1	-1.308913	0.199616	3.008413
1	-2.663565	-0.347638	4.014572
6	-3.700034	-2.880196	2.032920
1	-4.206220	-2.875581	3.008876
1	-4.433795	-3.205004	1.284543
1	-2.905274	-3.636173	2.079566
6	-4.471683	0.072067	1.608245
1	-5.129158	-0.082982	0.747489
1	-5.075834	-0.069063	2.516673
1	-4.134867	1.114108	1.590418

Rea-Ge=Ge-Triplet

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	1.161126	0.614289	0.495758
32	-1.161191	0.614156	-0.495992
6	-1.889643	-1.216144	0.021991
6	-0.627910	-2.082253	0.468408
6	0.627970	-2.082435	-0.467849
6	1.889684	-1.216075	-0.021828
1	-0.307872	-1.758851	1.466506
1	-0.961141	-3.123201	0.589920
1	0.961235	-3.123428	-0.588933
1	0.307914	-1.759479	-1.466085
6	-2.218545	2.239222	-0.127441
6	-3.448491	2.467904	-0.800828
6	-1.715843	3.278504	0.698686
6	-4.157470	3.671130	-0.641096
1	-3.855955	1.703375	-1.460548

6	-2.423165	4.486280	0.861121
1	-0.770991	3.151999	1.224019
6	-3.645745	4.687655	0.191787
1	-5.098329	3.817916	-1.167292
1	-2.017550	5.265662	1.502688
1	-4.188658	5.622732	0.310688
6	2.218433	2.239380	0.127101
6	3.448218	2.468275	0.800669
6	1.715779	3.278483	-0.699260
6	4.157071	3.671578	0.640965
1	3.855631	1.703884	1.460568
6	2.422966	4.486339	-0.861685
1	0.771041	3.151804	-1.224752
6	3.645377	4.687963	-0.192100
1	5.097795	3.818545	1.167352
1	2.017366	5.265610	-1.503397
1	4.188158	5.623125	-0.310948
14	3.046947	-1.172297	-1.597224
14	2.759051	-2.006819	1.541122
14	-2.758735	-2.007495	-1.540796
14	-3.047047	-1.171911	1.597274
6	4.528681	0.015582	-1.538526
1	4.206710	1.062257	-1.538821
1	5.183932	-0.136830	-0.675171
1	5.131096	-0.148567	-2.444381
6	3.721137	-2.929284	-1.932914
1	2.917227	-3.675020	-1.986572
1	4.242602	-2.939136	-2.900863
1	4.438403	-3.258916	-1.170616
6	2.035283	-0.678535	-3.138363
1	2.727523	-0.415568	-3.950928
1	1.402884	-1.498149	-3.503385
1	1.391574	0.192843	-2.959384
6	4.629486	-1.642765	1.599300
1	5.038518	-2.048230	2.535738
1	5.182468	-2.100423	0.770507
1	4.839538	-0.565018	1.590351
6	2.517852	-3.897636	1.552981
1	2.890352	-4.377187	0.639337
1	3.063616	-4.329892	2.403945

1	1.459872	-4.166632	1.671249
6	2.086974	-1.356365	3.204604
1	2.315647	-0.292010	3.348629
1	1.001999	-1.475420	3.308333
1	2.563909	-1.913083	4.025207
6	-2.086966	-1.356972	-3.204379
1	-2.316104	-0.292727	-3.348517
1	-1.001945	-1.475572	-3.308140
1	-2.563705	-1.913976	-4.024903
6	-2.516742	-3.898216	-1.552313
1	-2.889137	-4.377734	-0.638606
1	-3.062247	-4.330851	-2.403250
1	-1.458635	-4.166787	-1.670405
6	-4.629329	-1.644262	-1.599100
1	-5.038163	-2.050200	-2.535421
1	-5.182136	-2.101883	-0.770168
1	-4.839829	-0.566595	-1.590515
6	-2.035730	-0.676582	3.138118
1	-1.402452	-1.495394	3.503391
1	-1.392940	0.195381	2.958688
1	-2.728149	-0.413987	3.950650
6	-3.720374	-2.929028	1.933969
1	-4.242103	-2.938518	2.901775
1	-4.437253	-3.259538	1.171689
1	-2.916092	-3.674307	1.988339
6	-4.529366	0.015205	1.537794
1	-5.184657	-0.138109	0.674627
1	-5.131604	-0.148584	2.443830
1	-4.207882	1.062027	1.537335

Rea-Sn=Sn-Singlet

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	1.250192	0.738256	0.492639
50	-1.274053	0.706473	-0.636189
6	-1.939231	-1.295400	0.100585

6	-0.604533	-2.040337	0.544880
6	0.605313	-2.068137	-0.464812
6	1.941255	-1.295148	-0.068322
1	-0.255649	-1.594631	1.485435
1	-0.860044	-3.082977	0.786407
1	0.863546	-3.121316	-0.647845
1	0.254062	-1.675438	-1.427154
6	-2.677162	2.304811	-0.234470
6	-3.845721	2.437875	-1.029032
6	-2.413700	3.322404	0.719759
6	-4.723678	3.527335	-0.868788
1	-4.085006	1.689915	-1.785077
6	-3.289640	4.414873	0.884193
1	-1.526587	3.268094	1.348200
6	-4.448371	4.520443	0.091203
1	-5.614180	3.600645	-1.489556
1	-3.066663	5.177332	1.627625
1	-5.124293	5.363360	0.217474
6	2.702612	2.302596	0.174358
6	3.930598	2.319246	0.886876
6	2.403626	3.422927	-0.645652
6	4.828393	3.398468	0.776062
1	4.202876	1.487289	1.536076
6	3.302630	4.501616	-0.765426
1	1.469054	3.460875	-1.203625
6	4.517975	4.493086	-0.054097
1	5.763055	3.383358	1.332821
1	3.052942	5.342613	-1.408990
1	5.211103	5.326574	-0.143526
14	3.055300	-1.319775	-1.667306
14	2.779678	-2.163373	1.462535
14	-2.791754	-2.278197	-1.352453
14	-3.055688	-1.190681	1.694750
6	4.648709	-0.285391	-1.589985
1	4.439666	0.785089	-1.489302
1	5.318728	-0.576213	-0.774856
1	5.195495	-0.429591	-2.533576
6	3.557800	-3.120476	-2.072116
1	2.688565	-3.789645	-2.120850
1	4.051649	-3.149907	-3.053946

1	4.262119	-3.532807	-1.338000
6	2.081826	-0.681832	-3.178133
1	2.777342	-0.555538	-4.020177
1	1.300526	-1.381413	-3.501156
1	1.605015	0.289235	-2.993674
6	4.673380	-1.951905	1.517057
1	5.049740	-2.414817	2.440526
1	5.181784	-2.435873	0.674764
1	4.976325	-0.896843	1.532685
6	2.407972	-4.032950	1.448011
1	2.757961	-4.515969	0.527322
1	2.919288	-4.514912	2.293300
1	1.334464	-4.237774	1.551173
6	2.174394	-1.486691	3.144303
1	2.465689	-0.437898	3.301569
1	1.086922	-1.548830	3.266766
1	2.634341	-2.073541	3.953189
6	-2.083495	-1.882744	-3.083090
1	-2.195290	-0.824461	-3.357343
1	-1.019944	-2.134593	-3.174012
1	-2.629521	-2.474837	-3.832468
6	-2.569040	-4.157043	-1.110783
1	-2.971434	-4.507626	-0.153241
1	-3.097033	-4.693306	-1.912173
1	-1.511831	-4.449401	-1.161938
6	-4.657909	-1.917196	-1.492937
1	-5.053377	-2.439155	-2.375934
1	-5.225071	-2.265723	-0.621639
1	-4.867062	-0.846939	-1.623552
6	-2.055953	-0.518322	3.173610
1	-1.344555	-1.256525	3.565785
1	-1.496006	0.392166	2.925941
1	-2.751340	-0.269344	3.987834
6	-3.642093	-2.938120	2.206813
1	-4.111998	-2.884379	3.199367
1	-4.387136	-3.348153	1.512814
1	-2.811253	-3.652518	2.274331
6	-4.606819	-0.099826	1.556470
1	-5.231192	-0.332080	0.688041
1	-5.219486	-0.259116	2.456285

1	-4.353546	0.964518	1.510841

Rea-Sn=Sn-Triplet

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	1.293851	0.634122	0.612223
50	-1.294004	0.634003	-0.612666
6	-1.946319	-1.396799	0.041182
6	-0.613056	-2.145232	0.490769
6	0.613034	-2.145489	-0.490197
6	1.946293	-1.396831	-0.041001
1	-0.281644	-1.722122	1.447774
1	-0.874283	-3.193317	0.711001
1	0.874242	-3.193688	-0.709932
1	0.281613	-1.722844	-1.447406
6	-2.449476	2.379593	-0.111918
6	-3.702789	2.633088	-0.728436
6	-1.901211	3.395203	0.713309
6	-4.390024	3.842443	-0.515984
1	-4.149600	1.887152	-1.385249
6	-2.585686	4.607888	0.930198
1	-0.934877	3.250803	1.195434
6	-3.831511	4.835356	0.314354
1	-5.349399	4.011250	-1.000589
1	-2.144075	5.369500	1.569309
1	-4.356953	5.774409	0.472619
6	2.449469	2.379627	0.111575
6	3.702593	2.633207	0.728444
6	1.901417	3.395157	-0.713892
6	4.389842	3.842577	0.516118
1	4.149236	1.887345	1.385456
6	2.585904	4.607858	-0.930649
1	0.935235	3.250673	-1.196298
6	3.831533	4.835418	-0.314442
1	5.349063	4.011456	1.001003
1	2.144451	5.369414	-1.569937

1	4.356979	5.774488	-0.472598
14	3.068052	-1.340662	-1.634001
14	2.808617	-2.244193	1.482796
14	-2.808402	-2.244857	-1.482356
14	-3.068158	-1.340075	1.634107
6	4.542468	-0.142151	-1.577963
1	4.212789	0.902032	-1.537324
1	5.221552	-0.315278	-0.736777
1	5.122993	-0.269952	-2.503542
6	3.737407	-3.088202	-2.021792
1	2.931720	-3.832827	-2.068395
1	4.235558	-3.080728	-3.001872
1	4.471785	-3.430426	-1.281791
6	2.026516	-0.818047	-3.147136
1	2.702575	-0.555591	-3.973131
1	1.374346	-1.625422	-3.504456
1	1.398151	0.060560	-2.947718
6	4.675129	-1.857278	1.531863
1	5.101820	-2.263416	2.459969
1	5.228787	-2.294031	0.692366
1	4.863930	-0.774890	1.532740
6	2.567281	-4.134596	1.449850
1	2.934179	-4.592708	0.523346
1	3.115519	-4.587658	2.288538
1	1.509011	-4.404082	1.567349
6	2.162233	-1.649557	3.180677
1	2.430437	-0.601548	3.372967
1	1.074715	-1.736483	3.292182
1	2.627040	-2.257646	3.971298
6	-2.162326	-1.650394	-3.180418
1	-2.430805	-0.602484	-3.372874
1	-1.074800	-1.737076	-3.292028
1	-2.627070	-2.258737	-3.970880
6	-2.566277	-4.135156	-1.448837
1	-2.933180	-4.593136	-0.522265
1	-3.114143	-4.588696	-2.287508
1	-1.507861	-4.404217	-1.566005
6	-4.675079	-1.858762	-1.531520
1	-5.101643	-2.265620	-2.459370
1	-5.228503	-2.295268	-0.691741

1	-4.864347	-0.776457	-1.533029
6	-2.026864	-0.816079	3.146930
1	-1.374288	-1.622928	3.504692
1	-1.398927	0.062715	2.947004
1	-2.703031	-0.553484	3.972792
6	-3.736769	-3.087665	2.022937
1	-4.235129	-3.079774	3.002907
1	-4.470825	-3.430729	1.283009
1	-2.930744	-3.831883	2.070214
6	-4.543074	-0.142209	1.577311
1	-5.222157	-0.316155	0.736289
1	-5.123488	-0.269627	2.503012
1	-4.213818	0.902078	1.535972

Rea-Pb=Pb-Singlet

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	1.314370	0.677362	0.547666
82	-1.357650	0.638324	-0.728630
6	-1.963898	-1.428198	0.170900
6	-0.591177	-2.116342	0.584973
6	0.583549	-2.157737	-0.467770
6	1.958685	-1.443425	-0.104152
1	-0.219659	-1.628258	1.494878
1	-0.805849	-3.156195	0.877941
1	0.797832	-3.215894	-0.682227
1	0.213162	-1.737370	-1.410535
6	-2.841090	2.229543	-0.162245
6	-4.051826	2.362876	-0.888716
6	-2.531637	3.235242	0.790163
6	-4.927316	3.444812	-0.665686
1	-4.330257	1.621341	-1.638668
6	-3.405967	4.318038	1.021213
1	-1.607758	3.184280	1.365426
6	-4.606925	4.426131	0.293101
1	-5.851252	3.521011	-1.235756

1	-3.148007	5.072180	1.762550
1	-5.280248	5.262640	0.467785
6	2.910591	2.196961	0.150861
6	4.176067	2.167944	0.791624
6	2.596075	3.333254	-0.640630
6	5.096648	3.224822	0.639848
1	4.460974	1.318485	1.412673
6	3.520010	4.385071	-0.809071
1	1.628110	3.408989	-1.136999
6	4.772235	4.334442	-0.165667
1	6.060374	3.180059	1.143718
1	3.259780	5.238587	-1.432234
1	5.483150	5.148847	-0.287530
14	3.025857	-1.466895	-1.727125
14	2.808097	-2.320115	1.406292
14	-2.835464	-2.443704	-1.238282
14	-3.022648	-1.298420	1.793395
6	4.656207	-0.490781	-1.680825
1	4.488384	0.581621	-1.533060
1	5.346933	-0.834319	-0.903926
1	5.159987	-0.618771	-2.650376
6	3.453655	-3.275513	-2.184802
1	2.558955	-3.910881	-2.229597
1	3.930046	-3.304593	-3.175257
1	4.154267	-3.727834	-1.470164
6	2.030177	-0.760392	-3.194731
1	2.694866	-0.674126	-4.066374
1	1.191092	-1.405184	-3.486623
1	1.628977	0.241137	-2.988803
6	4.707684	-2.161899	1.417734
1	5.092398	-2.623816	2.338329
1	5.181354	-2.671932	0.570224
1	5.041995	-1.116067	1.410958
6	2.387632	-4.179579	1.426138
1	2.712949	-4.680611	0.505623
1	2.899121	-4.665270	2.269274
1	1.311009	-4.357299	1.545118
6	2.261990	-1.601357	3.094460
1	2.594286	-0.560846	3.234102
1	1.176483	-1.629889	3.246799

1	2.723078	-2.189759	3.901416
6	-2.204999	-2.026847	-2.997176
1	-2.408042	-0.985706	-3.287985
1	-1.129396	-2.202094	-3.119708
1	-2.728279	-2.668655	-3.721357
6	-2.544942	-4.314619	-1.003746
1	-2.900438	-4.671310	-0.029602
1	-3.085443	-4.871884	-1.782178
1	-1.481442	-4.573258	-1.092442
6	-4.715480	-2.140459	-1.319562
1	-5.126248	-2.682219	-2.183533
1	-5.241610	-2.496417	-0.425825
1	-4.960245	-1.077952	-1.452098
6	-1.983892	-0.556281	3.213366
1	-1.228607	-1.258411	3.590325
1	-1.471700	0.369894	2.920764
1	-2.650127	-0.312098	4.052958
6	-3.542345	-3.046938	2.377480
1	-3.983328	-2.982596	3.382659
1	-4.296282	-3.494997	1.716529
1	-2.689542	-3.736351	2.434582
6	-4.608387	-0.255673	1.689929
1	-5.259466	-0.530771	0.854063
1	-5.180479	-0.405392	2.617700
1	-4.386595	0.813013	1.603550

Rea-Pb=Pb-Triplet

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	1.346763	0.565990	0.657967
82	-1.346907	0.565892	-0.658366
6	-1.963316	-1.569774	0.102527
6	-0.590583	-2.246148	0.516041
6	0.590543	-2.246427	-0.515441
6	1.963277	-1.569848	-0.102275
1	-0.233946	-1.777350	1.441769

1	-0.807668	-3.293910	0.790791
1	0.807602	-3.294336	-0.789664
1	0.233907	-1.778091	-1.441408
6	-2.525448	2.355361	-0.035461
6	-3.797944	2.616188	-0.605064
6	-1.937790	3.358588	0.775404
6	-4.470445	3.828290	-0.356771
1	-4.271976	1.876570	-1.250204
6	-2.609303	4.572415	1.029658
1	-0.952188	3.205616	1.215026
6	-3.876012	4.810120	0.461523
1	-5.446038	4.006959	-0.804304
1	-2.140783	5.327031	1.658089
1	-4.390067	5.750498	0.646742
6	2.525556	2.355334	0.035209
6	3.797875	2.616198	0.605192
6	1.938137	3.358519	-0.775880
6	4.470433	3.828300	0.357060
1	4.271719	1.876627	1.250524
6	2.609706	4.572350	-1.029967
1	0.952674	3.205506	-1.215799
6	3.876234	4.810096	-0.461446
1	5.445884	4.007004	0.804891
1	2.141366	5.326939	-1.658563
1	4.390327	5.750480	-0.646529
14	3.035283	-1.473612	-1.722376
14	2.853801	-2.408124	1.401890
14	-2.853619	-2.408696	-1.401398
14	-3.035395	-1.472960	1.722546
6	4.505115	-0.269540	-1.688407
1	4.170742	0.771740	-1.618701
1	5.209595	-0.454006	-0.870866
1	5.058472	-0.376596	-2.633075
6	3.697084	-3.215187	-2.153541
1	2.890420	-3.959833	-2.183627
1	4.167181	-3.196618	-3.147223
1	4.451994	-3.563550	-1.437354
6	1.947604	-0.930666	-3.195115
1	2.597373	-0.673019	-4.043402
1	1.271631	-1.726836	-3.532684

1	1.340326	-0.043347	-2.969557
6	4.717905	-2.009210	1.402807
1	5.173075	-2.411897	2.318707
1	5.252219	-2.441086	0.548334
1	4.897072	-0.925197	1.398816
6	2.619514	-4.300046	1.369190
1	2.966311	-4.751717	0.431858
1	3.189123	-4.754758	2.192583
1	1.565273	-4.573874	1.510380
6	2.249363	-1.824712	3.119637
1	2.526907	-0.779119	3.313266
1	1.165336	-1.912053	3.261014
1	2.734780	-2.439288	3.892521
6	-2.249471	-1.825436	-3.119300
1	-2.527320	-0.779948	-3.313072
1	-1.165433	-1.912495	-3.260757
1	-2.734787	-2.440265	-3.892045
6	-2.618608	-4.300523	-1.368178
1	-2.965372	-4.752057	-0.430763
1	-3.187920	-4.755680	-2.191531
1	-1.564237	-4.573979	-1.509118
6	-4.717883	-2.010527	-1.402405
1	-5.172938	-2.413914	-2.318055
1	-5.251969	-2.442142	-0.547661
1	-4.897495	-0.926586	-1.399029
6	-1.947947	-0.928740	3.194985
1	-1.271606	-1.724427	3.532947
1	-1.341075	-0.041264	2.968972
1	-2.597818	-0.670957	4.043152
6	-3.696491	-3.214562	2.154682
1	-4.166783	-3.195593	3.148263
1	-4.451102	-3.563713	1.438566
1	-2.889497	-3.958826	2.185387
6	-4.505705	-0.269487	1.687874
1	-5.210160	-0.454698	0.870477
1	-5.058980	-0.376200	2.632629
1	-4.171743	0.771882	1.617558

Prec-H2O-C

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.212583	0.411405	2.822946
8	0.517017	1.043486	3.510963
6	0.654071	0.328162	0.070120
6	-0.735952	0.294122	0.067094
6	-1.494614	1.612016	0.176162
6	-1.464956	2.397920	1.354956
6	-2.151483	3.624785	1.431638
6	-2.884417	4.109024	0.332539
6	-2.916957	3.345886	-0.848292
6	-2.235047	2.118631	-0.917907
1	-0.887622	2.083673	2.216699
1	-2.098692	4.206719	2.349330
1	-3.405532	5.062230	0.389008
1	-3.457584	3.708398	-1.720444
1	-2.247938	1.582893	-1.857749
6	-1.585302	-0.995881	-0.093121
14	-3.014029	-1.213796	1.256401
6	-4.324906	0.156991	1.370027
1	-3.903295	1.090597	1.756441
1	-4.807446	0.378916	0.414143
1	-5.107297	-0.175853	2.068955
6	-3.928183	-2.856776	0.918132
1	-3.241333	-3.710354	0.850870
1	-4.616311	-3.054926	1.752465
1	-4.529223	-2.833173	0.001549
6	-2.304765	-1.400151	3.017096
1	-3.150122	-1.418265	3.721082
1	-1.753031	-2.340036	3.151859
1	-1.661597	-0.562744	3.316684
14	-2.400848	-1.177572	-1.912359
6	-4.201448	-0.568991	-2.084148
1	-4.493155	-0.691751	-3.137589
1	-4.909964	-1.146690	-1.479887
1	-4.320130	0.488324	-1.826466
6	-2.437174	-3.016064	-2.420364

1	-2.996111	-3.646995	-1.719933
1	-2.931599	-3.089460	-3.400014
1	-1.429782	-3.436589	-2.530998
6	-1.397610	-0.286379	-3.274393
1	-0.578397	0.317075	-2.875584
1	-0.960203	-1.021443	-3.962660
1	-2.046767	0.371978	-3.867736
6	-0.632805	-2.229942	0.081103
1	-0.374411	-2.358058	1.139566
1	-1.137790	-3.153308	-0.220663
6	0.672431	-2.063727	-0.727051
1	1.214058	-3.015277	-0.753158
1	0.412413	-1.831327	-1.767965
6	1.576205	-0.920538	-0.143701
14	2.496795	-1.720803	1.444276
6	1.530727	-1.901910	3.096570
1	1.880620	-1.172637	3.836635
1	0.441054	-1.850158	3.029879
1	1.777298	-2.899134	3.490134
6	2.919209	-3.550907	1.076985
1	3.405418	-3.730549	0.116394
1	3.604143	-3.897881	1.865103
1	2.021035	-4.180957	1.127818
6	4.123999	-0.867004	1.945697
1	4.466892	-1.316885	2.888848
1	4.920733	-1.007363	1.206650
1	4.003362	0.208813	2.114723
14	2.983557	-0.580517	-1.526357
6	2.230140	-0.180018	-3.228732
1	1.569328	-0.971551	-3.600451
1	1.680297	0.765110	-3.243258
1	3.063164	-0.086256	-3.940757
6	4.001408	-2.164677	-1.852714
1	4.594650	-1.983248	-2.760966
1	4.707672	-2.400074	-1.047806
1	3.381680	-3.049965	-2.041036
6	4.273136	0.774659	-1.176984
1	4.651806	0.770340	-0.151763
1	5.127386	0.603896	-1.849715
1	3.879825	1.775056	-1.380466

6	1.319751	1.693956	0.011407
6	2.140874	2.220976	1.031904
6	2.754745	3.481176	0.888470
6	2.563376	4.246066	-0.277504
6	1.732755	3.741849	-1.296554
6	1.123898	2.486539	-1.147359
1	2.255895	1.682539	1.966042
1	3.376283	3.869473	1.692647
1	3.039510	5.218085	-0.387338
1	1.552676	4.321929	-2.199368
1	0.469545	2.121827	-1.932591
1	0.756583	0.564617	4.328274

Prec-H2O-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.122512	0.939897	3.130288
8	1.082750	0.961000	3.356832
14	1.034239	0.559976	0.208965
14	-1.147630	0.697135	0.416255
6	1.712987	-1.188055	-0.227681
6	0.419807	-1.961623	-0.748877
6	-0.793876	-2.070582	0.236440
6	-1.981320	-1.019445	0.069694
1	0.074190	-1.481174	-1.670912
1	0.715012	-2.980657	-1.026275
1	-1.216885	-3.079760	0.135624
1	-0.409944	-2.004787	1.263417
6	2.184241	2.057242	0.276470
6	3.350437	2.109917	1.081804
6	1.898677	3.177325	-0.547800
6	4.209330	3.224194	1.045349
1	3.587068	1.281988	1.745108
6	2.752120	4.297098	-0.581507
1	1.006330	3.176566	-1.169909
6	3.915407	4.321324	0.210344

1	5.104296	3.237579	1.664057
1	2.510262	5.139291	-1.226150
1	4.581858	5.180828	0.179104
6	-1.989830	2.377851	0.130579
6	-3.099912	2.564754	-0.734296
6	-1.484649	3.533636	0.789333
6	-3.665877	3.836047	-0.947476
1	-3.527034	1.721244	-1.264330
6	-2.043536	4.806696	0.574599
1	-0.641571	3.441343	1.471086
6	-3.139548	4.967153	-0.296984
1	-4.510112	3.939968	-1.626523
1	-1.628341	5.670193	1.090459
1	-3.574867	5.950472	-0.461880
14	-3.259222	-1.468044	1.486851
14	-2.800583	-1.228501	-1.696839
14	2.607721	-2.301349	1.131005
14	2.877751	-0.992944	-1.813592
6	-4.605196	-0.150769	1.748856
1	-4.175749	0.808387	2.065648
1	-5.208730	0.031726	0.853937
1	-5.286118	-0.489256	2.543904
6	-4.095680	-3.151004	1.135360
1	-3.353524	-3.949911	1.003455
1	-4.722135	-3.428156	1.995363
1	-4.740220	-3.142554	0.249278
6	-2.385142	-1.701705	3.165309
1	-3.150581	-1.836726	3.943734
1	-1.745163	-2.593308	3.177667
1	-1.770854	-0.837091	3.446281
6	-4.670465	-0.832661	-1.742449
1	-5.015456	-0.949088	-2.780024
1	-5.266209	-1.512048	-1.122445
1	-4.909744	0.191739	-1.434609
6	-2.627909	-3.040397	-2.268418
1	-3.070824	-3.746590	-1.556067
1	-3.146015	-3.168188	-3.229483
1	-1.578709	-3.323729	-2.417926
6	-2.025520	-0.144646	-3.057999
1	-2.092837	0.926783	-2.837642

1	-0.969397	-0.374672	-3.228686
1	-2.562314	-0.326447	-4.000975
6	2.083023	-2.071154	2.943366
1	2.362380	-1.085951	3.330715
1	1.005298	-2.185754	3.108862
1	2.600376	-2.844924	3.532827
6	2.269036	-4.139718	0.734958
1	2.540108	-4.420883	-0.289152
1	2.866544	-4.759921	1.418791
1	1.214752	-4.401318	0.892926
6	4.506752	-2.105637	1.166029
1	4.893127	-2.756825	1.963654
1	4.991653	-2.411681	0.231749
1	4.824855	-1.080990	1.396548
6	1.951409	-0.113658	-3.227855
1	1.177729	-0.744085	-3.682256
1	1.481255	0.823447	-2.905595
1	2.676454	0.134926	-4.016272
6	3.350191	-2.717062	-2.477464
1	3.892061	-2.592465	-3.425813
1	4.002736	-3.274382	-1.795283
1	2.466802	-3.334447	-2.684130
6	4.479308	0.002441	-1.569793
1	5.110887	-0.361002	-0.755322
1	5.061869	-0.072175	-2.500210
1	4.273361	1.062615	-1.390726
1	1.250104	1.270765	4.273088

Prec-H2O-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.268949	1.086490	2.916935
8	1.069802	1.216265	3.483510
32	1.082172	0.516696	-0.050040
32	-1.184266	0.676226	0.533987
6	1.722313	-1.368440	-0.274281

6	0.391893	-2.117063	-0.740212
6	-0.825472	-2.156403	0.255569
6	-2.019753	-1.115558	0.061428
1	0.054747	-1.680846	-1.687195
1	0.656095	-3.158630	-0.968192
1	-1.256210	-3.166773	0.195201
1	-0.439385	-2.060204	1.278084
6	2.330638	2.022371	0.156534
6	3.431706	2.061533	1.045772
6	2.109233	3.139106	-0.690773
6	4.298485	3.170837	1.066715
1	3.603422	1.241802	1.737379
6	2.975181	4.249437	-0.671626
1	1.257933	3.146040	-1.369972
6	4.078330	4.263455	0.203285
1	5.141505	3.183825	1.754276
1	2.788301	5.090814	-1.335434
1	4.754754	5.115696	0.215342
6	-2.015017	2.406069	0.030127
6	-3.121626	2.554667	-0.842263
6	-1.459700	3.586337	0.593707
6	-3.643439	3.825878	-1.152370
1	-3.581338	1.682093	-1.294219
6	-1.973980	4.858026	0.281869
1	-0.614270	3.515536	1.276845
6	-3.069959	4.983831	-0.594711
1	-4.489724	3.908056	-1.831634
1	-1.522968	5.743975	0.723906
1	-3.470535	5.965808	-0.836018
14	-3.319543	-1.504130	1.471089
14	-2.792691	-1.322782	-1.719328
14	2.521000	-2.344144	1.228888
14	2.925756	-1.316925	-1.832432
6	-4.622761	-0.129005	1.647769
1	-4.163088	0.838879	1.887615
1	-5.226181	0.003660	0.743454
1	-5.308278	-0.380124	2.470034
6	-4.201864	-3.170860	1.177896
1	-3.483718	-3.995732	1.076868
1	-4.839381	-3.397823	2.044438

1	-4.842800	-3.171099	0.288783
6	-2.450195	-1.671787	3.159055
1	-3.209813	-1.736630	3.951394
1	-1.834119	-2.578280	3.218962
1	-1.807218	-0.811202	3.381867
6	-4.656723	-0.913884	-1.828579
1	-4.970309	-1.059498	-2.872622
1	-5.273778	-1.573962	-1.208014
1	-4.901133	0.120144	-1.559366
6	-2.642535	-3.150492	-2.252946
1	-3.125462	-3.827194	-1.536983
1	-3.136270	-3.288696	-3.225380
1	-1.598249	-3.466456	-2.364150
6	-1.969577	-0.266686	-3.074451
1	-2.045643	0.808253	-2.871614
1	-0.908153	-0.498194	-3.207855
1	-2.475582	-0.463275	-4.031537
6	1.839283	-1.927041	2.952443
1	1.956251	-0.871836	3.230253
1	0.774466	-2.172665	3.058451
1	2.389168	-2.539837	3.685388
6	2.201074	-4.210105	0.962989
1	2.532367	-4.567254	-0.019549
1	2.751009	-4.779123	1.726637
1	1.137313	-4.458116	1.073106
6	4.410513	-2.128706	1.361280
1	4.754451	-2.695385	2.238826
1	4.949109	-2.518415	0.488937
1	4.708556	-1.083110	1.509602
6	2.036781	-0.528212	-3.325768
1	1.234844	-1.159584	-3.727655
1	1.605371	0.453265	-3.087030
1	2.769218	-0.374022	-4.131350
6	3.424077	-3.078788	-2.355964
1	3.991214	-3.024528	-3.296138
1	4.060801	-3.574548	-1.613348
1	2.549956	-3.717582	-2.536482
6	4.505251	-0.286889	-1.588753
1	5.110484	-0.605137	-0.735946
1	5.123261	-0.389462	-2.492796

1	4.280515	0.777654	-1.461448
1	0.851896	1.681557	4.317501

Prec-H2O-Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.452733	0.996431	-3.365789
8	-1.414433	1.158067	-3.507214
50	-1.220565	0.624219	0.006931
50	1.430144	0.745122	-0.923928
6	2.354945	2.525828	-0.058089
6	1.567629	3.664296	0.263799
6	2.151730	4.866181	0.708414
6	3.551092	4.968473	0.838488
6	4.354513	3.860225	0.512146
6	3.762099	2.660348	0.066884
1	0.482581	3.621800	0.175058
1	1.517835	5.716514	0.953061
1	4.004975	5.894747	1.184199
1	5.437332	3.926582	0.600515
1	4.417462	1.832099	-0.191812
6	2.116022	-1.180505	0.030642
14	3.449578	-1.897771	-1.196381
6	4.818891	-0.646025	-1.637128
1	4.421122	0.242706	-2.146874
1	5.386596	-0.313716	-0.761038
1	5.528137	-1.121639	-2.329651
6	4.288351	-3.473307	-0.514902
1	3.551263	-4.237556	-0.234059
1	4.930779	-3.908867	-1.293664
1	4.917401	-3.274608	0.361083
6	2.640596	-2.412738	-2.845437
1	3.426306	-2.705742	-3.556608
1	1.968317	-3.272253	-2.726673
1	2.068863	-1.594922	-3.302818
14	2.778493	-1.053641	1.851506

6	4.622236	-0.574753	1.958755
1	4.921582	-0.605327	3.016510
1	5.282309	-1.258854	1.413341
1	4.804999	0.444851	1.600474
6	2.618222	-2.749278	2.722647
1	3.204853	-3.524626	2.214475
1	2.993739	-2.669496	3.752990
1	1.578636	-3.094726	2.776901
6	1.886644	0.232210	2.943088
1	1.881603	1.224338	2.475758
1	0.849873	-0.038490	3.175046
1	2.424425	0.317905	3.899203
6	0.874194	-2.176405	-0.085544
1	0.487159	-2.131870	-1.110699
1	1.263354	-3.201116	0.031531
6	-0.338119	-2.053675	0.909941
1	-0.532339	-3.065764	1.296791
1	-0.020856	-1.468800	1.780194
6	-1.730422	-1.473470	0.378283
14	-2.390576	-2.510353	-1.137291
6	-1.686555	-2.009991	-2.833779
1	-1.890351	-0.965371	-3.098808
1	-0.604191	-2.170153	-2.915335
1	-2.164917	-2.640119	-3.599143
6	-1.946002	-4.348090	-0.877614
1	-2.352991	-4.751620	0.056862
1	-2.358248	-4.941373	-1.706439
1	-0.859848	-4.504918	-0.870551
6	-4.282072	-2.392913	-1.339180
1	-4.563239	-2.921194	-2.261323
1	-4.832839	-2.858065	-0.512852
1	-4.625596	-1.355061	-1.436800
14	-2.956096	-1.539482	1.904350
6	-2.139049	-0.717017	3.424469
1	-1.255377	-1.262747	3.777855
1	-1.837746	0.324414	3.239966
1	-2.864413	-0.697893	4.250585
6	-3.332057	-3.341287	2.406900
1	-3.894996	-3.339704	3.351378
1	-3.942807	-3.863706	1.660117

1	-2.418556	-3.927854	2.568617
6	-4.614455	-0.639880	1.665485
1	-5.205935	-1.036198	0.835122
1	-5.206813	-0.763148	2.584090
1	-4.484628	0.435278	1.498473
6	-2.889637	1.974846	-0.206422
6	-3.852109	1.912304	-1.246262
6	-4.915316	2.835416	-1.302228
6	-5.039470	3.839083	-0.320432
6	-4.087069	3.924082	0.712381
6	-3.019856	3.004177	0.762056
1	-3.768016	1.157929	-2.024564
1	-5.643834	2.770221	-2.107797
1	-5.864206	4.547103	-0.362569
1	-4.169190	4.699492	1.471154
1	-2.290539	3.100539	1.567205
1	-1.559205	2.051594	-3.879919

Prec-H2O-Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.515534	1.469038	-3.521191
8	-1.466531	1.466048	-3.751313
82	-1.338250	0.660456	0.205738
82	1.554246	0.807502	-0.837068
6	2.662659	2.356194	0.383855
6	1.971313	3.433735	0.999891
6	2.660552	4.487766	1.633214
6	4.069129	4.499861	1.654702
6	4.778222	3.453352	1.035183
6	4.081450	2.398617	0.409034
1	0.881868	3.458859	0.994736
1	2.101942	5.294377	2.104679
1	4.603850	5.312325	2.141963
1	5.866723	3.455945	1.038053
1	4.663732	1.612639	-0.069427

6	2.097652	-1.360456	-0.098784
14	3.267540	-2.006256	-1.509190
6	4.694023	-0.799329	-1.899875
1	4.332963	0.140503	-2.343511
1	5.292762	-0.552404	-1.016369
1	5.366626	-1.258942	-2.638171
6	4.017212	-3.718530	-1.118804
1	3.239093	-4.447948	-0.856457
1	4.540697	-4.101326	-2.006750
1	4.739689	-3.687410	-0.294433
6	2.294039	-2.226864	-3.136592
1	2.988985	-2.506226	-3.941446
1	1.543701	-3.024226	-3.060587
1	1.777694	-1.310302	-3.451383
14	2.883652	-1.520647	1.661735
6	4.766387	-1.206584	1.670543
1	5.139604	-1.397127	2.687261
1	5.324369	-1.861330	0.991089
1	5.008432	-0.165137	1.427906
6	2.632360	-3.292462	2.339635
1	3.076643	-4.048117	1.679718
1	3.115293	-3.384158	3.323354
1	1.571230	-3.538836	2.467856
6	2.199157	-0.313689	2.971996
1	2.315949	0.729075	2.653594
1	1.142209	-0.480440	3.211170
1	2.769287	-0.441866	3.904197
6	0.729087	-2.153517	-0.269793
1	0.256055	-1.827933	-1.207546
1	0.960721	-3.219929	-0.430524
6	-0.341898	-2.091658	0.880024
1	-0.441190	-3.107832	1.292444
1	0.060548	-1.487172	1.701399
6	-1.795784	-1.554114	0.520112
14	-2.589851	-2.495148	-0.979923
6	-2.042276	-1.874477	-2.699016
1	-2.130431	-0.789883	-2.845463
1	-1.005320	-2.150581	-2.929393
1	-2.676991	-2.353963	-3.459362
6	-2.117727	-4.343464	-0.888434

1	-2.452709	-4.810055	0.046079
1	-2.588607	-4.886039	-1.720798
1	-1.033258	-4.491686	-0.969063
6	-4.493870	-2.401529	-0.980199
1	-4.865056	-2.873303	-1.901281
1	-4.943100	-2.937498	-0.135006
1	-4.865619	-1.369925	-0.963878
14	-2.861949	-1.680915	2.147720
6	-1.888932	-0.921700	3.609077
1	-0.976457	-1.484604	3.840987
1	-1.598661	0.126531	3.442274
1	-2.521811	-0.938125	4.507815
6	-3.199512	-3.499808	2.615602
1	-3.655295	-3.544184	3.615082
1	-3.890940	-3.985262	1.915611
1	-2.276736	-4.093742	2.645997
6	-4.525838	-0.759618	2.097967
1	-5.239101	-1.211666	1.401804
1	-4.974481	-0.792843	3.101598
1	-4.418059	0.295394	1.818822
6	-3.180712	1.844998	-0.264356
6	-4.065043	1.568599	-1.338193
6	-5.184802	2.389680	-1.583421
6	-5.447553	3.500017	-0.755912
6	-4.577113	3.794300	0.310823
6	-3.450811	2.978253	0.544963
1	-3.882602	0.726138	-2.000972
1	-5.848738	2.161495	-2.414949
1	-6.315439	4.128572	-0.942994
1	-4.768180	4.652836	0.951451
1	-2.785649	3.241061	1.369123
1	-1.829819	2.372407	-3.719709

TS-H2O-C

Atomic Number	Coordinates (Angstroms) X	Y	Z

1	0.613343	0.081227	-1.531631
8	-0.553129	0.289515	-2.499649
6	-0.730580	0.336429	-0.245560
6	0.781726	0.279041	-0.390543
6	1.504517	1.643511	-0.415724
6	1.525091	2.379214	-1.626145
6	2.197684	3.609423	-1.724715
6	2.871279	4.144825	-0.610526
6	2.849348	3.433808	0.602388
6	2.173544	2.202667	0.694248
1	0.983923	1.975574	-2.476558
1	2.193437	4.148608	-2.669746
1	3.395485	5.095083	-0.684134
1	3.352940	3.835797	1.479394
1	2.162372	1.702179	1.652397
6	1.615618	-0.974843	0.129326
14	3.075049	-1.356797	-1.152029
6	4.363373	0.022679	-1.374268
1	3.926400	0.906378	-1.851399
1	4.824364	0.344181	-0.436180
1	5.163350	-0.353227	-2.029603
6	3.995719	-2.946021	-0.628678
1	3.310708	-3.793008	-0.490324
1	4.696233	-3.221945	-1.429987
1	4.581755	-2.829525	0.290548
6	2.364462	-1.715906	-2.882755
1	3.189063	-1.696086	-3.609949
1	1.902707	-2.710439	-2.941426
1	1.618250	-0.975864	-3.194293
14	2.358514	-0.964366	1.969798
6	4.156937	-0.345936	2.131528
1	4.424281	-0.372767	3.198202
1	4.873197	-0.983987	1.601213
1	4.293299	0.680967	1.777437
6	2.399552	-2.748984	2.651817
1	2.969709	-3.437773	2.018146
1	2.887660	-2.727019	3.637232
1	1.395802	-3.169254	2.794320
6	1.338065	0.030073	3.251925
1	0.508763	0.593508	2.817288

1	0.912218	-0.651570	4.000091
1	1.981606	0.741266	3.788092
6	0.651054	-2.208957	0.052083
1	0.407075	-2.430010	-0.993742
1	1.141476	-3.104843	0.447535
6	-0.657586	-1.958661	0.826155
1	-1.211930	-2.896839	0.930264
1	-0.409432	-1.638507	1.846665
6	-1.573940	-0.879984	0.136559
14	-2.466772	-1.860294	-1.407366
6	-1.522825	-2.326058	-3.000338
1	-1.795578	-1.658744	-3.825136
1	-0.438509	-2.289275	-2.907550
1	-1.824903	-3.348594	-3.273786
6	-2.932672	-3.612866	-0.786223
1	-3.420144	-3.678574	0.186060
1	-3.622584	-4.036000	-1.532382
1	-2.046630	-4.262246	-0.771148
6	-4.076941	-1.013441	-1.964736
1	-4.428991	-1.533427	-2.867310
1	-4.874486	-1.079098	-1.215779
1	-3.936570	0.041435	-2.222907
14	-3.009841	-0.441153	1.484286
6	-2.264228	0.097283	3.153081
1	-1.599709	-0.657271	3.588623
1	-1.727480	1.048540	3.108354
1	-3.105550	0.231119	3.848841
6	-4.012252	-1.995255	1.952932
1	-4.598516	-1.729091	2.844714
1	-4.721883	-2.305839	1.178533
1	-3.387931	-2.855825	2.220421
6	-4.302661	0.874957	1.026641
1	-4.681539	0.790217	0.005273
1	-5.155069	0.746284	1.710870
1	-3.918554	1.890778	1.158138
6	-1.364239	1.711286	-0.214149
6	-2.214726	2.211943	-1.222115
6	-2.801225	3.482993	-1.113919
6	-2.550135	4.291651	0.010970
6	-1.694926	3.812015	1.018686

6	-1.104439	2.541690	0.902968
1	-2.357368	1.611393	-2.109678
1	-3.441691	3.846110	-1.914324
1	-2.997014	5.279635	0.091736
1	-1.468781	4.427934	1.885738
1	-0.426059	2.211956	1.681106
1	-0.992350	0.325434	-3.382207

	1
	A
Frequencies --	-561.7504
Red. masses --	1.5008
Frc consts --	0.2790
IR Inten --	64.0587

Atom	AN	X	Y	Z
1	1	0.54	-0.12	0.20
2	8	-0.03	0.00	0.05
3	6	-0.05	-0.01	-0.15
4	6	0.08	-0.02	-0.06
5	6	0.01	0.01	0.01
6	6	0.00	0.00	0.01
7	6	0.00	0.00	0.00
8	6	0.00	0.00	0.00
9	6	0.00	0.01	0.00
10	6	0.00	0.01	0.01
11	1	0.01	-0.02	0.01
12	1	0.00	0.00	0.00
13	1	0.00	0.00	0.00
14	1	0.01	0.01	0.00
15	1	0.01	0.00	0.01
16	6	0.02	-0.01	0.04
17	14	0.00	0.00	0.01
18	6	0.00	0.00	0.00
19	1	0.00	0.00	0.00
20	1	0.00	0.00	0.00
21	1	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	1	0.00	0.00	0.00
24	1	0.00	-0.01	0.00

25	1	0.00	0.00	0.00
26	6	0.00	0.00	0.01
27	1	0.00	0.01	0.01
28	1	0.00	0.00	0.00
29	1	-0.01	-0.01	0.00
30	14	0.00	0.00	0.01
31	6	0.00	0.00	0.00
32	1	0.00	0.00	0.00
33	1	0.00	0.00	0.00
34	1	0.00	0.00	0.00
35	6	0.00	0.00	0.01
36	1	0.00	0.00	0.00
37	1	0.00	-0.01	0.01
38	1	0.00	0.00	0.00
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	0.01	0.03	0.00
45	1	-0.01	-0.01	-0.01
46	6	0.00	0.01	-0.01
47	1	0.00	0.01	0.00
48	1	0.00	0.01	-0.01
49	6	-0.01	0.00	-0.01
50	14	0.00	-0.01	0.00
51	6	0.00	0.00	0.00
52	1	0.01	0.00	0.00
53	1	0.00	0.01	0.00
54	1	0.01	0.00	0.00
55	6	0.00	0.00	0.00
56	1	0.00	0.00	0.00
57	1	0.00	0.00	0.00
58	1	0.00	0.00	0.00
59	6	0.00	0.00	0.00
60	1	0.00	0.00	0.00
61	1	0.00	0.00	0.00
62	1	-0.01	0.00	0.00
63	14	0.00	0.00	0.00
64	6	0.00	0.00	0.00

65	1	0.00	0.00	0.00
66	1	0.00	0.00	0.00
67	1	0.00	0.00	0.00
68	6	0.00	0.00	0.00
69	1	0.00	0.00	0.00
70	1	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	-0.01	0.00	-0.01
77	6	-0.01	0.01	0.00
78	6	-0.01	0.01	0.00
79	6	0.00	0.00	0.00
80	6	0.00	-0.01	0.00
81	6	0.00	-0.01	0.00
82	1	-0.05	0.02	0.01
83	1	-0.01	0.01	0.00
84	1	0.01	0.00	0.01
85	1	0.01	-0.01	0.00
86	1	0.00	-0.01	-0.01
87	1	-0.67	0.17	0.36

TS-H2O-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.046331	0.720230	-2.649076
8	-0.958894	0.667939	-2.685993
14	-1.039215	0.579584	-0.315445
14	1.207924	0.700676	-0.543350
6	-1.730682	-1.148465	0.196411
6	-0.438153	-1.908646	0.749991
6	0.782287	-2.052624	-0.221558
6	1.987589	-1.020702	-0.062194
1	-0.098205	-1.400462	1.659536

1	-0.739246	-2.916789	1.059487
1	1.185862	-3.068186	-0.102717
1	0.407693	-1.996270	-1.253655
6	-2.204029	2.076154	-0.347822
6	-3.381304	2.120815	-1.137852
6	-1.901096	3.210314	0.447387
6	-4.225274	3.246012	-1.129957
1	-3.646306	1.270693	-1.763286
6	-2.742407	4.341401	0.457855
1	-1.000225	3.218789	1.057138
6	-3.908092	4.362545	-0.329688
1	-5.125028	3.253032	-1.741651
1	-2.484213	5.198965	1.075052
1	-4.559222	5.234064	-0.322796
6	2.011798	2.387854	-0.160157
6	3.102878	2.596843	0.723575
6	1.535088	3.530193	-0.865479
6	3.685641	3.868164	0.895864
1	3.510484	1.768622	1.291776
6	2.106561	4.802881	-0.690733
1	0.712083	3.420331	-1.569620
6	3.192722	4.980654	0.190083
1	4.521569	3.985618	1.583127
1	1.716517	5.649670	-1.252585
1	3.647130	5.961151	0.316077
14	3.272626	-1.542433	-1.449604
14	2.789091	-1.189600	1.709789
14	-2.647468	-2.321425	-1.099745
14	-2.894294	-0.913759	1.784272
6	4.641841	-0.258526	-1.756787
1	4.228946	0.687611	-2.131035
1	5.234181	-0.037070	-0.863335
1	5.330528	-0.647822	-2.522051
6	4.081480	-3.222789	-1.021451
1	3.324022	-4.003791	-0.868950
1	4.713488	-3.542106	-1.862478
1	4.714059	-3.190622	-0.127501
6	2.428107	-1.846643	-3.132732
1	3.210822	-2.020545	-3.886415
1	1.784551	-2.735985	-3.119909

1	1.828355	-0.990310	-3.464139
6	4.660828	-0.799658	1.747029
1	5.009446	-0.890669	2.785846
1	5.253944	-1.494334	1.141641
1	4.898205	0.216449	1.410858
6	2.602090	-2.983932	2.333175
1	3.036388	-3.712853	1.638488
1	3.118947	-3.093939	3.297179
1	1.549580	-3.251733	2.489920
6	2.017026	-0.064726	3.039799
1	2.103519	0.999846	2.795456
1	0.955390	-0.274490	3.204322
1	2.542042	-0.232638	3.992016
6	-2.181003	-2.183918	-2.939942
1	-2.516821	-1.239459	-3.381090
1	-1.106114	-2.278994	-3.131583
1	-2.696526	-3.004416	-3.464206
6	-2.299163	-4.142388	-0.638886
1	-2.562639	-4.384024	0.396798
1	-2.903085	-4.788294	-1.292717
1	-1.246710	-4.412906	-0.793407
6	-4.549271	-2.135367	-1.110428
1	-4.944354	-2.825144	-1.870527
1	-5.019626	-2.399283	-0.156298
1	-4.878177	-1.124476	-1.383600
6	-1.970766	0.002649	3.176626
1	-1.202897	-0.618683	3.652743
1	-1.494284	0.929793	2.835405
1	-2.700366	0.272857	3.953900
6	-3.357562	-2.619508	2.504923
1	-3.898224	-2.462955	3.449503
1	-4.010294	-3.205137	1.847191
1	-2.470854	-3.225510	2.731051
6	-4.504181	0.064772	1.522498
1	-5.140042	-0.327688	0.725099
1	-5.080087	0.014631	2.458694
1	-4.308092	1.120603	1.310842
1	-1.380327	0.928372	-3.536719

		1		
		A		
Frequencies --		-167.8726		
Red. masses --		6.3924		
Frc consts --		0.1061		
IR Inten --		54.8475		
Atom	AN	X	Y	Z
1	1	0.06	-0.06	0.26
2	8	0.00	-0.12	0.48
3	14	-0.03	0.00	-0.16
4	14	0.08	0.00	-0.15
5	6	-0.01	0.02	-0.04
6	6	0.00	0.04	-0.02
7	6	0.00	0.02	-0.01
8	6	0.01	0.00	0.00
9	1	0.00	0.07	-0.03
10	1	0.00	0.05	0.01
11	1	-0.01	0.01	0.00
12	1	0.02	0.01	-0.01
13	6	-0.04	0.00	-0.01
14	6	-0.05	0.02	0.01
15	6	-0.02	-0.01	0.00
16	6	-0.03	0.03	0.01
17	1	-0.09	0.02	0.02
18	6	0.00	0.00	0.01
19	1	0.00	-0.03	-0.02
20	6	0.00	0.02	0.01
21	1	-0.04	0.05	0.02
22	1	0.02	-0.01	0.01
23	1	0.01	0.03	0.02
24	6	0.00	0.01	0.03
25	6	0.00	0.01	0.03
26	6	0.01	0.01	0.03
27	6	0.00	0.01	0.02
28	1	0.00	0.01	0.03
29	6	0.00	0.01	0.02
30	1	0.02	0.00	0.01
31	6	0.01	0.01	0.02
32	1	0.01	0.01	0.02
33	1	0.01	0.01	0.01

34	1	0.01	0.01	0.01
35	14	0.01	-0.01	0.00
36	14	0.00	0.00	0.00
37	14	-0.01	-0.01	0.00
38	14	0.00	0.01	-0.02
39	6	0.01	-0.01	0.00
40	1	0.00	-0.01	0.01
41	1	0.01	-0.01	0.00
42	1	0.01	0.00	0.00
43	6	0.01	-0.01	0.01
44	1	0.01	-0.01	0.01
45	1	0.01	-0.01	0.01
46	1	0.01	-0.01	0.01
47	6	0.02	-0.03	0.00
48	1	0.03	-0.05	0.01
49	1	0.01	-0.02	0.01
50	1	0.04	-0.02	-0.01
51	6	0.00	0.00	0.01
52	1	0.00	0.01	0.01
53	1	0.00	0.00	0.01
54	1	0.00	0.00	0.00
55	6	0.00	0.00	0.01
56	1	0.00	0.00	0.01
57	1	0.00	0.00	0.01
58	1	0.00	0.00	0.01
59	6	-0.01	0.00	0.00
60	1	-0.01	0.00	-0.01
61	1	-0.01	0.00	0.00
62	1	-0.01	0.01	0.00
63	6	-0.02	-0.01	-0.01
64	1	-0.11	-0.06	-0.05
65	1	-0.02	0.07	-0.02
66	1	0.04	-0.06	0.01
67	6	0.01	0.00	0.00
68	1	0.01	0.00	0.00
69	1	0.01	-0.01	0.00
70	1	0.01	0.01	0.00
71	6	-0.01	-0.01	0.00
72	1	-0.01	-0.01	0.00
73	1	0.00	-0.01	0.00

74	1	-0.01	-0.01	0.00
75	6	0.01	0.02	-0.03
76	1	0.00	0.02	-0.02
77	1	0.01	0.02	-0.03
78	1	0.01	0.03	-0.03
79	6	0.01	0.01	-0.01
80	1	0.02	0.02	-0.01
81	1	0.01	0.01	0.00
82	1	0.01	0.02	-0.01
83	6	-0.01	0.00	0.00
84	1	-0.01	0.00	0.00
85	1	0.00	-0.01	0.00
86	1	-0.02	0.01	0.00
87	1	-0.34	-0.13	0.64

TS-H2O-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.193736	0.818255	-2.825758
8	-1.180802	0.805179	-2.933972
32	-1.088240	0.522875	-0.138021
32	1.254095	0.692436	-0.698231
6	-1.707548	-1.344224	0.272540
6	-0.359128	-2.019246	0.805351
6	0.858412	-2.118368	-0.182251
6	2.053207	-1.075907	-0.028872
1	-0.032793	-1.489003	1.706357
1	-0.601491	-3.040175	1.130542
1	1.279770	-3.129455	-0.076818
1	0.476640	-2.066135	-1.209877
6	-2.400020	1.996229	-0.254835
6	-3.548284	1.988166	-1.084013
6	-2.161044	3.139889	0.547592
6	-4.434836	3.080793	-1.101138
1	-3.747075	1.131141	-1.722562
6	-3.049008	4.234692	0.536164

1	-1.276201	3.187830	1.180098
6	-4.189446	4.206576	-0.287470
1	-5.312852	3.055318	-1.743109
1	-2.845973	5.100549	1.162349
1	-4.876512	5.049891	-0.299238
6	1.980986	2.453888	-0.098673
6	3.066956	2.652860	0.788994
6	1.411278	3.611606	-0.695592
6	3.556428	3.943422	1.075730
1	3.544466	1.804461	1.267044
6	1.888581	4.902628	-0.407052
1	0.587005	3.505699	-1.400327
6	2.969005	5.075581	0.481527
1	4.392571	4.060275	1.762610
1	1.427385	5.766851	-0.881206
1	3.347981	6.071607	0.699895
14	3.369600	-1.556338	-1.396487
14	2.806014	-1.182084	1.763979
14	-2.491032	-2.485993	-1.117963
14	-2.900176	-1.212453	1.838890
6	4.659944	-0.181883	-1.656515
1	4.186703	0.758463	-1.968935
1	5.249932	0.023346	-0.757033
1	5.358380	-0.478506	-2.452224
6	4.264666	-3.192935	-0.988537
1	3.551060	-4.014865	-0.840622
1	4.909973	-3.469340	-1.834798
1	4.898665	-3.132227	-0.096677
6	2.522218	-1.853178	-3.078428
1	3.292247	-1.984306	-3.852295
1	1.899718	-2.757364	-3.076690
1	1.892382	-1.004964	-3.372437
6	4.663883	-0.743594	1.864051
1	4.973170	-0.822421	2.916463
1	5.292044	-1.432176	1.287214
1	4.896969	0.274957	1.532991
6	2.673233	-2.982034	2.392925
1	3.172654	-3.689586	1.719457
1	3.155522	-3.063643	3.377546
1	1.630753	-3.303861	2.507569

6	1.961126	-0.079009	3.068649
1	2.000601	0.985073	2.809670
1	0.909873	-0.339509	3.227287
1	2.481467	-0.209193	4.029447
6	-1.812132	-2.332192	-2.888799
1	-2.318364	-1.543943	-3.458627
1	-0.739922	-2.111969	-2.931572
1	-1.978854	-3.299770	-3.391740
6	-2.144470	-4.311051	-0.671403
1	-2.456363	-4.585050	0.342165
1	-2.695405	-4.951729	-1.375452
1	-1.078666	-4.552069	-0.778278
6	-4.383094	-2.296744	-1.261360
1	-4.727380	-2.919938	-2.099270
1	-4.915219	-2.632855	-0.362999
1	-4.689376	-1.264136	-1.472481
6	-2.015145	-0.307869	3.267071
1	-1.215972	-0.908871	3.717329
1	-1.582755	0.654245	2.962037
1	-2.750681	-0.097520	4.056831
6	-3.338086	-2.947765	2.494676
1	-3.874364	-2.839201	3.448322
1	-3.989698	-3.505970	1.811878
1	-2.445625	-3.556227	2.688111
6	-4.523583	-0.259856	1.570410
1	-5.123412	-0.633924	0.736381
1	-5.127169	-0.359165	2.484800
1	-4.346205	0.808055	1.405792
1	-1.493088	1.475007	-3.579636

	1
	A
Frequencies --	-108.8652
Red. masses --	7.0113
Frc consts --	0.0490
IR Inten --	25.2385

Atom	AN	X	Y	Z
1	1	0.05	-0.07	0.13
2	8	0.00	-0.14	0.51

3	32	-0.02	0.01	-0.11
4	32	0.05	0.01	-0.06
5	6	-0.01	0.02	-0.03
6	6	-0.01	0.04	-0.01
7	6	0.00	0.02	-0.01
8	6	0.01	0.00	0.01
9	1	-0.01	0.06	-0.03
10	1	0.00	0.04	0.02
11	1	-0.03	0.01	-0.02
12	1	0.00	0.04	-0.01
13	6	-0.05	0.00	0.02
14	6	-0.06	0.02	0.04
15	6	-0.02	0.00	0.01
16	6	-0.04	0.03	0.04
17	1	-0.11	0.00	0.07
18	6	0.00	0.02	0.01
19	1	0.00	-0.01	-0.01
20	6	-0.01	0.03	0.03
21	1	-0.06	0.04	0.06
22	1	0.02	0.02	0.01
23	1	0.01	0.05	0.03
24	6	0.00	0.00	0.04
25	6	0.00	0.01	0.05
26	6	0.01	0.00	0.03
27	6	0.00	0.02	0.03
28	1	0.00	0.02	0.06
29	6	0.01	0.01	0.02
30	1	0.02	0.00	0.02
31	6	0.01	0.01	0.02
32	1	0.00	0.02	0.03
33	1	0.01	0.00	0.01
34	1	0.01	0.01	0.01
35	14	0.01	-0.01	0.01
36	14	0.00	-0.01	0.00
37	14	0.00	-0.01	0.00
38	14	0.00	0.02	-0.02
39	6	0.01	-0.01	0.01
40	1	0.01	-0.01	0.01
41	1	0.01	-0.01	0.00
42	1	0.01	-0.01	0.00

43	6	0.01	−0.01	0.01
44	1	0.01	−0.01	0.01
45	1	0.01	−0.01	0.02
46	1	0.00	−0.01	0.02
47	6	0.02	−0.02	0.01
48	1	0.03	−0.06	0.02
49	1	−0.01	0.00	0.02
50	1	0.05	0.00	−0.01
51	6	0.00	0.00	0.01
52	1	0.00	0.00	0.01
53	1	0.00	−0.01	0.01
54	1	0.00	0.00	0.00
55	6	0.00	0.00	0.01
56	1	0.00	−0.01	0.01
57	1	−0.01	−0.01	0.01
58	1	−0.01	0.00	0.00
59	6	−0.01	−0.01	0.01
60	1	−0.03	−0.01	−0.01
61	1	0.00	−0.03	0.02
62	1	0.01	0.02	0.00
63	6	−0.02	−0.05	−0.02
64	1	−0.14	−0.16	−0.07
65	1	−0.05	0.09	−0.04
66	1	0.10	−0.10	0.05
67	6	0.00	0.00	0.02
68	1	0.01	0.00	0.02
69	1	0.01	−0.02	0.03
70	1	0.01	0.00	0.02
71	6	−0.01	−0.02	0.00
72	1	−0.01	−0.02	0.01
73	1	0.00	−0.01	0.00
74	1	−0.01	−0.02	−0.01
75	6	0.00	0.02	−0.03
76	1	−0.01	0.02	−0.02
77	1	0.02	0.02	−0.04
78	1	0.00	0.04	−0.03
79	6	0.01	0.02	−0.01
80	1	0.02	0.02	0.00
81	1	0.00	0.01	0.00
82	1	0.02	0.02	−0.01

83	6	-0.01	0.00	-0.01
84	1	-0.01	0.00	-0.01
85	1	-0.01	-0.02	-0.01
86	1	-0.03	0.00	0.01
87	1	-0.33	-0.23	0.57

TS-H2O-Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.321547	1.101884	-3.077685
8	-1.274920	1.257654	-3.292632
50	-1.226516	0.619717	-0.003588
50	1.435896	0.739029	-0.917318
6	2.355080	2.522244	-0.053002
6	1.563170	3.661655	0.255331
6	2.141885	4.869001	0.691862
6	3.540280	4.975721	0.828342
6	4.348183	3.866924	0.515424
6	3.761279	2.661683	0.077437
1	0.478479	3.615932	0.161745
1	1.504522	5.719886	0.925381
1	3.990033	5.905975	1.168571
1	5.430361	3.936837	0.608508
1	4.420000	1.833428	-0.172718
6	2.114951	-1.185638	0.034063
14	3.453834	-1.902370	-1.187928
6	4.824082	-0.650110	-1.623939
1	4.427459	0.239144	-2.133701
1	5.389679	-0.318593	-0.746167
1	5.535038	-1.124832	-2.315311
6	4.289004	-3.477805	-0.502434
1	3.550167	-4.241030	-0.223422
1	4.933546	-3.914624	-1.278729
1	4.915306	-3.278961	0.375436
6	2.651145	-2.417998	-2.840063
1	3.439740	-2.711849	-3.547738

1	1.978419	-3.277468	-2.723430
1	2.081404	-1.600923	-3.301102
14	2.767595	-1.055493	1.856996
6	4.610015	-0.573757	1.971967
1	4.904706	-0.602125	3.031085
1	5.273351	-1.257894	1.430614
1	4.792796	0.445380	1.612400
6	2.604311	-2.748658	2.731603
1	3.194737	-3.524238	2.228143
1	2.973577	-2.666276	3.763971
1	1.564818	-3.095274	2.780312
6	1.867265	0.234183	2.937216
1	1.858716	1.222841	2.462037
1	0.830957	-0.039474	3.168320
1	2.402043	0.330179	3.894177
6	0.873072	-2.181524	-0.088719
1	0.490519	-2.135812	-1.115542
1	1.262384	-3.206129	0.028448
6	-0.344605	-2.061742	0.901435
1	-0.541837	-3.075758	1.281482
1	-0.031455	-1.482177	1.776898
6	-1.734243	-1.479038	0.364354
14	-2.386618	-2.513926	-1.155938
6	-1.673447	-2.005090	-2.846237
1	-1.855300	-0.952437	-3.095718
1	-0.593981	-2.183329	-2.929324
1	-2.162153	-2.616863	-3.619896
6	-1.941203	-4.351565	-0.895470
1	-2.356092	-4.755915	0.035319
1	-2.345772	-4.944933	-1.728079
1	-0.854982	-4.507514	-0.878628
6	-4.277411	-2.401638	-1.367237
1	-4.552602	-2.934973	-2.288428
1	-4.830708	-2.865161	-0.541567
1	-4.623660	-1.365213	-1.470935
14	-2.969763	-1.540211	1.883381
6	-2.162194	-0.705345	3.402118
1	-1.279862	-1.247664	3.764116
1	-1.860476	0.335113	3.211198
1	-2.891929	-0.679852	4.224284

6	-3.348239	-3.338878	2.395296
1	-3.917980	-3.331220	3.335791
1	-3.953901	-3.866421	1.647849
1	-2.436175	-3.924553	2.567821
6	-4.627101	-0.643369	1.627439
1	-5.212015	-1.044113	0.794540
1	-5.226351	-0.762421	2.542122
1	-4.496527	0.430982	1.455870
6	-2.897040	1.969369	-0.219517
6	-3.858815	1.904763	-1.260241
6	-4.921653	2.827851	-1.319691
6	-5.046466	3.834088	-0.340530
6	-4.095324	3.921168	0.693114
6	-3.028610	3.000587	0.746737
1	-3.774317	1.149080	-2.037126
1	-5.648990	2.760540	-2.126270
1	-5.870951	4.542213	-0.385753
1	-4.177878	4.698788	1.449541
1	-2.300126	3.098519	1.552555
1	-1.409744	2.176262	-3.605981

		1		
		A		
Frequencies --		-63.9424		
Red. masses --		8.3824		
Frc consts --		0.0202		
IR Inten --		11.0284		
Atom	AN	X	Y	Z
1	1	0.04	-0.04	0.18
2	8	-0.06	-0.10	0.56
3	50	-0.02	0.01	-0.10
4	50	0.05	0.00	-0.03
5	6	0.01	0.00	0.04
6	6	0.00	-0.01	0.05
7	6	0.00	0.00	0.04
8	6	0.00	0.01	0.03
9	6	0.00	0.02	0.02
10	6	0.01	0.01	0.03
11	1	0.00	-0.02	0.06

12	1	-0.01	-0.01	0.04
13	1	-0.01	0.02	0.02
14	1	0.00	0.03	0.01
15	1	0.02	0.02	0.02
16	6	0.01	0.00	0.00
17	14	0.01	-0.01	0.01
18	6	0.02	-0.02	0.01
19	1	0.02	-0.02	0.00
20	1	0.01	-0.01	0.01
21	1	0.02	-0.02	0.02
22	6	0.00	-0.01	0.02
23	1	0.00	-0.01	0.02
24	1	0.00	-0.02	0.02
25	1	0.00	-0.01	0.02
26	6	0.02	-0.02	0.01
27	1	0.02	-0.02	0.02
28	1	0.01	-0.01	0.01
29	1	0.02	-0.02	0.00
30	14	0.00	0.00	0.00
31	6	0.00	-0.01	0.01
32	1	-0.01	-0.01	0.01
33	1	0.00	-0.01	0.02
34	1	0.00	-0.01	0.01
35	6	-0.01	0.00	0.01
36	1	-0.02	0.00	0.02
37	1	-0.02	0.00	0.01
38	1	-0.02	0.01	0.00
39	6	0.00	0.01	0.00
40	1	0.00	0.00	-0.01
41	1	0.00	0.01	0.00
42	1	-0.01	0.01	0.00
43	6	0.00	0.02	-0.01
44	1	0.00	0.03	-0.01
45	1	-0.02	0.01	-0.01
46	6	0.00	0.04	-0.01
47	1	0.00	0.05	0.02
48	1	-0.01	0.06	-0.03
49	6	-0.01	0.01	-0.03
50	14	0.00	-0.03	0.00
51	6	0.00	-0.08	-0.01

52	1	0.02	-0.08	-0.01
53	1	-0.01	-0.11	-0.02
54	1	-0.02	-0.08	0.00
55	6	0.00	-0.03	0.05
56	1	0.00	-0.01	0.05
57	1	0.01	-0.05	0.06
58	1	0.00	-0.02	0.05
59	6	0.00	-0.03	0.00
60	1	0.00	-0.06	0.01
61	1	0.00	-0.01	0.01
62	1	0.00	-0.04	-0.03
63	14	0.00	0.03	-0.02
64	6	0.00	0.04	-0.03
65	1	-0.01	0.05	-0.03
66	1	0.00	0.04	-0.05
67	1	0.00	0.06	-0.04
68	6	0.01	0.03	0.00
69	1	0.03	0.04	0.01
70	1	0.00	0.02	0.02
71	1	0.01	0.03	-0.01
72	6	-0.01	0.01	-0.02
73	1	0.00	0.02	-0.03
74	1	-0.02	-0.02	-0.03
75	1	-0.03	0.01	0.00
76	6	-0.04	0.01	0.02
77	6	-0.08	0.00	0.06
78	6	-0.07	0.01	0.08
79	6	-0.03	0.03	0.06
80	6	0.01	0.03	0.03
81	6	0.00	0.02	0.01
82	1	-0.13	-0.03	0.08
83	1	-0.11	0.00	0.11
84	1	-0.02	0.04	0.08
85	1	0.04	0.04	0.02
86	1	0.03	0.03	-0.02
87	1	-0.25	-0.13	0.57

TS-H2O-Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.350267	1.366434	-3.158870
8	-1.289652	1.394343	-3.441733
82	-1.342595	0.665129	0.188856
82	1.559106	0.797806	-0.841524
6	2.664792	2.351535	0.371915
6	1.974080	3.438945	0.970627
6	2.663695	4.497606	1.595522
6	4.072264	4.505142	1.624030
6	4.780826	3.449821	1.018816
6	4.083356	2.390453	0.401417
1	0.884757	3.469208	0.957860
1	2.105602	5.311703	2.054567
1	4.607375	5.321209	2.104821
1	5.869310	3.449532	1.025654
1	4.664937	1.598928	-0.068418
6	2.091862	-1.364711	-0.087139
14	3.265879	-2.024046	-1.488652
6	4.695802	-0.823126	-1.885592
1	4.338127	0.112718	-2.340143
1	5.292234	-0.568042	-1.002929
1	5.370139	-1.291172	-2.616954
6	4.010525	-3.734887	-1.082940
1	3.230135	-4.459671	-0.814884
1	4.533351	-4.126762	-1.967281
1	4.732814	-3.699054	-0.258566
6	2.296067	-2.254681	-3.116671
1	2.992054	-2.543116	-3.917402
1	1.543158	-3.049090	-3.035809
1	1.783407	-1.339167	-3.440419
14	2.869440	-1.513785	1.678403
6	4.753678	-1.211991	1.692716
1	5.121174	-1.397629	2.712365
1	5.310119	-1.875352	1.020477
1	5.003023	-0.173817	1.444142
6	2.602989	-3.277679	2.369485
1	3.045404	-4.041604	1.717940

1	3.080442	-3.364677	3.356292
1	1.539564	-3.515686	2.494183
6	2.187455	-0.289340	2.973577
1	2.309192	0.749073	2.643127
1	1.129461	-0.448315	3.212624
1	2.754944	-0.409364	3.908414
6	0.720441	-2.154673	-0.259467
1	0.252050	-1.833871	-1.201393
1	0.949195	-3.222717	-0.412801
6	-0.355447	-2.083171	0.885624
1	-0.457065	-3.096645	1.303938
1	0.043912	-1.473711	1.704834
6	-1.807297	-1.545096	0.516123
14	-2.597596	-2.497328	-0.979980
6	-2.041071	-1.897022	-2.702697
1	-2.121031	-0.813440	-2.859218
1	-1.004861	-2.180539	-2.927182
1	-2.675858	-2.381218	-3.460122
6	-2.131950	-4.346191	-0.868124
1	-2.472114	-4.803425	0.069149
1	-2.600955	-4.894639	-1.697680
1	-1.047641	-4.498262	-0.943018
6	-4.501393	-2.396401	-0.990291
1	-4.869805	-2.876166	-1.908369
1	-4.957429	-2.921626	-0.142073
1	-4.868798	-1.363118	-0.987015
14	-2.881100	-1.655476	2.139592
6	-1.912791	-0.885656	3.598423
1	-1.002716	-1.448620	3.839299
1	-1.619020	0.160295	3.423344
1	-2.549632	-0.892054	4.494418
6	-3.225454	-3.469363	2.620695
1	-3.687016	-3.504097	3.617870
1	-3.914383	-3.958555	1.920992
1	-2.304372	-4.065341	2.660955
6	-4.542185	-0.729895	2.074137
1	-5.254016	-1.186238	1.379320
1	-4.994892	-0.753208	3.076184
1	-4.430448	0.322380	1.786251
6	-3.179698	1.853314	-0.298470

6	-4.060604	1.570887	-1.373744
6	-5.175076	2.395058	-1.632420
6	-5.436406	3.514659	-0.817002
6	-4.569819	3.814664	0.251307
6	-3.448793	2.995117	0.499025
1	-3.878977	0.721151	-2.027465
1	-5.835856	2.162274	-2.465194
1	-6.300059	4.145778	-1.014752
1	-4.759851	4.680307	0.882612
1	-2.786851	3.262532	1.324266
1	-1.630407	2.310062	-3.399614

	1
	A
Frequencies --	-65.2819
Red. masses --	11.2754
Frc consts --	0.0283
IR Inten --	23.5945

Atom	AN	X	Y	Z
1	1	0.10	0.08	0.03
2	8	-0.11	-0.11	0.71
3	82	-0.01	0.01	-0.08
4	82	0.04	0.01	-0.02
5	6	0.01	-0.01	0.05
6	6	0.00	-0.01	0.04
7	6	0.00	0.00	0.03
8	6	0.00	0.01	0.02
9	6	0.00	0.02	0.03
10	6	0.01	0.01	0.04
11	1	0.00	-0.02	0.05
12	1	-0.01	0.00	0.03
13	1	-0.01	0.02	0.02
14	1	0.00	0.03	0.02
15	1	0.01	0.01	0.04
16	6	0.00	0.00	0.01
17	14	0.00	-0.01	0.01
18	6	0.01	-0.02	0.01
19	1	0.01	-0.02	0.00
20	1	0.00	-0.01	0.01

21	1	0.01	−0.02	0.02
22	6	0.00	−0.01	0.01
23	1	0.00	−0.01	0.01
24	1	0.00	−0.01	0.01
25	1	0.00	−0.01	0.01
26	6	0.01	−0.01	0.01
27	1	0.01	−0.01	0.01
28	1	0.01	−0.01	0.01
29	1	0.01	−0.01	0.01
30	14	−0.01	−0.01	0.01
31	6	0.00	−0.01	0.01
32	1	−0.01	−0.01	0.01
33	1	0.00	−0.01	0.01
34	1	0.00	−0.01	0.01
35	6	−0.01	−0.01	0.01
36	1	−0.01	−0.01	0.01
37	1	−0.01	−0.01	0.01
38	1	−0.01	−0.01	0.01
39	6	0.00	−0.01	0.01
40	1	0.00	−0.01	0.00
41	1	0.00	−0.01	0.01
42	1	0.00	0.00	0.01
43	6	−0.01	0.01	0.00
44	1	0.00	0.03	0.00
45	1	−0.02	0.01	−0.01
46	6	0.00	0.03	0.00
47	1	0.01	0.03	0.02
48	1	−0.01	0.05	−0.02
49	6	−0.01	0.01	−0.01
50	14	0.00	−0.03	0.01
51	6	0.01	−0.08	−0.01
52	1	0.07	−0.08	−0.01
53	1	−0.01	−0.15	−0.01
54	1	−0.03	−0.06	0.01
55	6	−0.01	−0.03	0.05
56	1	−0.02	−0.01	0.06
57	1	0.00	−0.04	0.06
58	1	−0.01	−0.03	0.07
59	6	0.00	−0.02	0.00
60	1	0.00	−0.03	0.01

61	1	-0.01	0.00	0.01
62	1	0.00	-0.02	-0.02
63	14	-0.01	0.02	-0.01
64	6	0.00	0.04	-0.02
65	1	-0.01	0.04	-0.01
66	1	0.00	0.04	-0.03
67	1	0.00	0.05	-0.02
68	6	0.01	0.02	0.01
69	1	0.02	0.03	0.02
70	1	0.00	0.02	0.03
71	1	0.01	0.03	0.01
72	6	-0.01	0.01	-0.01
73	1	-0.01	0.00	-0.01
74	1	-0.01	0.00	-0.01
75	1	-0.02	0.01	0.00
76	6	-0.05	0.01	0.05
77	6	-0.06	0.01	0.05
78	6	-0.05	0.02	0.06
79	6	-0.04	0.03	0.05
80	6	-0.03	0.02	0.04
81	6	-0.03	0.01	0.04
82	1	-0.07	0.00	0.06
83	1	-0.06	0.02	0.06
84	1	-0.03	0.04	0.05
85	1	-0.02	0.03	0.04
86	1	-0.03	0.01	0.04
87	1	-0.14	-0.11	0.50

Pro-H2O-C

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.852268	0.377133	-0.595104
6	0.724852	-0.095681	-0.653464
1	0.625716	-0.870461	-1.424164
6	1.406151	-0.913183	0.547196
6	-1.792492	-0.700362	0.109337

6	-1.034413	-1.393427	1.294612
1	-1.671650	-2.187978	1.706386
1	-0.877437	-0.682641	2.119655
6	0.334761	-2.001709	0.918991
1	0.685813	-2.629326	1.745331
1	0.187976	-2.678661	0.065893
14	-2.350769	-2.072917	-1.239279
14	-3.487526	0.026924	0.873145
8	-1.282804	0.319144	-2.015213
1	-0.651071	0.814519	-2.581558
14	2.945319	-1.906057	-0.264928
14	2.138145	-0.166638	2.254793
6	2.394779	-3.022177	-1.708581
1	3.304987	-3.478354	-2.125411
1	1.901973	-2.481623	-2.523969
1	1.737790	-3.841350	-1.392690
6	3.727816	-3.134994	0.968407
1	4.459080	-3.741734	0.414780
1	2.986035	-3.825470	1.389565
1	4.259052	-2.656003	1.797405
6	4.340235	-0.827112	-0.994938
1	5.303294	-1.340113	-0.857130
1	4.421977	0.166306	-0.549206
1	4.186313	-0.689253	-2.071707
6	2.053440	-1.548837	3.574681
1	2.487799	-2.503185	3.264948
1	1.017663	-1.733383	3.889684
1	2.605788	-1.205754	4.461593
6	3.965575	0.379451	2.124767
1	4.647457	-0.403452	1.780672
1	4.290138	0.680692	3.131160
1	4.090381	1.246811	1.465684
6	1.384106	1.295114	3.236298
1	2.043318	1.408430	4.110163
1	0.378001	1.093418	3.622591
1	1.371764	2.253057	2.709095
6	-1.115707	-2.701679	-2.550816
1	-0.259190	-3.232180	-2.127404
1	-0.753486	-1.897687	-3.198207
1	-1.660982	-3.421803	-3.180291

6	-3.860833	-1.542084	-2.272919
1	-3.576612	-0.706233	-2.922086
1	-4.738114	-1.239525	-1.693348
1	-4.161727	-2.385155	-2.912070
6	-2.767902	-3.687915	-0.295619
1	-1.860520	-4.140131	0.128323
1	-3.184298	-4.411068	-1.012448
1	-3.494717	-3.570689	0.512423
6	-4.766605	-1.359784	1.197359
1	-4.410388	-2.074798	1.950694
1	-5.080089	-1.922373	0.314382
1	-5.661389	-0.873334	1.613210
6	-4.312817	1.335819	-0.235597
1	-4.000354	2.346877	0.049277
1	-5.405577	1.276274	-0.132466
1	-4.062496	1.196566	-1.291981
6	-3.306902	0.747725	2.637521
1	-2.645709	0.149328	3.278311
1	-4.303015	0.733867	3.103765
1	-2.953346	1.781849	2.643988
6	-1.022775	1.849585	-0.151908
6	-1.238063	4.578921	0.661226
6	-0.857547	2.229843	1.189756
6	-1.324346	2.871900	-1.082994
6	-1.427310	4.216143	-0.685639
6	-0.958233	3.570840	1.600133
1	-0.661534	1.470109	1.928617
1	-1.512891	2.627037	-2.121723
1	-1.660702	4.976613	-1.427528
1	-0.824204	3.822210	2.650071
1	-1.316436	5.618450	0.970806
6	1.572795	1.008038	-1.292138
6	3.088626	3.046477	-2.590405
6	2.090550	2.106332	-0.568362
6	1.833502	0.959712	-2.682772
6	2.579417	1.964407	-3.329745
6	2.840613	3.108710	-1.204663
1	1.892089	2.196810	0.493223
1	1.480615	0.107045	-3.262245
1	2.766793	1.894611	-4.398907

1	3.223945	3.943380	-0.622133
1	3.668202	3.824712	-3.081267

Pro-H2O-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-1.127574	0.635780	-0.775409
14	1.224040	0.215458	-0.843792
1	1.375684	-0.361854	-2.217746
6	1.682988	-1.227120	0.376181
6	-1.960115	-0.928888	0.001407
6	-0.934172	-1.639587	0.989194
1	-1.453864	-2.496504	1.443430
1	-0.709258	-0.962832	1.821209
6	0.414633	-2.188930	0.419579
1	0.682640	-3.064260	1.030452
1	0.231127	-2.585896	-0.585756
14	-2.469029	-2.171066	-1.436910
14	-3.547616	-0.523648	1.087751
8	-1.659376	0.791203	-2.417881
1	-1.221560	0.356228	-3.167439
14	3.123597	-2.292691	-0.443056
14	2.197441	-0.715076	2.188519
6	2.474245	-3.265508	-1.948473
1	3.324161	-3.774475	-2.425926
1	2.011335	-2.620632	-2.704620
1	1.747368	-4.038476	-1.668075
6	3.818709	-3.625156	0.733681
1	4.533177	-4.241910	0.169298
1	3.036304	-4.296914	1.109670
1	4.353004	-3.208845	1.595171
6	4.583180	-1.242049	-1.063722
1	5.433029	-1.904902	-1.281784
1	4.919027	-0.493798	-0.339418
1	4.331983	-0.715414	-1.991617
6	1.950258	-2.187977	3.376588

1	2.495310	-3.088242	3.076817
1	0.888614	-2.451570	3.474320
1	2.307633	-1.900090	4.375814
6	4.007109	-0.130302	2.286747
1	4.731630	-0.907271	2.018620
1	4.223040	0.179257	3.319316
1	4.183180	0.738212	1.639118
6	1.207059	0.698914	3.004578
1	1.562015	0.784030	4.042441
1	0.128268	0.512836	3.049748
1	1.378408	1.669363	2.527688
6	-1.252834	-2.278615	-2.919097
1	-0.245753	-1.898262	-2.722991
1	-1.662120	-1.739698	-3.784808
1	-1.145410	-3.331149	-3.216535
6	-4.137907	-1.732528	-2.236006
1	-4.107553	-0.713239	-2.640084
1	-4.991544	-1.811048	-1.554165
1	-4.319474	-2.421719	-3.073477
6	-2.557779	-3.950029	-0.750552
1	-1.575509	-4.305335	-0.412648
1	-2.888576	-4.620324	-1.557273
1	-3.261867	-4.060213	0.079998
6	-4.551080	-2.098844	1.498009
1	-3.933115	-2.870889	1.974860
1	-5.044876	-2.545816	0.627778
1	-5.337156	-1.821898	2.215549
6	-4.736175	0.725730	0.290043
1	-4.299041	1.728553	0.243236
1	-5.649145	0.786981	0.900200
1	-5.032940	0.440609	-0.724871
6	-3.054646	0.147748	2.803136
1	-2.458226	-0.574853	3.375106
1	-3.974226	0.336298	3.376148
1	-2.505326	1.092381	2.751340
6	-1.595248	2.367009	-0.132466
6	-2.287049	5.013807	0.671798
6	-1.288769	2.842886	1.164974
6	-2.245894	3.257552	-1.023881
6	-2.589750	4.563444	-0.627211

6	-1.631333	4.148195	1.567324
1	-0.774765	2.203967	1.877229
1	-2.474297	2.913321	-2.027875
1	-3.090388	5.225097	-1.330866
1	-1.386680	4.484679	2.572794
1	-2.553163	6.022685	0.979817
6	2.297449	1.788566	-0.929190
6	3.880102	4.149150	-1.224784
6	2.248916	2.834031	0.027102
6	3.146540	1.975428	-2.051663
6	3.929362	3.135283	-2.199999
6	3.031531	3.995736	-0.112256
1	1.575533	2.765777	0.875521
1	3.191431	1.212652	-2.826246
1	4.569260	3.246604	-3.072744
1	2.966619	4.781296	0.637481
1	4.483068	5.047584	-1.335857

Pro-H2O-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-1.175251	0.630875	-0.698713
32	1.281625	0.208960	-0.792111
1	1.486595	-0.352526	-2.234475
6	1.702000	-1.332103	0.448687
6	-2.002386	-1.036415	0.069269
6	-0.939671	-1.732082	1.030277
1	-1.439888	-2.598702	1.489244
1	-0.712882	-1.058022	1.863616
6	0.412197	-2.266777	0.441810
1	0.663966	-3.171210	1.017560
1	0.231930	-2.620938	-0.579737
14	-2.492499	-2.242301	-1.397362
14	-3.576326	-0.652163	1.174800
8	-1.778401	0.833844	-2.404985
1	-1.343199	0.401781	-3.160709

14	3.139725	-2.383869	-0.381927
14	2.189965	-0.838414	2.268981
6	2.493413	-3.332662	-1.903466
1	3.342392	-3.836449	-2.387924
1	2.033893	-2.673689	-2.649599
1	1.763496	-4.107511	-1.636433
6	3.831820	-3.726839	0.784265
1	4.550323	-4.339469	0.220649
1	3.046604	-4.400684	1.150913
1	4.359733	-3.315564	1.652331
6	4.593992	-1.312778	-0.980390
1	5.444767	-1.965250	-1.224339
1	4.932617	-0.585489	-0.235941
1	4.334411	-0.759821	-1.890825
6	1.922033	-2.320350	3.440141
1	2.487553	-3.210620	3.146058
1	0.861288	-2.598061	3.502783
1	2.246161	-2.039031	4.452526
6	4.000539	-0.261895	2.395138
1	4.724836	-1.037193	2.121223
1	4.207979	0.030225	3.434515
1	4.186573	0.616695	1.763905
6	1.192632	0.583842	3.063246
1	1.556343	0.704024	4.094804
1	0.115932	0.388736	3.123727
1	1.348835	1.541753	2.555855
6	-1.277338	-2.284206	-2.883692
1	-0.279015	-1.881955	-2.684983
1	-1.703929	-1.735354	-3.734400
1	-1.143987	-3.326484	-3.205964
6	-4.172651	-1.810530	-2.175671
1	-4.160255	-0.782906	-2.559534
1	-5.019374	-1.915507	-1.488408
1	-4.351690	-2.484936	-3.025600
6	-2.552776	-4.037232	-0.750317
1	-1.567062	-4.381627	-0.411222
1	-2.866568	-4.698310	-1.571171
1	-3.260884	-4.173989	0.073472
6	-4.565100	-2.237927	1.576628
1	-3.935358	-3.014314	2.030787

1	-5.064931	-2.672028	0.702819
1	-5.345236	-1.980649	2.307788
6	-4.774043	0.601244	0.396238
1	-4.340109	1.606296	0.356307
1	-5.682965	0.655887	1.013077
1	-5.077484	0.325651	-0.619337
6	-3.059073	0.020073	2.882597
1	-2.452029	-0.700237	3.446214
1	-3.968438	0.210227	3.471106
1	-2.511497	0.966011	2.820382
6	-1.676072	2.408758	-0.003824
6	-2.359758	5.039138	0.837052
6	-1.348328	2.866619	1.294352
6	-2.342071	3.301669	-0.879407
6	-2.682218	4.602731	-0.462563
6	-1.688377	4.166871	1.715080
1	-0.821007	2.219753	1.990961
1	-2.582273	2.966871	-1.884509
1	-3.194152	5.271744	-1.151005
1	-1.429638	4.494259	2.720069
1	-2.622980	6.044230	1.159563
6	2.400376	1.839760	-0.805108
6	3.967765	4.213805	-1.013911
6	2.294951	2.875357	0.156101
6	3.295855	2.037958	-1.888047
6	4.072381	3.207287	-1.993009
6	3.072086	4.045415	0.059471
1	1.584768	2.794235	0.973975
1	3.383262	1.280401	-2.664663
1	4.749039	3.331939	-2.836062
1	2.966452	4.825098	0.810904
1	4.565175	5.119335	-1.092640

Pro-H2O-Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z

50	-1.367390	0.586744	-0.742754
50	1.445081	0.315230	-0.932847
1	1.814186	-0.229083	-2.534776
6	1.875139	-1.366911	0.417715
6	-1.971827	-1.286140	0.221251
6	-0.753568	-1.786376	1.119613
1	-1.126661	-2.630935	1.720825
1	-0.505587	-1.009179	1.850715
6	0.574507	-2.290659	0.444284
1	0.852388	-3.213533	0.978754
1	0.350086	-2.615603	-0.577778
14	-2.422872	-2.591742	-1.153726
14	-3.470161	-0.999552	1.440405
8	-2.248729	0.696856	-2.488178
1	-1.986067	0.252279	-3.311211
14	3.270565	-2.480248	-0.374927
14	2.351637	-0.756850	2.201287
6	2.595444	-3.427948	-1.884475
1	3.425091	-3.959610	-2.372231
1	2.150376	-2.758915	-2.631404
1	1.844625	-4.178625	-1.606976
6	3.889575	-3.809579	0.847744
1	4.543697	-4.513094	0.313035
1	3.062353	-4.392126	1.274175
1	4.468012	-3.387158	1.678238
6	4.777374	-1.494499	-0.993393
1	5.564725	-2.199423	-1.296591
1	5.201661	-0.833113	-0.230652
1	4.527279	-0.893533	-1.877438
6	1.999921	-2.119914	3.488806
1	2.593220	-3.023879	3.308401
1	0.941222	-2.408357	3.505866
1	2.255929	-1.748678	4.491406
6	4.188800	-0.272145	2.345449
1	4.873570	-1.102163	2.136033
1	4.382301	0.060843	3.375236
1	4.444880	0.562512	1.680653
6	1.401709	0.798508	2.776874
1	1.778154	1.083977	3.770202
1	0.321559	0.636662	2.877532

1	1.569833	1.655465	2.112612
6	-1.325916	-2.507310	-2.730846
1	-0.384369	-1.957778	-2.619424
1	-1.886399	-2.050245	-3.557741
1	-1.063804	-3.527669	-3.043998
6	-4.198903	-2.388563	-1.801557
1	-4.346831	-1.378767	-2.204497
1	-4.967263	-2.575471	-1.042814
1	-4.362672	-3.103536	-2.620752
6	-2.220792	-4.357189	-0.459078
1	-1.182517	-4.566277	-0.172018
1	-2.502802	-5.085463	-1.233046
1	-2.855716	-4.538446	0.415008
6	-4.230037	-2.649195	2.033989
1	-3.478128	-3.318399	2.473110
1	-4.747712	-3.197258	1.237312
1	-4.970450	-2.432073	2.817574
6	-4.862550	0.062072	0.700580
1	-4.551123	1.104596	0.569407
1	-5.719544	0.059405	1.389650
1	-5.213837	-0.308505	-0.267769
6	-2.871270	-0.128796	3.027921
1	-2.150153	-0.736976	3.589136
1	-3.735222	0.043591	3.685804
1	-2.419514	0.849721	2.827941
6	-2.093769	2.458199	0.002999
6	-3.075842	5.005711	0.805783
6	-1.693744	3.039327	1.231750
6	-2.987416	3.186894	-0.823243
6	-3.474863	4.447364	-0.424212
6	-2.181393	4.299479	1.632977
1	-0.994159	2.524950	1.888934
1	-3.289315	2.763231	-1.778174
1	-4.160367	4.989426	-1.072366
1	-1.863131	4.724710	2.582621
1	-3.453082	5.978628	1.113662
6	2.543495	2.145400	-0.660643
6	3.957146	4.609711	-0.388726
6	1.869825	3.345107	-0.313983
6	3.943934	2.217749	-0.877573

6	4.644398	3.432441	-0.741152
6	2.566499	4.563122	-0.178682
1	0.793438	3.349655	-0.154673
1	4.502791	1.329706	-1.162565
1	5.718442	3.457606	-0.913425
1	2.021786	5.467053	0.084927
1	4.496455	5.548638	-0.284547

Pro-H2O-Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-1.510142	0.533239	-0.621721
82	1.594357	0.295200	-0.833077
1	1.911486	-0.219817	-2.470875
6	1.895563	-1.470010	0.538187
6	-1.980162	-1.443915	0.328000
6	-0.739091	-1.912276	1.201590
1	-1.087472	-2.770881	1.799771
1	-0.505015	-1.136315	1.938891
6	0.592708	-2.381112	0.506153
1	0.866361	-3.332888	0.992875
1	0.373256	-2.651147	-0.532663
14	-2.401740	-2.704316	-1.094807
14	-3.478511	-1.178163	1.547150
8	-2.367679	0.646896	-2.412448
1	-2.027693	0.249468	-3.236159
14	3.313785	-2.537691	-0.273127
14	2.337047	-0.865337	2.329282
6	2.660048	-3.451541	-1.812194
1	3.497064	-3.964909	-2.306906
1	2.216520	-2.766227	-2.545132
1	1.911785	-4.213782	-1.560493
6	3.935813	-3.887320	0.925908
1	4.604589	-4.572118	0.385143
1	3.108175	-4.486950	1.327388
1	4.498923	-3.477815	1.773617

6	4.811354	-1.512853	-0.849362
1	5.612156	-2.198707	-1.161067
1	5.217226	-0.865763	-0.064875
1	4.563359	-0.892734	-1.720673
6	1.976095	-2.243170	3.598371
1	2.567560	-3.146741	3.409133
1	0.916239	-2.528257	3.604638
1	2.227100	-1.886039	4.607337
6	4.168580	-0.367926	2.488879
1	4.861109	-1.194849	2.291819
1	4.352034	-0.022865	3.516549
1	4.420534	0.462129	1.816416
6	1.370650	0.680381	2.904303
1	1.723691	0.950944	3.910392
1	0.288328	0.517630	2.977167
1	1.553262	1.547945	2.257613
6	-1.303110	-2.549891	-2.663546
1	-0.385036	-1.964801	-2.537720
1	-1.880230	-2.093777	-3.478972
1	-1.001274	-3.552668	-2.997266
6	-4.179172	-2.511041	-1.739672
1	-4.335552	-1.496699	-2.127637
1	-4.947451	-2.720567	-0.986648
1	-4.331464	-3.214633	-2.570939
6	-2.173605	-4.485972	-0.447200
1	-1.134037	-4.685917	-0.157552
1	-2.437775	-5.198174	-1.242182
1	-2.812138	-4.701512	0.417017
6	-4.221784	-2.845839	2.110869
1	-3.460729	-3.515465	2.533416
1	-4.732175	-3.381003	1.300963
1	-4.964504	-2.655069	2.898980
6	-4.872590	-0.115791	0.813827
1	-4.566328	0.930249	0.698949
1	-5.734698	-0.132610	1.496308
1	-5.214054	-0.474522	-0.162531
6	-2.880414	-0.324641	3.144141
1	-2.150564	-0.934322	3.692616
1	-3.742412	-0.168842	3.808623
1	-2.437468	0.660780	2.956595

6	-2.193499	2.427644	0.155843
6	-3.221540	4.934742	0.993690
6	-1.796789	2.991632	1.391408
6	-3.101542	3.141129	-0.663048
6	-3.613166	4.386091	-0.243744
6	-2.310456	4.236612	1.810227
1	-1.085533	2.480414	2.038849
1	-3.396470	2.721432	-1.621935
1	-4.311720	4.923952	-0.881582
1	-1.999770	4.655855	2.765211
1	-3.617670	5.895403	1.316104
6	2.587650	2.176415	-0.480792
6	3.948351	4.646865	-0.099091
6	1.882592	3.343768	-0.098904
6	3.987171	2.273071	-0.676206
6	4.662501	3.495963	-0.485401
6	2.555751	4.568352	0.091084
1	0.804182	3.320064	0.045267
1	4.565381	1.405085	-0.984597
1	5.738096	3.548054	-0.641794
1	1.992175	5.452672	0.380756
1	4.468778	5.591103	0.045950

TS–C_4H_6–C

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.765388	0.403761	-0.572768
6	-1.060726	0.283131	-2.248035
6	-0.499632	1.297905	-3.145837
6	0.855113	1.220442	-3.512116
6	1.659598	0.174272	-3.074238
6	0.791922	0.366518	-0.318450
6	1.525423	-0.883701	0.307896
14	3.055164	-1.834052	-0.619277
6	4.603422	-0.850686	-1.140515
1	4.387839	0.019655	-1.766916

1	5.191124	-0.506998	-0.281479
1	5.242842	-1.535266	-1.718472
6	3.702798	-3.225320	0.533102
1	2.929658	-3.975018	0.744846
1	4.506396	-3.742085	-0.012400
1	4.121650	-2.892302	1.486277
6	2.548576	-2.894850	-2.133059
1	3.436461	-3.492928	-2.392408
1	1.748712	-3.607430	-1.892843
1	2.264076	-2.340252	-3.029906
14	2.164564	-0.565893	2.232367
6	4.042282	-0.273808	2.501245
1	4.252260	-0.522930	3.552158
1	4.707228	-0.886915	1.886419
1	4.312766	0.778290	2.356315
6	1.768122	-2.097341	3.308054
1	2.305550	-2.996611	2.988264
1	2.091963	-1.869627	4.334148
1	0.699516	-2.334226	3.348060
6	1.380603	0.906855	3.146898
1	1.573652	1.858161	2.640073
1	0.304148	0.795521	3.312109
1	1.857789	0.959120	4.136493
6	0.517750	-2.070461	0.435227
1	0.284472	-2.483855	-0.553367
1	0.968499	-2.888700	1.004196
6	-0.782771	-1.622232	1.098423
1	-1.319818	-2.492064	1.491617
1	-0.544806	-0.996353	1.965494
6	-1.680810	-0.834834	0.098897
14	-2.443885	-2.250812	-1.136971
6	-1.527717	-2.805285	-2.734397
1	-1.752926	-2.168094	-3.597452
1	-0.438759	-2.881876	-2.639678
1	-1.899809	-3.815027	-2.964772
6	-2.539770	-3.927604	-0.218016
1	-3.046785	-3.911344	0.747821
1	-3.087662	-4.627206	-0.866282
1	-1.535168	-4.346748	-0.070097
6	-4.191085	-1.808562	-1.768439

1	-4.526681	-2.610146	-2.442122
1	-4.935252	-1.713787	-0.971098
1	-4.200272	-0.874756	-2.346584
14	-3.213799	-0.314866	1.307613
6	-2.653100	0.364087	3.004819
1	-2.116955	-0.398904	3.584626
1	-2.042542	1.266094	2.961537
1	-3.566072	0.614832	3.565501
6	-4.146723	-1.883033	1.900086
1	-4.871003	-1.532620	2.650414
1	-4.711841	-2.410336	1.125382
1	-3.492318	-2.604293	2.403600
6	-4.595325	0.813862	0.640838
1	-4.779630	0.691445	-0.431416
1	-5.524804	0.555958	1.169431
1	-4.383349	1.870450	0.825184
6	-1.427602	1.768950	-0.160773
6	-2.393722	2.431293	-0.958429
6	-2.930348	3.679657	-0.596981
6	-2.533760	4.310208	0.595489
6	-1.597175	3.658817	1.417556
6	-1.059773	2.417599	1.038182
1	-2.746353	1.996708	-1.884584
1	-3.661650	4.152159	-1.249512
1	-2.939600	5.280281	0.872139
1	-1.263009	4.124491	2.341831
1	-0.304048	1.967052	1.662034
6	1.568248	1.636218	-0.416799
6	1.071922	2.877035	-0.939184
6	1.856670	4.039995	-0.988286
6	3.176206	4.055032	-0.505209
6	3.704731	2.847516	-0.005456
6	2.927051	1.686436	0.021874
1	0.068457	2.956650	-1.316045
1	1.414154	4.950249	-1.388243
1	3.768454	4.966880	-0.511544
1	4.729766	2.807828	0.358712
1	3.404711	0.787270	0.366310
1	1.219284	-0.737107	-2.701500
1	2.740833	0.196337	-3.180626

1	1.309595	2.054157	-4.047060
1	-1.095928	2.151762	-3.457606
1	-2.149964	0.236539	-2.321528
1	-0.663528	-0.694575	-2.487310

	1
	A
Frequencies --	-141.1700
Red. masses --	4.3846
Frc consts --	0.0515
IR Inten --	4.4383

Atom	AN	X	Y	Z
1	6	-0.03	0.00	-0.11
2	6	-0.11	-0.01	0.03
3	6	-0.07	-0.03	-0.03
4	6	-0.06	-0.04	0.15
5	6	-0.15	-0.05	0.38
6	6	0.06	-0.01	-0.17
7	6	0.02	0.01	-0.05
8	14	0.02	-0.01	0.00
9	6	0.04	-0.02	0.02
10	1	0.08	0.00	0.04
11	1	0.04	-0.05	0.04
12	1	0.04	-0.03	0.02
13	6	0.00	-0.01	0.00
14	1	0.00	-0.01	0.00
15	1	0.01	-0.02	0.02
16	1	-0.01	-0.01	0.01
17	6	0.04	0.00	-0.02
18	1	0.01	-0.05	0.03
19	1	-0.02	0.05	-0.06
20	1	0.11	0.02	-0.03
21	14	-0.01	0.02	-0.03
22	6	-0.01	0.01	-0.01
23	1	-0.02	0.02	0.00
24	1	0.00	-0.01	0.01
25	1	0.00	0.00	-0.02
26	6	-0.01	0.02	-0.03
27	1	-0.01	0.01	-0.02

28	1	-0.01	0.02	-0.03
29	1	-0.01	0.01	-0.03
30	6	0.00	0.01	-0.01
31	1	-0.01	0.02	-0.01
32	1	0.00	0.01	0.00
33	1	0.01	0.00	-0.02
34	6	0.01	0.02	-0.03
35	1	0.00	0.01	-0.03
36	1	0.01	0.02	-0.03
37	6	0.02	0.03	-0.03
38	1	0.02	0.03	-0.01
39	1	0.02	0.04	-0.04
40	6	0.00	0.00	-0.03
41	14	-0.01	-0.02	0.00
42	6	-0.01	-0.03	0.00
43	1	-0.04	-0.05	-0.01
44	1	-0.01	-0.01	-0.01
45	1	0.01	-0.04	0.02
46	6	0.00	-0.01	0.01
47	1	0.01	0.00	0.02
48	1	0.00	-0.02	0.02
49	1	0.01	0.00	0.01
50	6	-0.01	-0.02	0.00
51	1	-0.01	-0.03	0.01
52	1	-0.01	-0.01	0.00
53	1	-0.01	-0.03	0.00
54	14	0.01	0.00	-0.02
55	6	0.01	0.00	-0.01
56	1	0.01	0.00	-0.02
57	1	0.00	0.01	-0.01
58	1	0.01	-0.01	-0.01
59	6	0.01	0.01	-0.01
60	1	0.01	0.01	-0.01
61	1	0.01	0.00	0.00
62	1	0.01	0.01	0.00
63	6	0.00	0.00	-0.01
64	1	0.00	0.00	-0.01
65	1	0.01	0.01	0.00
66	1	0.01	0.00	-0.02
67	6	0.01	0.00	-0.04

68	6	0.00	0.03	-0.02
69	6	0.01	0.02	0.01
70	6	0.02	-0.01	0.03
71	6	0.03	-0.03	0.00
72	6	0.02	-0.03	-0.03
73	1	0.00	0.06	-0.03
74	1	0.01	0.04	0.03
75	1	0.03	-0.01	0.05
76	1	0.04	-0.05	0.01
77	1	0.02	-0.04	-0.04
78	6	0.03	0.03	-0.03
79	6	0.03	0.04	0.00
80	6	0.02	0.04	0.04
81	6	0.02	0.03	0.04
82	6	0.02	0.02	0.02
83	6	0.02	0.02	-0.01
84	1	0.04	0.04	-0.02
85	1	0.02	0.05	0.05
86	1	0.02	0.03	0.06
87	1	0.01	0.02	0.03
88	1	0.01	0.01	-0.02
89	1	-0.23	-0.15	0.03
90	1	-0.12	-0.04	0.62
91	1	0.05	-0.07	0.19
92	1	-0.06	-0.06	-0.13
93	1	-0.11	0.02	-0.01
94	1	-0.17	-0.02	-0.04

TS-C_4H_6-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.122511	0.477540	0.401225
6	1.337027	1.276500	3.216200
6	0.666899	2.481486	3.215196
6	-0.773558	2.605485	3.158737
6	-1.652573	1.549701	3.135535

14	-1.091097	0.531126	0.164085
6	-1.860522	-1.214557	-0.155220
14	-3.214351	-1.805561	1.130877
6	-4.627441	-0.569949	1.435729
1	-4.259067	0.408111	1.765079
1	-5.257464	-0.415548	0.552144
1	-5.272342	-0.968651	2.232146
6	-3.993482	-3.465123	0.586284
1	-3.232170	-4.244532	0.449707
1	-4.671160	-3.810667	1.380637
1	-4.578523	-3.399839	-0.337895
6	-2.433628	-2.207247	2.823637
1	-3.240182	-2.376536	3.552303
1	-1.833521	-3.125353	2.782421
1	-1.799953	-1.405375	3.216482
14	-2.532178	-1.367343	-2.010621
6	-4.409292	-1.075308	-2.219880
1	-4.686906	-1.433927	-3.222157
1	-5.030939	-1.615163	-1.498422
1	-4.672828	-0.012707	-2.176208
6	-2.205462	-3.130767	-2.661277
1	-2.725771	-3.895017	-2.071006
1	-2.578181	-3.198721	-3.693509
1	-1.138359	-3.382202	-2.679752
6	-1.720217	-0.145738	-3.225223
1	-1.887775	0.896533	-2.928101
1	-0.640316	-0.294658	-3.329812
1	-2.173643	-0.284502	-4.218089
6	-0.670144	-2.257369	0.042375
1	-0.390921	-2.280224	1.101330
1	-1.062573	-3.258343	-0.183297
6	0.629632	-2.061598	-0.802566
1	0.992748	-3.063205	-1.072733
1	0.358129	-1.570803	-1.743684
6	1.835460	-1.264938	-0.141231
14	2.575714	-2.339800	1.325086
6	1.710004	-2.167914	3.018687
1	2.151286	-1.360972	3.614077
1	0.631259	-1.991440	2.955044
1	1.859389	-3.104402	3.575721

6	2.447316	-4.199276	0.909629
1	2.893017	-4.467503	-0.053466
1	2.971005	-4.771203	1.689502
1	1.401892	-4.535964	0.906157
6	4.403684	-1.940835	1.689901
1	4.709180	-2.499784	2.586222
1	5.081657	-2.224973	0.876606
1	4.557911	-0.874240	1.901442
14	3.148978	-1.094391	-1.598773
6	2.329208	-0.412893	-3.178075
1	1.661748	-1.144582	-3.650630
1	1.762293	0.506050	-2.994540
1	3.119290	-0.173657	-3.904767
6	3.812818	-2.819906	-2.085378
1	4.389999	-2.715519	-3.015669
1	4.483911	-3.248010	-1.330568
1	3.009320	-3.542106	-2.278029
6	4.671684	-0.005578	-1.257737
1	5.069421	-0.108164	-0.243991
1	5.467802	-0.300456	-1.957395
1	4.453359	1.053337	-1.426812
6	2.114214	2.032781	-0.102231
6	3.222489	2.507606	0.644405
6	3.956946	3.638483	0.241927
6	3.596647	4.337673	-0.926518
6	2.497233	3.891239	-1.683795
6	1.770091	2.755705	-1.275712
1	3.525872	1.988235	1.549139
1	4.805323	3.970477	0.836908
1	4.161269	5.213246	-1.239878
1	2.203785	4.419987	-2.588332
1	0.922452	2.433636	-1.876203
6	-2.054478	2.115359	-0.185245
6	-1.417010	3.383992	-0.102008
6	-2.114374	4.573841	-0.371007
6	-3.475760	4.538490	-0.734262
6	-4.128178	3.294415	-0.816409
6	-3.427498	2.105324	-0.542689
1	-0.370233	3.448716	0.177242
1	-1.593440	5.526469	-0.299540

1	-4.014687	5.459360	-0.945180
1	-5.181015	3.246901	-1.087336
1	-3.964563	1.165910	-0.595773
1	-1.333033	0.535947	3.350034
1	-2.723162	1.712847	3.041289
1	-1.176129	3.612841	3.046096
1	1.245895	3.403417	3.152474
1	2.422220	1.236303	3.281465
1	0.816951	0.344122	3.394136

	1
	A
Frequencies --	-156.9680
Red. masses --	7.5975
Frc consts --	0.1103
IR Inten --	2.1634

Atom	AN	X	Y	Z
1	14	-0.03	-0.05	-0.17
2	6	0.03	0.20	0.41
3	6	-0.01	0.12	0.20
4	6	-0.06	0.11	0.14
5	6	-0.06	0.16	0.27
6	14	0.05	-0.04	-0.18
7	6	0.00	-0.02	-0.03
8	14	0.01	0.01	-0.01
9	6	0.01	0.01	0.00
10	1	0.02	0.00	0.01
11	1	0.01	0.02	0.00
12	1	0.02	0.00	0.00
13	6	0.00	0.00	0.01
14	1	0.00	0.00	0.01
15	1	0.01	0.01	0.01
16	1	0.00	0.00	0.01
17	6	0.02	0.03	-0.01
18	1	0.02	0.05	0.00
19	1	0.02	0.03	0.00
20	1	0.03	0.04	-0.03
21	14	-0.01	-0.03	-0.02
22	6	-0.01	-0.01	-0.01

23	1	-0.02	0.00	-0.01
24	1	-0.01	-0.01	0.00
25	1	0.00	-0.01	0.00
26	6	-0.01	-0.02	-0.02
27	1	-0.01	-0.02	-0.02
28	1	-0.01	-0.03	-0.02
29	1	-0.01	-0.02	-0.02
30	6	-0.02	-0.02	-0.02
31	1	-0.02	-0.02	-0.02
32	1	-0.02	-0.02	-0.02
33	1	-0.02	-0.02	-0.02
34	6	0.00	-0.03	-0.02
35	1	0.00	0.00	-0.02
36	1	-0.01	-0.03	0.00
37	6	0.01	-0.06	-0.03
38	1	0.00	-0.07	0.01
39	1	0.01	-0.09	-0.04
40	6	0.01	-0.04	-0.05
41	14	0.00	0.00	-0.01
42	6	-0.01	0.04	-0.02
43	1	-0.01	0.06	-0.04
44	1	-0.01	0.04	-0.03
45	1	-0.01	0.05	0.00
46	6	0.01	-0.01	0.01
47	1	0.01	-0.01	0.01
48	1	0.01	0.00	0.02
49	1	0.01	-0.01	0.01
50	6	0.00	0.01	-0.01
51	1	-0.01	0.01	0.00
52	1	0.00	0.00	0.00
53	1	-0.01	0.01	-0.01
54	14	0.01	-0.03	-0.03
55	6	0.01	-0.01	-0.02
56	1	0.00	0.00	-0.02
57	1	0.02	-0.01	-0.01
58	1	0.01	-0.01	-0.03
59	6	0.02	-0.02	-0.03
60	1	0.02	-0.03	-0.02
61	1	0.01	-0.02	-0.02
62	1	0.02	-0.02	-0.02

63	6	0.00	-0.01	-0.01
64	1	-0.01	-0.01	-0.01
65	1	0.01	-0.01	0.00
66	1	-0.01	-0.02	-0.01
67	6	-0.01	-0.02	-0.03
68	6	-0.02	-0.04	0.00
69	6	-0.01	-0.03	0.03
70	6	0.00	-0.01	0.04
71	6	0.01	0.02	0.02
72	6	0.00	0.01	-0.01
73	1	-0.03	-0.06	-0.01
74	1	-0.02	-0.04	0.04
75	1	0.01	0.00	0.06
76	1	0.02	0.03	0.02
77	1	0.01	0.02	-0.03
78	6	0.01	-0.02	0.01
79	6	0.00	-0.02	0.03
80	6	0.01	-0.02	0.03
81	6	0.01	-0.01	0.02
82	6	0.01	-0.01	0.02
83	6	0.00	-0.01	0.02
84	1	0.01	-0.02	0.03
85	1	0.01	-0.02	0.03
86	1	0.01	-0.01	0.02
87	1	0.01	-0.01	0.02
88	1	0.01	-0.01	0.01
89	1	-0.06	0.13	0.16
90	1	-0.06	0.16	0.22
91	1	-0.03	0.11	0.05
92	1	-0.05	0.14	0.17
93	1	0.03	0.24	0.35
94	1	0.05	0.14	0.18

TS-C_4H_6-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z

32	1.218160	0.459979	0.529344
6	1.331891	1.451126	3.312418
6	0.634148	2.631252	3.167660
6	-0.801582	2.716196	3.008928
6	-1.663999	1.646987	2.980524
32	-1.103998	0.522870	-0.016282
6	-1.882331	-1.334192	-0.132232
14	-3.172244	-1.861565	1.238775
6	-4.605343	-0.640589	1.501299
1	-4.252999	0.359678	1.777475
1	-5.246707	-0.543647	0.617738
1	-5.234263	-1.010275	2.323898
6	-3.926162	-3.573195	0.837129
1	-3.148354	-4.339131	0.717949
1	-4.560044	-3.883843	1.680411
1	-4.550091	-3.583512	-0.063440
6	-2.317803	-2.133767	2.922220
1	-3.087660	-2.213649	3.703397
1	-1.747481	-3.071721	2.928688
1	-1.638703	-1.325466	3.211615
14	-2.603435	-1.622441	-1.945218
6	-4.488198	-1.360130	-2.098069
1	-4.786205	-1.688287	-3.104598
1	-5.079431	-1.936368	-1.379122
1	-4.770187	-0.304960	-2.009606
6	-2.257714	-3.415858	-2.490578
1	-2.735203	-4.149053	-1.829077
1	-2.664595	-3.565342	-3.501011
1	-1.185009	-3.640848	-2.530733
6	-1.858160	-0.461504	-3.260908
1	-2.060653	0.594733	-3.040953
1	-0.775306	-0.577951	-3.378298
1	-2.323975	-0.688143	-4.231773
6	-0.637147	-2.299081	0.110676
1	-0.327454	-2.212118	1.157659
1	-0.989383	-3.333418	-0.011057
6	0.631799	-2.120893	-0.791481
1	0.961772	-3.127976	-1.087488
1	0.329732	-1.616451	-1.716291
6	1.884786	-1.360437	-0.184535

14	2.658252	-2.421066	1.267230
6	1.867010	-2.155951	2.983116
1	2.228419	-1.232036	3.449325
1	0.771971	-2.118036	2.965910
1	2.161226	-2.992536	3.635137
6	2.472252	-4.283979	0.894969
1	2.890824	-4.571353	-0.075874
1	2.999447	-4.860150	1.669059
1	1.419361	-4.595902	0.916099
6	4.507227	-2.051727	1.546963
1	4.843973	-2.601645	2.437593
1	5.142808	-2.359063	0.708239
1	4.686441	-0.984468	1.734145
14	3.127354	-1.182171	-1.688195
6	2.226946	-0.502894	-3.224861
1	1.611101	-1.269546	-3.713015
1	1.586868	0.354929	-2.988979
1	2.974621	-0.166594	-3.957833
6	3.774306	-2.909001	-2.199464
1	4.319453	-2.813109	-3.149682
1	4.468256	-3.335986	-1.464653
1	2.961141	-3.629089	-2.358609
6	4.657602	-0.089045	-1.404700
1	5.139137	-0.254085	-0.436008
1	5.396630	-0.323300	-2.185344
1	4.414674	0.974962	-1.483254
6	2.209536	2.060235	-0.140951
6	3.307885	2.572324	0.595627
6	4.028979	3.700116	0.159139
6	3.659514	4.358742	-1.029852
6	2.565536	3.876542	-1.773088
6	1.852985	2.742705	-1.333390
1	3.612658	2.086699	1.519900
1	4.872021	4.062145	0.744174
1	4.212938	5.231574	-1.369652
1	2.266339	4.375349	-2.692797
1	1.015376	2.390361	-1.930938
6	-2.203315	2.124069	-0.329760
6	-1.574363	3.398222	-0.334256
6	-2.303405	4.569030	-0.605514

6	-3.682740	4.499866	-0.888488
6	-4.322022	3.246012	-0.892246
6	-3.590714	2.075186	-0.614201
1	-0.512148	3.482252	-0.120668
1	-1.794922	5.530873	-0.599203
1	-4.246568	5.405383	-1.100856
1	-5.386866	3.176867	-1.104917
1	-4.114490	1.125956	-0.607351
1	-1.342105	0.645717	3.243791
1	-2.729983	1.793221	2.830606
1	-1.213692	3.709249	2.826190
1	1.196292	3.558685	3.059166
1	2.413902	1.451613	3.424103
1	0.830487	0.520851	3.553951

	1
	A
Frequencies --	-125.2886
Red. masses --	7.6388
Frc consts --	0.0706
IR Inten --	4.7737

Atom	AN	X	Y	Z
1	32	-0.02	-0.03	-0.05
2	6	0.01	0.22	0.39
3	6	-0.01	0.14	0.22
4	6	-0.05	0.12	0.18
5	6	-0.05	0.16	0.27
6	32	0.04	-0.03	-0.13
7	6	0.00	-0.01	-0.02
8	14	0.01	0.01	0.00
9	6	0.01	0.01	0.00
10	1	0.02	0.01	0.01
11	1	0.01	0.02	0.01
12	1	0.01	0.01	0.00
13	6	0.00	0.01	0.01
14	1	0.00	0.01	0.01
15	1	0.01	0.01	0.02
16	1	0.00	0.00	0.02
17	6	0.02	0.04	0.00

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

58	1	0.00	0.00	-0.02
59	6	0.01	-0.02	-0.02
60	1	0.01	-0.02	-0.02
61	1	0.01	-0.01	-0.02
62	1	0.01	-0.02	-0.02
63	6	-0.01	-0.01	-0.01
64	1	-0.01	-0.01	-0.01
65	1	0.00	0.00	-0.01
66	1	-0.01	-0.01	-0.01
67	6	-0.01	-0.02	-0.01
68	6	-0.02	-0.02	0.01
69	6	-0.01	-0.02	0.02
70	6	0.00	-0.01	0.03
71	6	0.01	0.00	0.01
72	6	0.00	0.00	-0.01
73	1	-0.03	-0.03	0.01
74	1	-0.02	-0.03	0.04
75	1	0.01	0.00	0.04
76	1	0.01	0.01	0.02
77	1	0.01	0.00	-0.02
78	6	0.00	-0.02	0.04
79	6	0.00	-0.02	0.04
80	6	0.01	-0.02	0.03
81	6	0.01	-0.01	0.02
82	6	0.00	-0.01	0.02
83	6	0.00	-0.01	0.03
84	1	0.00	-0.02	0.04
85	1	0.01	-0.02	0.03
86	1	0.02	-0.01	0.01
87	1	0.01	-0.01	0.01
88	1	0.00	-0.01	0.03
89	1	-0.04	0.14	0.17
90	1	-0.05	0.16	0.22
91	1	-0.03	0.12	0.12
92	1	-0.04	0.16	0.17
93	1	0.01	0.25	0.35
94	1	0.04	0.16	0.23

TS–C_4H_6–Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	1.433518	0.530488	0.692368
6	1.261236	2.026065	3.528410
6	0.419489	3.039043	3.141561
6	-1.005994	2.902073	2.884690
6	-1.736260	1.742546	2.948280
50	-1.212230	0.513550	-0.143902
6	-1.868442	-1.586855	-0.093529
14	-3.071710	-2.087457	1.350274
6	-4.577582	-0.942580	1.549574
1	-4.285072	0.091560	1.769514
1	-5.223217	-0.931713	0.664187
1	-5.184610	-1.299219	2.393961
6	-3.713369	-3.875178	1.134072
1	-2.885934	-4.590907	1.038089
1	-4.288266	-4.159906	2.027115
1	-4.370353	-4.001131	0.265814
6	-2.140322	-2.110467	3.015202
1	-2.865742	-2.105064	3.841116
1	-1.534845	-3.020483	3.117051
1	-1.474797	-1.250470	3.151717
14	-2.593573	-2.055690	-1.849480
6	-4.489031	-1.873338	-1.960032
1	-4.803884	-2.186613	-2.965823
1	-5.034544	-2.491188	-1.238580
1	-4.810209	-0.832183	-1.833027
6	-2.156372	-3.859567	-2.278005
1	-2.565627	-4.567795	-1.547295
1	-2.577602	-4.113609	-3.261190
1	-1.071854	-4.016717	-2.333274
6	-1.941950	-0.955316	-3.269482
1	-2.245550	0.095174	-3.157234
1	-0.852258	-0.982264	-3.382253
1	-2.378252	-1.311824	-4.214748
6	-0.514535	-2.385575	0.195761
1	-0.189769	-2.160170	1.217660

1	-0.759568	-3.459077	0.198126
6	0.711776	-2.184471	-0.773300
1	1.006597	-3.186347	-1.127154
1	0.364947	-1.645812	-1.663236
6	2.018812	-1.463896	-0.229754
14	2.838556	-2.508883	1.197325
6	2.078920	-2.250340	2.933506
1	2.277475	-1.239296	3.313131
1	0.994851	-2.413313	2.971014
1	2.545522	-2.965724	3.628111
6	2.693012	-4.378523	0.841843
1	3.123254	-4.658724	-0.126123
1	3.226613	-4.941147	1.621670
1	1.645843	-4.710405	0.856881
6	4.680177	-2.075149	1.436576
1	5.063195	-2.615768	2.314327
1	5.303752	-2.350584	0.577879
1	4.822159	-1.001901	1.626899
14	3.190700	-1.263218	-1.769479
6	2.215681	-0.602554	-3.270268
1	1.583661	-1.376401	-3.725500
1	1.580894	0.252777	-3.008845
1	2.924440	-0.263172	-4.038894
6	3.884273	-2.962895	-2.314630
1	4.389236	-2.852348	-3.285137
1	4.619878	-3.360532	-1.603631
1	3.091415	-3.712811	-2.437919
6	4.682348	-0.106489	-1.525342
1	5.214132	-0.272459	-0.582378
1	5.397687	-0.281110	-2.342787
1	4.384626	0.946904	-1.563690
6	2.345952	2.269520	-0.267092
6	3.409573	2.924285	0.408384
6	4.009842	4.090511	-0.106736
6	3.548535	4.646989	-1.315390
6	2.486956	4.025374	-2.000098
6	1.897255	2.853907	-1.481982
1	3.782225	2.524384	1.351131
1	4.829095	4.561392	0.433120
1	4.007075	5.548741	-1.715507

1	2.119005	4.445380	-2.934384
1	1.084050	2.393947	-2.039104
6	-2.631904	2.092615	-0.487056
6	-2.095482	3.405502	-0.585146
6	-2.917404	4.512196	-0.867955
6	-4.300438	4.331837	-1.069796
6	-4.850865	3.038748	-0.983112
6	-4.025253	1.933485	-0.693805
1	-1.029052	3.573174	-0.439281
1	-2.479301	5.506016	-0.934129
1	-4.937411	5.185219	-1.291834
1	-5.917691	2.889075	-1.136717
1	-4.483200	0.951257	-0.622198
1	-1.313981	0.817503	3.328794
1	-2.804889	1.747999	2.749548
1	-1.522153	3.807539	2.561973
1	0.855393	4.014989	2.927599
1	2.324587	2.205481	3.669111
1	0.896190	1.052237	3.839990

	1
	A
Frequencies --	-77.9225
Red. masses --	6.7301
Frc consts --	0.0241
IR Inten --	3.5964

Atom	AN	X	Y	Z
1	50	-0.02	-0.02	0.00
2	6	0.01	0.24	0.30
3	6	0.00	0.17	0.19
4	6	-0.01	0.14	0.17
5	6	-0.02	0.17	0.27
6	50	0.02	-0.03	-0.10
7	6	0.00	-0.01	-0.03
8	14	0.01	0.02	-0.01
9	6	0.01	0.02	-0.01
10	1	0.01	0.01	0.00
11	1	0.01	0.02	-0.01
12	1	0.01	0.01	-0.01

13	6	0.01	0.01	0.03
14	1	0.01	0.01	0.03
15	1	0.03	0.02	0.04
16	1	0.00	0.00	0.04
17	6	0.03	0.08	-0.02
18	1	0.05	0.13	-0.01
19	1	0.02	0.08	0.01
20	1	0.04	0.08	-0.08
21	14	-0.01	-0.03	-0.02
22	6	-0.01	-0.02	0.00
23	1	-0.02	-0.02	0.00
24	1	-0.01	-0.02	0.00
25	1	-0.01	-0.02	0.00
26	6	-0.01	-0.03	-0.01
27	1	-0.01	-0.02	-0.01
28	1	-0.02	-0.03	-0.01
29	1	-0.01	-0.02	-0.02
30	6	-0.02	-0.03	-0.02
31	1	-0.03	-0.03	-0.03
32	1	-0.02	-0.01	-0.02
33	1	-0.01	-0.04	-0.02
34	6	0.00	-0.02	-0.02
35	1	-0.01	-0.02	-0.02
36	1	-0.01	-0.02	-0.02
37	6	0.00	-0.03	-0.02
38	1	0.01	-0.03	0.01
39	1	0.01	-0.05	-0.03
40	6	0.00	-0.01	-0.02
41	14	0.00	-0.01	-0.01
42	6	-0.01	-0.01	-0.01
43	1	-0.03	0.00	-0.02
44	1	0.00	-0.03	-0.02
45	1	0.01	0.00	-0.01
46	6	0.01	-0.01	-0.01
47	1	0.01	-0.01	-0.01
48	1	0.02	0.00	-0.01
49	1	0.01	-0.01	0.00
50	6	0.00	0.00	-0.01
51	1	0.00	0.00	-0.01
52	1	0.00	0.01	0.00

53	1	-0.01	0.00	-0.01
54	14	0.00	-0.01	-0.01
55	6	0.00	0.00	-0.01
56	1	0.00	0.00	-0.02
57	1	0.00	0.00	-0.01
58	1	0.00	0.00	-0.01
59	6	0.00	0.00	-0.02
60	1	0.00	0.00	-0.02
61	1	0.00	0.00	-0.01
62	1	0.00	-0.01	-0.02
63	6	0.00	-0.01	-0.01
64	1	-0.01	0.00	-0.01
65	1	0.00	-0.01	-0.01
66	1	-0.01	-0.01	-0.01
67	6	0.00	-0.02	-0.01
68	6	-0.01	-0.02	0.01
69	6	-0.01	-0.02	0.02
70	6	0.00	-0.01	0.02
71	6	0.00	0.00	0.01
72	6	0.00	-0.01	0.00
73	1	-0.02	-0.03	0.01
74	1	-0.01	-0.02	0.03
75	1	0.00	0.00	0.03
76	1	0.01	0.00	0.01
77	1	0.01	-0.01	-0.02
78	6	-0.01	-0.02	0.03
79	6	0.00	-0.02	0.04
80	6	0.00	-0.02	0.05
81	6	0.00	-0.01	0.04
82	6	0.00	-0.01	0.03
83	6	-0.01	-0.01	0.02
84	1	0.00	-0.02	0.04
85	1	0.01	-0.02	0.05
86	1	0.01	-0.01	0.04
87	1	0.00	0.00	0.02
88	1	-0.01	-0.01	0.01
89	1	-0.01	0.17	0.28
90	1	-0.01	0.14	0.21
91	1	0.00	0.12	0.10
92	1	-0.02	0.17	0.16

93	1	0.00	0.28	0.30
94	1	0.04	0.21	0.23

TS–C_4H_6–Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-1.665329	0.442645	-0.781712
6	-1.168527	1.630765	-3.420032
6	-0.272820	2.632614	-3.084540
6	1.124706	2.420280	-2.812417
6	1.793088	1.199316	-2.781278
82	1.242795	0.499876	-0.112414
6	1.936528	-1.686358	0.177184
14	3.146924	-2.338810	-1.188084
6	4.646184	-1.203633	-1.486861
1	4.349658	-0.187193	-1.772302
1	5.292992	-1.128387	-0.605280
1	5.253271	-1.611714	-2.307504
6	3.810294	-4.086485	-0.782313
1	2.989401	-4.796130	-0.611874
1	4.393441	-4.459440	-1.636895
1	4.463198	-4.110384	0.097988
6	2.235960	-2.568991	-2.850584
1	2.973352	-2.733692	-3.649396
1	1.582268	-3.450648	-2.821199
1	1.622783	-1.709797	-3.144052
14	2.652508	-1.926205	1.974359
6	4.550137	-1.753259	2.082962
1	4.851698	-2.006953	3.109886
1	5.094269	-2.423428	1.408471
1	4.884623	-0.726161	1.893194
6	2.222486	-3.672659	2.612708
1	2.644858	-4.456480	1.971507
1	2.639819	-3.806648	3.621100
1	1.139620	-3.835639	2.678309
6	2.003746	-0.670057	3.260088

1	2.261085	0.365038	2.997256
1	0.921600	-0.724994	3.423168
1	2.487983	-0.882183	4.225039
6	0.561689	-2.469620	-0.019886
1	0.203704	-2.293663	-1.039974
1	0.782916	-3.549150	0.022809
6	-0.621741	-2.193381	0.985008
1	-0.855206	-3.158479	1.471927
1	-0.251817	-1.547123	1.789003
6	-1.981288	-1.594066	0.447005
14	-2.811409	-2.704527	-0.910663
6	-2.068616	-2.543110	-2.671907
1	-2.353049	-1.592743	-3.142554
1	-0.975929	-2.622624	-2.708432
1	-2.477665	-3.351534	-3.296183
6	-2.694498	-4.556772	-0.472610
1	-3.122403	-4.783990	0.510134
1	-3.240742	-5.146561	-1.223084
1	-1.651875	-4.902866	-0.478338
6	-4.641501	-2.227042	-1.161695
1	-5.051813	-2.792272	-2.010788
1	-5.269257	-2.433929	-0.287264
1	-4.744174	-1.159316	-1.403986
14	-3.111985	-1.281677	1.990741
6	-2.092150	-0.558413	3.431559
1	-1.442372	-1.310085	3.898640
1	-1.470368	0.288354	3.115776
1	-2.776958	-0.187642	4.207538
6	-3.838886	-2.929393	2.640776
1	-4.329590	-2.757321	3.609571
1	-4.590440	-3.347532	1.958669
1	-3.059602	-3.688154	2.792787
6	-4.576498	-0.096155	1.710689
1	-5.127697	-0.289532	0.783886
1	-5.285233	-0.211700	2.544087
1	-4.249903	0.949600	1.698673
6	-2.289276	2.309315	0.351961
6	-3.348224	3.016226	-0.275585
6	-3.861807	4.214831	0.260186
6	-3.312049	4.746525	1.442707

6	-2.249261	4.072263	2.076431
6	-1.745795	2.870181	1.535504
1	-3.791260	2.630152	-1.195613
1	-4.682713	4.724748	-0.240976
1	-3.704773	5.670380	1.862110
1	-1.814170	4.478067	2.988065
1	-0.925518	2.375403	2.052476
6	2.694146	2.095601	0.453235
6	2.145408	3.400152	0.559709
6	2.958672	4.512541	0.853490
6	4.342411	4.339810	1.054047
6	4.903259	3.050742	0.960365
6	4.085690	1.941007	0.660222
1	1.078267	3.561750	0.408121
1	2.513906	5.503558	0.922479
1	4.973693	5.196980	1.278049
1	5.971212	2.908737	1.114494
1	4.549358	0.961364	0.577721
1	1.336623	0.302996	-3.193368
1	2.875193	1.186760	-2.680175
1	1.697876	3.307745	-2.540544
1	-0.659826	3.637715	-2.924636
1	-2.213909	1.856610	-3.615341
1	-0.835965	0.643795	-3.730568

	1
	A
Frequencies --	-99.6864
Red. masses --	7.6745
Frc consts --	0.0449
IR Inten --	44.0057

Atom	AN	X	Y	Z
1	82	0.04	0.02	0.02
2	6	-0.08	-0.27	0.37
3	6	-0.07	-0.17	0.20
4	6	-0.10	-0.11	0.16
5	6	-0.07	-0.14	0.29
6	82	0.01	0.01	-0.06
7	6	-0.01	0.00	-0.01

8	14	0.00	-0.01	0.00
9	6	0.00	-0.01	0.00
10	1	0.00	-0.01	0.00
11	1	0.00	-0.01	0.00
12	1	0.00	-0.01	0.00
13	6	0.00	0.00	0.01
14	1	0.00	0.00	0.01
15	1	0.00	-0.01	0.02
16	1	-0.01	0.00	0.02
17	6	0.01	-0.04	-0.01
18	1	0.02	-0.06	0.01
19	1	0.01	-0.04	0.01
20	1	0.02	-0.05	-0.03
21	14	-0.01	0.00	-0.01
22	6	-0.01	0.00	0.00
23	1	-0.02	0.00	0.00
24	1	-0.01	0.00	0.00
25	1	-0.01	0.00	0.00
26	6	-0.01	0.00	-0.01
27	1	-0.01	0.00	-0.01
28	1	-0.02	0.00	-0.01
29	1	-0.01	0.00	-0.01
30	6	-0.01	0.00	0.00
31	1	-0.03	0.00	-0.01
32	1	-0.01	-0.02	0.01
33	1	0.00	0.00	-0.01
34	6	-0.01	0.01	-0.02
35	1	0.00	0.02	-0.03
36	1	-0.03	0.01	-0.02
37	6	-0.01	0.04	-0.03
38	1	-0.01	0.05	0.00
39	1	-0.01	0.07	-0.05
40	6	-0.02	0.00	-0.04
41	14	-0.01	0.00	-0.03
42	6	-0.01	0.02	-0.02
43	1	0.01	0.04	-0.01
44	1	-0.01	0.00	-0.02
45	1	-0.02	0.04	-0.04
46	6	0.01	0.01	-0.02
47	1	0.00	0.01	-0.02

48	1	0.02	0.00	−0.02
49	1	0.01	0.02	−0.01
50	6	−0.02	0.00	−0.02
51	1	−0.02	0.00	−0.01
52	1	−0.01	−0.01	−0.01
53	1	−0.02	0.00	−0.01
54	14	−0.01	0.01	−0.02
55	6	−0.01	0.00	−0.02
56	1	0.00	0.00	−0.03
57	1	−0.01	0.01	−0.01
58	1	−0.01	−0.01	−0.02
59	6	0.00	0.00	−0.03
60	1	0.00	0.00	−0.03
61	1	0.00	0.00	−0.03
62	1	0.00	0.01	−0.04
63	6	−0.01	0.01	−0.02
64	1	−0.01	0.02	−0.02
65	1	−0.02	0.00	−0.02
66	1	−0.02	0.01	0.00
67	6	−0.03	0.01	−0.06
68	6	−0.04	0.01	−0.03
69	6	−0.03	0.01	−0.01
70	6	−0.01	−0.01	−0.01
71	6	−0.01	−0.02	−0.03
72	6	−0.01	−0.01	−0.06
73	1	−0.05	0.02	−0.03
74	1	−0.03	0.02	0.01
75	1	−0.01	−0.02	0.01
76	1	0.01	−0.03	−0.03
77	1	0.01	−0.01	−0.09
78	6	−0.04	0.02	0.03
79	6	−0.02	0.03	0.03
80	6	0.00	0.02	0.02
81	6	0.00	0.00	0.01
82	6	−0.02	−0.01	0.01
83	6	−0.04	0.00	0.02
84	1	−0.02	0.04	0.03
85	1	0.01	0.02	0.01
86	1	0.01	0.00	0.00
87	1	−0.02	−0.02	0.00

88	1	-0.05	0.00	0.02
89	1	-0.03	-0.12	0.20
90	1	-0.05	-0.08	0.12
91	1	-0.09	-0.08	0.07
92	1	-0.10	-0.17	0.12
93	1	-0.07	-0.28	0.29
94	1	-0.03	-0.22	0.26

Pro–C_4H_6–C

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.920461	0.432094	-0.705908
6	0.800533	0.119681	-0.783950
6	-1.826242	-0.622371	0.194613
6	-0.963816	-1.114491	1.391000
1	-0.679206	-0.268072	2.029342
1	-1.545983	-1.789842	2.031510
6	0.297385	-1.843789	0.909685
1	0.689176	-2.461777	1.723054
1	-0.001510	-2.548486	0.124048
6	1.431717	-0.902651	0.373572
6	1.693929	1.414325	-0.923123
6	3.541360	3.575074	-1.434454
6	3.081794	1.304913	-0.677498
6	1.277939	2.647404	-1.488579
6	2.172453	3.704571	-1.726892
6	3.990502	2.351369	-0.913339
1	3.486261	0.378004	-0.309880
1	0.248769	2.808822	-1.758003
1	1.788250	4.631492	-2.147282
1	5.045918	2.199810	-0.695777
1	4.232812	4.394318	-1.616884
6	-1.177546	1.869327	-0.162604
6	-1.506305	4.528179	0.866863
6	-2.012135	2.818030	-0.804831
6	-0.533834	2.301577	1.012019

6	−0.678033	3.600263	1.522014
6	−2.177362	4.121063	−0.300265
1	−2.531759	2.573735	−1.723400
1	0.123188	1.616104	1.516306
1	−0.139057	3.886067	2.422036
1	−2.822270	4.818691	−0.830623
1	−1.621002	5.539584	1.249126
6	−1.521119	0.319956	−2.164334
1	−1.661769	−0.740392	−2.366417
1	−2.524963	0.749104	−2.173820
6	−0.673198	0.821542	−3.307769
1	−1.075481	1.504320	−4.053183
6	0.581904	0.335351	−3.356360
1	1.291081	0.607896	−4.134018
6	1.023702	−0.554408	−2.212354
1	0.475279	−1.500364	−2.245968
1	2.085163	−0.782091	−2.328744
14	2.754292	−2.314333	−0.268309
14	2.325815	−0.137067	2.059278
14	−2.530664	−2.287166	−0.733125
14	−3.473734	0.161474	1.045659
6	2.064959	−3.625908	−1.479102
1	1.186340	−4.148858	−1.084501
1	2.856327	−4.381913	−1.591971
1	1.828682	−3.247796	−2.477870
6	3.222466	−3.450504	1.203348
1	3.620795	−2.949880	2.088513
1	3.994943	−4.147440	0.846311
1	2.363708	−4.058611	1.516372
6	4.387589	−1.766167	−1.100886
1	5.054896	−1.190583	−0.452157
1	4.227114	−1.184197	−2.015994
1	4.921540	−2.684452	−1.387215
6	4.246156	−0.250288	2.102224
1	4.530307	−0.206893	3.164217
1	4.702436	0.617657	1.611437
1	4.693134	−1.154898	1.687378
6	1.757103	−1.149835	3.583392
1	2.234234	−0.701397	4.467237
1	2.057083	−2.203052	3.548692

1	0.673129	-1.111353	3.744179
6	2.117022	1.673153	2.655984
1	2.956335	1.843348	3.346212
1	1.196688	1.840199	3.227893
1	2.186568	2.418984	1.859904
6	-4.240694	-2.039254	-1.554195
1	-5.026542	-1.662420	-0.894825
1	-4.568775	-3.017903	-1.934125
1	-4.175373	-1.363767	-2.417169
6	-2.665691	-3.716450	0.531436
1	-1.673505	-4.113701	0.782602
1	-3.233705	-4.532742	0.061773
1	-3.169632	-3.460268	1.465517
6	-1.584139	-3.151388	-2.164732
1	-0.549232	-3.409278	-1.935301
1	-1.596934	-2.599186	-3.111993
1	-2.120181	-4.097101	-2.338822
6	-4.689927	1.044647	-0.137151
1	-5.719884	0.793650	0.153570
1	-4.571379	0.763173	-1.188398
1	-4.575088	2.131151	-0.061949
6	-4.487115	-1.218936	1.911978
1	-3.916454	-1.706100	2.713352
1	-4.887898	-1.995030	1.255027
1	-5.342642	-0.717796	2.388129
6	-3.154862	1.327765	2.521326
1	-2.310282	1.004723	3.142501
1	-4.052762	1.311943	3.156562
1	-2.973016	2.361091	2.217674

Pro-C_4H_6-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-1.201752	0.572862	-0.725711
14	1.200061	0.332086	-0.748947
6	-1.978787	-1.003617	0.156996

6	-0.842995	-1.612737	1.088720
1	-0.554967	-0.863039	1.834176
1	-1.279243	-2.442713	1.664680
6	0.447782	-2.162538	0.395788
1	0.734840	-3.080780	0.926915
1	0.188081	-2.485103	-0.618218
6	1.732668	-1.217646	0.320594
6	2.207872	1.936688	-0.450317
6	3.771518	4.326401	-0.245184
6	3.597487	1.894081	-0.170245
6	1.629616	3.218657	-0.635523
6	2.396002	4.395803	-0.533560
6	4.371081	3.065690	-0.066915
1	4.096137	0.940156	-0.044289
1	0.574469	3.310058	-0.867139
1	1.915652	5.360985	-0.679028
1	5.435539	2.992023	0.146903
1	4.364752	5.234766	-0.165177
6	-1.756263	2.284416	-0.048655
6	-2.531256	4.874979	0.891814
6	-2.660060	3.099373	-0.777359
6	-1.240337	2.822221	1.156856
6	-1.621483	4.092406	1.627414
6	-3.045620	4.373643	-0.318817
1	-3.077492	2.745176	-1.716160
1	-0.510060	2.258903	1.729343
1	-1.201036	4.470767	2.556622
1	-3.743187	4.969198	-0.904034
1	-2.827076	5.858483	1.250203
6	-1.583473	0.653876	-2.623355
1	-1.528503	-0.362119	-3.022959
1	-2.608760	1.002351	-2.799725
6	-0.580914	1.535849	-3.343243
1	-0.953676	2.433419	-3.835816
6	0.750484	1.271541	-3.377229
1	1.413857	1.969655	-3.885607
6	1.391000	0.089184	-2.676632
1	0.901233	-0.846525	-2.975295
1	2.449944	0.007052	-2.948245
14	3.099483	-2.342553	-0.534169

14	2.279693	-0.804242	2.167783
14	-2.596103	-2.415815	-1.068768
14	-3.463321	-0.555968	1.376755
6	2.442679	-3.244860	-2.081866
1	1.553892	-3.852715	-1.872870
1	3.228204	-3.931453	-2.429844
1	2.209056	-2.569276	-2.910971
6	3.640953	-3.765205	0.621716
1	4.141509	-3.427729	1.535703
1	4.348990	-4.405223	0.075616
1	2.792552	-4.397570	0.914614
6	4.676183	-1.430129	-1.089999
1	5.250519	-1.017269	-0.252965
1	4.467808	-0.617240	-1.795800
1	5.325270	-2.152513	-1.605807
6	4.156082	-0.565126	2.434960
1	4.333927	-0.557518	3.520341
1	4.511703	0.393707	2.043000
1	4.774945	-1.363169	2.011895
6	1.771061	-2.238074	3.322764
1	2.095152	-1.994753	4.344923
1	2.237763	-3.190666	3.047088
1	0.685237	-2.387168	3.349910
6	1.495501	0.769226	2.904409
1	1.941000	0.943420	3.894822
1	0.412561	0.677604	3.049478
1	1.696991	1.655841	2.293079
6	-4.349671	-2.079569	-1.736690
1	-5.121980	-2.068682	-0.960009
1	-4.609629	-2.872845	-2.452172
1	-4.398695	-1.124360	-2.276441
6	-2.582863	-4.098584	-0.167215
1	-1.554819	-4.420647	0.045896
1	-3.029458	-4.853433	-0.830716
1	-3.141607	-4.109350	0.771748
6	-1.568314	-2.778412	-2.652234
1	-0.529978	-2.436387	-2.626987
1	-2.041868	-2.346974	-3.543257
1	-1.546133	-3.868648	-2.793186
6	-4.790244	0.577618	0.619866

1	-5.671514	0.575354	1.277699
1	-5.120391	0.247204	-0.371339
1	-4.440611	1.610806	0.535883
6	-4.376097	-2.108538	2.022385
1	-3.700022	-2.804936	2.534893
1	-4.916727	-2.664231	1.248131
1	-5.116622	-1.771205	2.762448
6	-2.827533	0.252938	2.981071
1	-2.148128	-0.411653	3.530644
1	-3.691283	0.446253	3.633761
1	-2.323337	1.208214	2.814549

Pro-C_4H_6-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-1.246759	0.562568	-0.662356
32	1.255668	0.321891	-0.682402
6	-2.009551	-1.120903	0.220811
6	-0.840385	-1.707560	1.126707
1	-0.557261	-0.953748	1.869686
1	-1.253513	-2.546869	1.707634
6	0.454957	-2.240060	0.418964
1	0.719733	-3.188397	0.909609
1	0.201732	-2.510874	-0.611618
6	1.763668	-1.326239	0.398714
6	2.309748	1.973002	-0.331393
6	3.838955	4.370118	-0.044676
6	3.707677	1.933688	-0.101331
6	1.700514	3.250672	-0.419969
6	2.452300	4.433759	-0.278525
6	4.465263	3.112174	0.041321
1	4.222847	0.980883	-0.044501
1	0.634150	3.334824	-0.604158
1	1.952960	5.397853	-0.350803
1	5.537611	3.046501	0.214564
1	4.420695	5.282812	0.065346

6	-1.854607	2.313270	0.076678
6	-2.660028	4.874867	1.055794
6	-2.773678	3.121524	-0.638980
6	-1.337886	2.836921	1.288304
6	-1.735419	4.095817	1.777565
6	-3.174700	4.384171	-0.159728
1	-3.189046	2.771630	-1.581298
1	-0.599268	2.273811	1.853639
1	-1.317657	4.467399	2.710961
1	-3.883624	4.979045	-0.732249
1	-2.968177	5.848961	1.429543
6	-1.599295	0.708586	-2.643070
1	-1.540403	-0.298271	-3.065135
1	-2.615331	1.077292	-2.828575
6	-0.564744	1.613320	-3.280404
1	-0.916450	2.551749	-3.709075
6	0.768231	1.344483	-3.317108
1	1.433397	2.082065	-3.764700
6	1.415774	0.124691	-2.699875
1	0.902560	-0.796291	-3.002992
1	2.466807	0.039961	-2.997564
14	3.125609	-2.423268	-0.481936
14	2.287204	-0.924183	2.245885
14	-2.595571	-2.495111	-1.051084
14	-3.488103	-0.709902	1.451195
6	2.460365	-3.271337	-2.055528
1	1.590339	-3.908622	-1.854519
1	3.252433	-3.922138	-2.453879
1	2.190887	-2.564202	-2.847121
6	3.672007	-3.873679	0.636228
1	4.183479	-3.554326	1.551205
1	4.370428	-4.509330	0.073041
1	2.821575	-4.504429	0.927338
6	4.692619	-1.479393	-1.010419
1	5.242114	-1.054984	-0.162781
1	4.476134	-0.670779	-1.719432
1	5.367110	-2.184698	-1.517029
6	4.159349	-0.661148	2.505029
1	4.338948	-0.590605	3.587849
1	4.510652	0.275306	2.058167

1	4.779957	-1.480628	2.126703
6	1.785192	-2.374224	3.381718
1	2.108366	-2.150576	4.408527
1	2.253300	-3.320344	3.086222
1	0.699230	-2.525457	3.404566
6	1.480394	0.640840	2.980083
1	1.901184	0.808395	3.982513
1	0.393900	0.547206	3.097379
1	1.693775	1.534644	2.382324
6	-4.353632	-2.166729	-1.710747
1	-5.126697	-2.194759	-0.934921
1	-4.599773	-2.939952	-2.452581
1	-4.418539	-1.195034	-2.218994
6	-2.556715	-4.205651	-0.204224
1	-1.525279	-4.511281	0.016710
1	-2.976965	-4.950904	-0.895059
1	-3.129320	-4.253657	0.725919
6	-1.553390	-2.766563	-2.641863
1	-0.527297	-2.390512	-2.600312
1	-2.040286	-2.315802	-3.516013
1	-1.493468	-3.848826	-2.826465
6	-4.824298	0.423735	0.710604
1	-5.704381	0.410927	1.369949
1	-5.154554	0.102373	-0.283499
1	-4.479994	1.459961	0.637445
6	-4.377858	-2.285388	2.071171
1	-3.686853	-2.988527	2.554181
1	-4.919905	-2.824384	1.285640
1	-5.114302	-1.979464	2.828872
6	-2.846017	0.093464	3.055676
1	-2.169138	-0.574948	3.603819
1	-3.705928	0.295277	3.710875
1	-2.334784	1.045190	2.885292

Pro-C_4H_6-Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z

50	-1.360916	0.599889	-0.636213
50	1.385924	0.282406	-0.662900
6	-2.105715	-1.258135	0.293765
6	-0.894596	-1.823268	1.168568
1	-0.601146	-1.060133	1.897874
1	-1.291541	-2.657759	1.769441
6	0.400152	-2.375064	0.451397
1	0.607745	-3.356601	0.906484
1	0.152019	-2.593927	-0.592186
6	1.770401	-1.548496	0.488665
6	2.553260	2.026725	-0.230496
6	4.026001	4.434231	0.174275
6	3.946302	1.999591	0.025530
6	1.916085	3.294088	-0.275656
6	2.642207	4.484696	-0.079707
6	4.676574	3.186572	0.228317
1	4.479197	1.052663	0.057645
1	0.847474	3.363548	-0.466100
1	2.126399	5.441550	-0.124768
1	5.745555	3.134147	0.423414
1	4.588794	5.352322	0.326381
6	-1.947627	2.470249	0.242909
6	-2.588179	5.027144	1.332351
6	-2.823568	3.356065	-0.431431
6	-1.386371	2.909626	1.469294
6	-1.704777	4.168199	2.013820
6	-3.142998	4.619715	0.103686
1	-3.264051	3.066253	-1.384369
1	-0.678517	2.281216	2.007575
1	-1.258699	4.475004	2.957576
1	-3.818579	5.279635	-0.436087
1	-2.835051	6.000714	1.749323
6	-1.648723	0.835131	-2.792794
1	-1.611336	-0.166637	-3.232028
1	-2.632879	1.262834	-3.016804
6	-0.535912	1.718905	-3.308638
1	-0.826345	2.715559	-3.642275
6	0.792178	1.405806	-3.352407
1	1.475820	2.174155	-3.713852

6	1.432369	0.130049	-2.865278
1	0.863093	-0.762001	-3.154449
1	2.456540	0.023106	-3.238832
14	3.101022	-2.633661	-0.422940
14	2.277151	-1.159221	2.329250
14	-2.678205	-2.563911	-1.031540
14	-3.568279	-0.836043	1.522210
6	2.403086	-3.387872	-2.029008
1	1.525209	-4.021566	-1.851236
1	3.177004	-4.023149	-2.483956
1	2.129347	-2.627943	-2.770703
6	3.657206	-4.117449	0.639426
1	4.170014	-3.817666	1.560934
1	4.352305	-4.742409	0.061130
1	2.803224	-4.748765	0.919317
6	4.643226	-1.638735	-0.935595
1	5.183420	-1.217521	-0.080410
1	4.393975	-0.817113	-1.620689
1	5.337410	-2.302874	-1.470306
6	4.150500	-0.895112	2.574462
1	4.345206	-0.825189	3.655179
1	4.490555	0.045927	2.124432
1	4.770327	-1.710401	2.183836
6	1.750768	-2.604963	3.455711
1	2.076048	-2.403570	4.486167
1	2.198341	-3.556234	3.144185
1	0.661284	-2.732414	3.472811
6	1.488944	0.421831	3.059180
1	1.905884	0.581688	4.064685
1	0.399695	0.352579	3.168670
1	1.724561	1.315778	2.468170
6	-4.410636	-2.160929	-1.717095
1	-5.203258	-2.188500	-0.961351
1	-4.664779	-2.896289	-2.493618
1	-4.429649	-1.169759	-2.191468
6	-2.683158	-4.305474	-0.254115
1	-1.661446	-4.626972	-0.010718
1	-3.090545	-5.026244	-0.977444
1	-3.283683	-4.370370	0.658339
6	-1.595204	-2.742288	-2.607940

1	-0.586282	-2.325682	-2.531758
1	-2.083829	-2.273017	-3.471509
1	-1.485924	-3.811673	-2.838448
6	-4.841223	0.371095	0.778660
1	-5.735941	0.388260	1.417578
1	-5.164883	0.088813	-0.229756
1	-4.449698	1.393439	0.738398
6	-4.521567	-2.386901	2.098040
1	-3.860483	-3.125378	2.569851
1	-5.063506	-2.884636	1.285225
1	-5.262675	-2.080067	2.850183
6	-2.900051	-0.051101	3.124899
1	-2.232815	-0.730593	3.670706
1	-3.748647	0.176370	3.786172
1	-2.368031	0.888868	2.944624

Pro-C_4H_6-Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-1.405660	0.559014	-0.559876
82	1.413692	0.274487	-0.568657
6	-2.114689	-1.416495	0.368885
6	-0.871441	-1.945195	1.210107
1	-0.578777	-1.172596	1.929147
1	-1.238040	-2.784631	1.825222
6	0.418763	-2.472359	0.467376
1	0.613551	-3.481796	0.867425
1	0.176407	-2.631370	-0.588011
6	1.793562	-1.672390	0.562371
6	2.615809	2.057347	-0.076980
6	4.059157	4.460065	0.419156
6	4.010422	2.031110	0.165144
6	1.958687	3.313598	-0.064271
6	2.672583	4.504102	0.178175
6	4.726565	3.219803	0.413204
1	4.554420	1.089456	0.152293

1	0.887295	3.375756	-0.243610
1	2.144957	5.455740	0.178978
1	5.798101	3.175025	0.597525
1	4.611167	5.378085	0.607775
6	-2.051785	2.449858	0.388274
6	-2.710231	4.965146	1.550205
6	-2.952183	3.334220	-0.252704
6	-1.476912	2.860816	1.616921
6	-1.805353	4.101857	2.197528
6	-3.279514	4.580362	0.320555
1	-3.403691	3.061857	-1.205737
1	-0.752940	2.226504	2.127004
1	-1.350513	4.391697	3.142682
1	-3.972346	5.245238	-0.191115
1	-2.962957	5.925263	1.994384
6	-1.651455	0.856046	-2.791025
1	-1.575761	-0.142498	-3.231613
1	-2.640750	1.268075	-3.016620
6	-0.541833	1.775044	-3.223708
1	-0.834870	2.791090	-3.490606
6	0.792802	1.478421	-3.265658
1	1.470802	2.278876	-3.563497
6	1.443444	0.190745	-2.853961
1	0.871100	-0.700119	-3.138776
1	2.467507	0.097970	-3.228574
14	3.134803	-2.706298	-0.388083
14	2.286250	-1.308319	2.408075
14	-2.662584	-2.679593	-1.001954
14	-3.567120	-1.035543	1.618433
6	2.435828	-3.403899	-2.018150
1	1.582047	-4.074024	-1.856493
1	3.220068	-3.989340	-2.519836
1	2.122398	-2.615487	-2.713439
6	3.707551	-4.220751	0.623988
1	4.225879	-3.944991	1.550291
1	4.402738	-4.823793	0.022610
1	2.860088	-4.866053	0.891920
6	4.666271	-1.675733	-0.858131
1	5.185616	-1.264167	0.014233
1	4.409173	-0.843669	-1.527652

1	5.380479	-2.314243	-1.397611
6	4.156360	-1.021359	2.646283
1	4.353163	-0.920833	3.724173
1	4.487008	-0.089705	2.169460
1	4.781326	-1.842057	2.274976
6	1.781703	-2.786364	3.503229
1	2.104892	-2.606366	4.538340
1	2.242739	-3.723142	3.167633
1	0.693992	-2.930590	3.517633
6	1.479621	0.250647	3.164107
1	1.881972	0.388862	4.178651
1	0.389100	0.177589	3.255855
1	1.721333	1.158441	2.596514
6	-4.408700	-2.293241	-1.661259
1	-5.194060	-2.367204	-0.900620
1	-4.651707	-3.007972	-2.460378
1	-4.456104	-1.287026	-2.100899
6	-2.637084	-4.448915	-0.287023
1	-1.614328	-4.756587	-0.030486
1	-3.012622	-5.153781	-1.042819
1	-3.257348	-4.557619	0.608648
6	-1.575163	-2.758806	-2.582242
1	-0.595103	-2.279151	-2.495105
1	-2.096190	-2.297294	-3.431238
1	-1.397800	-3.812257	-2.841875
6	-4.865599	0.163995	0.910197
1	-5.754715	0.156091	1.557160
1	-5.193141	-0.105986	-0.100302
1	-4.489578	1.192939	0.885110
6	-4.487787	-2.617123	2.167553
1	-3.808500	-3.360686	2.604780
1	-5.035862	-3.097135	1.347886
1	-5.221272	-2.345296	2.940598
6	-2.887337	-0.268537	3.224418
1	-2.209395	-0.950948	3.753196
1	-3.728760	-0.053707	3.898817
1	-2.362111	0.676960	3.049648

TS-PdPCy$_3$-C

Atomic Number	Coordinates (Angstroms) X	Y	Z
46	0.848339	-0.146130	0.239063
6	-2.051215	0.709682	0.447727
6	-2.176890	-0.682373	0.288973
6	-2.260206	-1.630931	1.505789
6	-3.435290	-1.738483	2.292297
6	-3.586631	-2.730986	3.277615
6	-2.554047	-3.652594	3.524733
6	-1.355812	-3.531745	2.796698
6	-1.215397	-2.536107	1.810728
1	-4.252812	-1.048185	2.147756
1	-4.516565	-2.786088	3.840677
1	-2.680399	-4.440881	4.264588
1	-0.538221	-4.225402	2.983471
1	-0.280390	-2.455215	1.258662
6	-2.113482	1.287892	1.875160
6	-3.387037	1.576288	2.422303
6	-3.554522	2.080182	3.722008
6	-2.431292	2.302001	4.538630
6	-1.154478	2.001794	4.027962
6	-0.999053	1.505756	2.716880
1	-4.269733	1.396352	1.826854
1	-4.557062	2.286882	4.093768
1	-2.551993	2.689028	5.548484
1	-0.277467	2.149665	4.654612
1	-0.006180	1.257600	2.347569
6	-2.332540	1.772167	-0.732412
14	-0.640580	2.538734	-1.452344
6	0.452383	3.313069	-0.102790
1	1.311066	3.809980	-0.577135
1	-0.083272	4.061586	0.490852
1	0.837450	2.548935	0.581945
6	-0.922196	3.889350	-2.784412
1	-1.395673	4.814978	-2.445246
1	0.075249	4.147897	-3.171548
1	-1.496851	3.495874	-3.633862

6	0.388298	1.324678	-2.502447
1	0.627353	0.392901	-1.976222
1	-0.123021	1.084392	-3.444062
1	1.338166	1.813089	-2.759135
14	-3.542037	3.372200	-0.474231
6	-2.700871	4.906955	0.277670
1	-2.322742	4.718845	1.289889
1	-1.875049	5.287870	-0.333173
1	-3.453247	5.706774	0.343355
6	-4.211973	3.866918	-2.205131
1	-4.922830	3.114634	-2.572855
1	-4.770138	4.807666	-2.088666
1	-3.458420	4.024085	-2.977888
6	-5.216414	3.224073	0.445145
1	-5.828283	4.058303	0.068978
1	-5.760742	2.299864	0.222893
1	-5.135486	3.338252	1.529256
6	-3.058261	1.038425	-1.913465
1	-2.990720	1.645062	-2.824529
1	-4.132295	0.949938	-1.692734
6	-2.513205	-0.359133	-2.213365
1	-1.448899	-0.282368	-2.436577
1	-2.999898	-0.736208	-3.119885
6	-2.718603	-1.357347	-1.032529
14	-1.824069	-2.985879	-1.737972
6	-0.062472	-2.560463	-2.307570
1	-0.059279	-1.883717	-3.171229
1	0.509960	-2.082279	-1.500280
1	0.457516	-3.482292	-2.606884
6	-2.733575	-3.539109	-3.330563
1	-2.106332	-4.293701	-3.826898
1	-3.707358	-4.004243	-3.136294
1	-2.884341	-2.721421	-4.045757
6	-1.663334	-4.578012	-0.708222
1	-2.594198	-4.898951	-0.231049
1	-1.350068	-5.371212	-1.405324
1	-0.899030	-4.496867	0.069031
14	-4.682345	-1.740176	-0.932908
6	-5.723480	-0.520441	0.111921
1	-5.164191	0.024850	0.871409

1	-6.192533	0.221888	-0.547709
1	-6.530428	-1.069529	0.619047
6	-5.508107	-1.541499	-2.644846
1	-5.161216	-2.244282	-3.407318
1	-6.587867	-1.702563	-2.505596
1	-5.383816	-0.522802	-3.034977
6	-5.071914	-3.503285	-0.326796
1	-6.153572	-3.586285	-0.147288
1	-4.804351	-4.262164	-1.072479
1	-4.558884	-3.746758	0.609824
15	3.284875	-0.148297	0.086884
6	4.302940	1.527571	0.088107
6	4.053679	2.323787	-1.220411
6	4.638814	3.754935	-1.133952
6	6.150921	3.730979	-0.819229
6	6.427895	2.921005	0.467076
6	5.828687	1.491843	0.389291
1	3.819054	2.085480	0.906041
1	4.525105	1.800600	-2.066445
1	2.980622	2.374157	-1.431612
1	4.454748	4.289187	-2.077481
1	4.113288	4.313751	-0.343365
1	6.691516	3.273728	-1.664024
1	6.536277	4.755440	-0.714121
1	7.511834	2.850625	0.643410
1	5.999213	3.454269	1.330094
1	6.353149	0.943445	-0.400573
1	6.032335	0.969358	1.330309
6	3.832815	-1.052988	1.725774
6	3.741653	-0.083346	2.934542
6	3.947288	-0.826785	4.276635
6	5.276727	-1.615179	4.292824
6	5.362951	-2.578765	3.088472
6	5.174247	-1.831170	1.744719
1	3.028923	-1.796740	1.846666
1	4.512858	0.695534	2.844175
1	2.767189	0.425296	2.935659
1	3.924777	-0.104771	5.105625
1	3.109479	-1.522812	4.436696
1	6.122230	-0.909121	4.254267

1	5.373733	-2.174909	5.234020
1	6.330730	-3.101710	3.086382
1	4.583379	-3.350796	3.186290
1	6.020073	-1.144846	1.602075
1	5.207774	-2.558361	0.923701
6	4.034319	-1.272896	-1.328644
6	5.562882	-1.235539	-1.603862
6	5.970441	-2.340883	-2.611806
6	5.202115	-2.204435	-3.945697
6	3.677320	-2.151912	-3.704135
6	3.293070	-1.060555	-2.675490
1	3.780472	-2.285484	-0.969643
1	5.824273	-0.261157	-2.040942
1	6.147336	-1.344052	-0.686364
1	7.054532	-2.292228	-2.793078
1	5.766207	-3.329745	-2.171283
1	5.521801	-1.280087	-4.453129
1	5.453835	-3.038270	-4.616893
1	3.148888	-1.969564	-4.650876
1	3.332574	-3.129938	-3.332512
1	3.556345	-0.072801	-3.083931
1	2.211392	-1.063447	-2.526667

	1
	A
Frequencies --	-56.4429
Red. masses --	13.0254
Frc consts --	0.0244
IR Inten --	1.8748

Atom	AN	X	Y	Z
1	46	0.28	-0.01	0.03
2	6	-0.07	0.00	-0.03
3	6	-0.08	0.03	-0.02
4	6	-0.02	0.03	-0.02
5	6	-0.02	-0.04	-0.04
6	6	0.02	-0.04	-0.04
7	6	0.08	0.03	-0.02
8	6	0.08	0.10	0.00
9	6	0.04	0.10	0.00

10	1	−0.06	−0.09	−0.06
11	1	0.02	−0.09	−0.05
12	1	0.11	0.02	−0.01
13	1	0.12	0.15	0.02
14	1	0.04	0.16	0.01
15	6	−0.01	0.00	−0.03
16	6	0.01	−0.01	0.01
17	6	0.05	−0.01	0.01
18	6	0.08	−0.01	−0.02
19	6	0.06	−0.01	−0.06
20	6	0.02	−0.01	−0.07
21	1	−0.01	−0.01	0.04
22	1	0.06	−0.01	0.05
23	1	0.11	−0.01	−0.02
24	1	0.08	−0.01	−0.09
25	1	0.01	−0.01	−0.11
26	6	−0.03	0.00	−0.02
27	14	−0.02	0.00	−0.01
28	6	−0.01	−0.04	−0.01
29	1	−0.09	0.11	−0.02
30	1	−0.03	−0.17	0.13
31	1	0.12	−0.09	−0.14
32	6	−0.03	0.02	0.00
33	1	−0.02	0.02	0.01
34	1	−0.02	0.01	0.00
35	1	−0.03	0.02	0.00
36	6	−0.06	−0.01	−0.02
37	1	−0.10	−0.02	−0.02
38	1	−0.06	0.02	−0.03
39	1	−0.04	−0.04	−0.01
40	14	−0.02	0.00	−0.01
41	6	0.00	−0.02	0.00
42	1	−0.04	−0.02	0.01
43	1	0.03	−0.04	0.02
44	1	0.02	0.00	−0.03
45	6	−0.02	0.01	0.00
46	1	−0.02	0.01	−0.01
47	1	−0.03	0.00	0.00
48	1	−0.02	0.02	0.00
49	6	−0.01	−0.01	0.00

50	1	-0.01	0.00	0.02
51	1	-0.01	0.00	0.00
52	1	0.00	-0.01	0.00
53	6	-0.02	0.01	-0.03
54	1	0.00	0.01	-0.03
55	1	-0.02	0.01	-0.05
56	6	-0.02	0.00	-0.02
57	1	-0.02	0.00	-0.02
58	1	-0.02	0.00	-0.02
59	6	-0.03	0.01	-0.02
60	14	-0.02	0.00	0.01
61	6	-0.02	0.00	0.02
62	1	-0.01	-0.02	0.00
63	1	-0.03	0.02	0.02
64	1	-0.01	-0.01	0.04
65	6	-0.01	-0.01	0.01
66	1	-0.02	-0.03	0.03
67	1	-0.02	0.01	0.01
68	1	0.01	-0.02	0.00
69	6	-0.03	0.02	0.04
70	1	-0.03	0.02	0.02
71	1	0.00	0.01	0.06
72	1	-0.05	0.04	0.06
73	14	-0.03	0.00	-0.03
74	6	-0.01	0.01	-0.02
75	1	0.02	0.03	-0.05
76	1	-0.04	-0.01	-0.02
77	1	0.01	0.02	0.02
78	6	-0.02	0.01	-0.03
79	1	-0.01	0.01	-0.03
80	1	-0.02	0.01	-0.03
81	1	-0.02	0.01	-0.03
82	6	-0.03	0.01	-0.03
83	1	-0.03	0.01	-0.03
84	1	-0.04	0.00	-0.03
85	1	-0.04	0.00	-0.03
86	15	-0.13	-0.02	0.02
87	6	-0.13	-0.01	0.02
88	6	-0.11	0.00	0.02
89	6	-0.09	-0.01	0.01

90	6	−0.09	−0.03	0.02
91	6	−0.11	−0.02	0.03
92	6	−0.13	−0.02	0.03
93	1	−0.13	0.00	0.01
94	1	−0.12	−0.01	0.02
95	1	−0.11	0.01	0.01
96	1	−0.08	−0.01	0.01
97	1	−0.09	0.00	0.01
98	1	−0.09	−0.04	0.03
99	1	−0.08	−0.03	0.02
100	1	−0.12	−0.04	0.04
101	1	−0.11	−0.01	0.02
102	1	−0.13	−0.02	0.03
103	1	−0.14	−0.01	0.03
104	6	−0.10	−0.02	0.01
105	6	−0.09	−0.02	0.01
106	6	−0.05	−0.01	0.01
107	6	−0.04	0.00	−0.01
108	6	−0.06	0.00	−0.01
109	6	−0.09	−0.01	−0.01
110	1	−0.09	−0.02	0.02
111	1	−0.10	−0.01	0.00
112	1	−0.09	−0.03	0.03
113	1	−0.05	−0.01	0.01
114	1	−0.04	−0.02	0.03
115	1	−0.05	0.01	−0.03
116	1	−0.02	0.00	−0.01
117	1	−0.06	0.01	−0.03
118	1	−0.05	−0.01	0.01
119	1	−0.10	0.00	−0.03
120	1	−0.10	−0.01	−0.01
121	6	−0.11	0.00	0.01
122	6	−0.10	0.01	0.03
123	6	−0.08	0.01	0.04
124	6	−0.05	0.01	0.02
125	6	−0.06	0.02	−0.01
126	6	−0.08	0.01	−0.01
127	1	−0.11	0.00	−0.01
128	1	−0.10	0.01	0.03
129	1	−0.12	0.01	0.04

130	1	-0.08	0.02	0.06
131	1	-0.09	0.01	0.03
132	1	-0.04	0.01	0.03
133	1	-0.04	0.01	0.03
134	1	-0.04	0.02	-0.02
135	1	-0.07	0.02	-0.02
136	1	-0.06	0.01	0.00
137	1	-0.08	0.02	-0.04

TS-PdPCy$_3$-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-1.792403	0.934156	0.975037
14	-2.457555	-1.259451	0.399488
6	-3.728059	-1.142702	-1.166087
6	-3.428406	0.283316	-1.788160
6	-3.796981	1.541988	-0.943872
6	-2.587437	2.308697	-0.248110
1	-2.359941	0.323886	-2.015227
1	-3.942512	0.366252	-2.758833
1	-4.329008	2.246889	-1.598806
1	-4.522673	1.253183	-0.173321
6	-2.879246	-2.628430	1.786025
6	-3.201788	-2.211524	3.112053
6	-2.896159	-4.046018	1.572015
6	-3.498745	-3.122156	4.150018
1	-3.248470	-1.150615	3.338798
6	-3.202877	-4.961350	2.609192
1	-2.667740	-4.473606	0.599338
6	-3.498225	-4.507801	3.909377
1	-3.739843	-2.746566	5.143177
1	-3.205581	-6.034128	2.410954
1	-3.723469	-5.211957	4.711415
6	-0.519867	1.583252	2.346314
6	0.234663	2.791547	2.213879
6	-0.339812	0.885939	3.578455

6	1.109510	3.255711	3.222851
1	0.169526	3.389064	1.315058
6	0.530639	1.348962	4.591061
1	-0.884440	-0.035141	3.765721
6	1.267620	2.536548	4.421677
1	1.675237	4.176358	3.073226
1	0.634843	0.784122	5.516212
1	1.943223	2.891474	5.201060
14	-3.496237	3.715223	0.837242
14	-1.524167	3.182605	-1.666891
14	-5.633011	-1.325446	-0.693724
14	-3.332109	-2.357377	-2.687277
6	-2.451223	5.266220	1.209822
1	-1.509053	5.022349	1.712188
1	-2.225442	5.861773	0.316600
1	-3.028308	5.908256	1.891668
6	-5.094003	4.349428	-0.013478
1	-5.859358	3.568384	-0.106019
1	-5.520320	5.144388	0.618327
1	-4.927926	4.779327	-1.007851
6	-4.051052	3.012903	2.514141
1	-3.196970	2.819394	3.174001
1	-4.704068	3.742712	3.014814
1	-4.616316	2.078666	2.406139
6	0.032403	4.097774	-1.066988
1	0.459641	4.628552	-1.930381
1	-0.164347	4.842681	-0.289686
1	0.792427	3.392452	-0.709309
6	-2.586976	4.485836	-2.595563
1	-2.857014	5.352168	-1.979472
1	-1.995092	4.864634	-3.443074
1	-3.512431	4.067962	-3.013572
6	-0.879144	2.034515	-3.043655
1	-0.291647	1.192745	-2.656136
1	-1.677165	1.640978	-3.684026
1	-0.213890	2.634763	-3.682801
6	-6.061364	-0.674883	1.041435
1	-5.468697	-1.175289	1.814152
1	-5.907896	0.406220	1.138551
1	-7.122487	-0.878245	1.246104

6	-6.760688	-0.364898	-1.911479
1	-6.703253	-0.737381	-2.940370
1	-7.804994	-0.478452	-1.581310
1	-6.542327	0.710763	-1.928714
6	-6.219092	-3.140479	-0.709848
1	-7.267147	-3.173720	-0.377502
1	-6.179616	-3.602367	-1.703677
1	-5.635447	-3.760436	-0.018103
6	-1.729713	-1.839062	-3.573877
1	-1.839240	-0.889266	-4.112625
1	-0.882210	-1.743219	-2.883916
1	-1.474173	-2.606901	-4.319528
6	-4.672534	-2.298850	-4.071824
1	-4.291424	-2.884981	-4.923583
1	-5.635617	-2.740379	-3.787334
1	-4.866213	-1.285496	-4.448704
6	-3.130941	-4.185795	-2.212178
1	-3.966757	-4.571114	-1.619533
1	-3.069908	-4.786816	-3.131430
1	-2.199897	-4.344095	-1.653993
46	1.441058	-0.479355	-0.292221
15	3.843463	-0.277012	-0.276644
6	4.631569	-1.556783	-1.508171
6	6.152477	-1.567781	-1.819596
6	4.147442	-2.981587	-1.131739
1	4.116010	-1.279814	-2.441805
6	6.453992	-2.578496	-2.961612
1	6.729496	-1.853226	-0.929906
1	6.501971	-0.572395	-2.123327
6	4.448563	-3.991129	-2.262168
1	4.651965	-3.312108	-0.210111
1	3.069761	-2.954867	-0.920351
6	5.950506	-4.001797	-2.625529
1	7.534754	-2.599181	-3.166722
1	5.962288	-2.233162	-3.885280
1	4.121070	-4.996672	-1.960937
1	3.859263	-3.716656	-3.151557
1	6.130648	-4.676956	-3.474898
1	6.526363	-4.400161	-1.774690
6	4.512796	1.473440	-0.796120

6	5.960055	1.868341	-0.401304
6	4.267812	1.718436	-2.307172
1	3.832948	2.138678	-0.239801
6	6.254095	3.340518	-0.793552
1	6.688634	1.214793	-0.901586
1	6.111186	1.751624	0.679737
6	4.573577	3.183915	-2.700384
1	4.913727	1.052182	-2.899773
1	3.227621	1.467682	-2.557585
6	6.009272	3.592406	-2.298744
1	7.290550	3.597108	-0.528558
1	5.601527	4.007387	-0.207221
1	4.429324	3.315529	-3.782709
1	3.854225	3.850660	-2.198998
1	6.184672	4.650794	-2.540982
1	6.733715	3.007191	-2.888112
6	4.575317	-0.533257	1.508371
6	3.617332	-1.425661	2.340182
6	6.034865	-1.039080	1.658324
1	4.527484	0.485606	1.930391
6	4.033094	-1.476098	3.828084
1	3.622855	-2.446037	1.926771
1	2.590379	-1.051977	2.235925
6	6.455685	-1.072548	3.152453
1	6.115037	-2.057670	1.251993
1	6.736400	-0.412632	1.094889
6	5.496623	-1.942878	3.996261
1	3.354593	-2.145383	4.376682
1	3.916592	-0.473283	4.269554
1	7.485837	-1.449040	3.240265
1	6.457420	-0.045637	3.552756
1	5.787782	-1.911739	5.056520
1	5.581988	-2.993162	3.673626

	1
	A
Frequencies --	-47.4048
Red. masses --	9.3021
Frc consts --	0.0099

IR Inten -- 0.2701

Atom	AN	X	Y	Z
1	14	0.14	-0.01	-0.06
2	14	0.10	-0.01	-0.03
3	6	0.08	-0.01	-0.02
4	6	0.07	-0.01	-0.02
5	6	0.08	-0.01	0.00
6	6	0.09	-0.01	-0.02
7	1	0.06	0.00	-0.04
8	1	0.05	0.00	-0.01
9	1	0.06	-0.01	0.01
10	1	0.09	-0.02	0.01
11	6	0.10	-0.01	-0.02
12	6	0.09	0.00	-0.03
13	6	0.08	-0.01	-0.02
14	6	0.07	0.01	-0.03
15	1	0.10	0.00	-0.03
16	6	0.06	0.00	-0.02
17	1	0.09	-0.01	-0.02
18	6	0.06	0.01	-0.03
19	1	0.07	0.01	-0.03
20	1	0.06	0.00	-0.02
21	1	0.04	0.01	-0.03
22	6	0.09	0.00	-0.02
23	6	0.11	-0.01	-0.02
24	6	0.05	0.03	0.00
25	6	0.09	0.00	-0.01
26	1	0.14	-0.02	-0.04
27	6	0.03	0.04	0.01
28	1	0.03	0.04	0.00
29	6	0.05	0.02	0.01
30	1	0.10	-0.01	-0.01
31	1	0.00	0.05	0.03
32	1	0.03	0.03	0.02
33	14	0.09	-0.03	0.00
34	14	0.06	0.01	-0.03
35	14	0.08	-0.01	0.00
36	14	0.06	-0.01	-0.02
37	6	0.08	-0.03	0.02
38	1	0.09	-0.03	0.00

39	1	0.06	−0.01	0.02
40	1	0.08	−0.04	0.03
41	6	0.08	−0.03	0.02
42	1	0.08	−0.03	0.03
43	1	0.08	−0.03	0.03
44	1	0.07	−0.02	0.02
45	6	0.10	−0.06	0.00
46	1	0.10	−0.05	−0.01
47	1	0.09	−0.08	0.01
48	1	0.12	−0.07	−0.01
49	6	0.05	0.02	−0.03
50	1	0.04	0.04	−0.03
51	1	0.05	0.00	−0.02
52	1	0.06	0.02	−0.05
53	6	0.04	0.01	−0.01
54	1	0.04	0.00	−0.01
55	1	0.02	0.01	−0.02
56	1	0.03	0.00	0.00
57	6	0.05	0.02	−0.04
58	1	0.05	0.02	−0.04
59	1	0.04	0.02	−0.04
60	1	0.04	0.02	−0.04
61	6	0.09	0.00	0.00
62	1	0.11	0.02	0.00
63	1	0.06	0.00	−0.01
64	1	0.10	−0.03	0.02
65	6	0.07	−0.01	0.01
66	1	0.06	−0.01	0.01
67	1	0.08	−0.01	0.02
68	1	0.07	−0.01	0.01
69	6	0.08	−0.01	0.01
70	1	0.08	−0.01	0.01
71	1	0.08	−0.01	0.01
72	1	0.08	−0.01	0.01
73	6	0.05	0.00	−0.04
74	1	0.04	−0.01	−0.04
75	1	0.05	0.01	−0.05
76	1	0.05	−0.01	−0.04
77	6	0.04	−0.01	−0.01
78	1	0.04	−0.01	−0.01

79	1	0.05	-0.01	0.00
80	1	0.04	-0.01	-0.01
81	6	0.06	-0.01	-0.02
82	1	0.07	-0.01	-0.01
83	1	0.06	-0.01	-0.02
84	1	0.07	0.00	-0.03
85	46	-0.16	0.00	0.05
86	15	-0.12	0.01	0.02
87	6	-0.11	0.01	0.01
88	6	-0.11	0.03	0.01
89	6	-0.09	0.01	0.02
90	1	-0.12	0.00	0.01
91	6	-0.10	0.03	0.01
92	1	-0.10	0.04	0.01
93	1	-0.12	0.03	0.00
94	6	-0.08	0.01	0.02
95	1	-0.09	0.02	0.02
96	1	-0.09	-0.01	0.02
97	6	-0.08	0.02	0.02
98	1	-0.10	0.04	0.01
99	1	-0.11	0.02	0.01
100	1	-0.07	0.00	0.03
101	1	-0.08	-0.01	0.02
102	1	-0.07	0.02	0.02
103	1	-0.07	0.03	0.02
104	6	-0.11	0.01	0.01
105	6	-0.11	0.00	0.02
106	6	-0.10	0.00	0.01
107	1	-0.11	0.01	0.01
108	6	-0.09	0.00	0.01
109	1	-0.11	0.00	0.03
110	1	-0.12	0.01	0.02
111	6	-0.08	0.00	0.00
112	1	-0.10	-0.01	0.02
113	1	-0.10	0.01	0.00
114	6	-0.08	-0.01	0.01
115	1	-0.09	-0.01	0.02
116	1	-0.09	0.01	0.00
117	1	-0.07	-0.01	0.00
118	1	-0.08	0.01	-0.01

119	1	-0.07	-0.02	0.00
120	1	-0.08	-0.02	0.02
121	6	-0.09	0.01	0.01
122	6	-0.08	0.00	0.02
123	6	-0.09	0.02	-0.01
124	1	-0.10	0.01	0.01
125	6	-0.06	-0.01	0.01
126	1	-0.07	0.00	0.01
127	1	-0.08	-0.01	0.03
128	6	-0.07	0.02	-0.01
129	1	-0.08	0.02	-0.01
130	1	-0.10	0.03	-0.01
131	6	-0.05	0.00	0.00
132	1	-0.05	-0.01	0.02
133	1	-0.06	-0.01	0.02
134	1	-0.07	0.03	-0.02
135	1	-0.08	0.02	-0.01
136	1	-0.04	0.00	-0.01
137	1	-0.05	0.01	-0.01

TS-PdPCy$_3$-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-1.698384	1.012268	0.983467
32	-2.202613	-1.387624	0.255392
6	-3.643753	-1.111791	-1.279166
6	-3.289293	0.317094	-1.863883
6	-3.659346	1.590624	-1.033358
6	-2.458509	2.400097	-0.362403
1	-2.213246	0.337271	-2.061473
1	-3.768049	0.419869	-2.851911
1	-4.206228	2.277845	-1.696452
1	-4.377461	1.309310	-0.253025
6	-2.812063	-2.657191	1.781159
6	-3.135067	-2.187792	3.086994
6	-2.835884	-4.073866	1.602332

6	-3.438380	-3.067644	4.149274
1	-3.167325	-1.119220	3.283017
6	-3.150564	-4.956941	2.660681
1	-2.602410	-4.518098	0.637283
6	-3.443538	-4.459775	3.945012
1	-3.674854	-2.664568	5.132857
1	-3.157557	-6.033024	2.488060
1	-3.670576	-5.139709	4.765804
6	-0.328086	1.690485	2.339427
6	0.442635	2.877669	2.190962
6	-0.177000	0.983584	3.566644
6	1.318567	3.328640	3.201037
1	0.382498	3.459202	1.280559
6	0.693880	1.434430	4.581696
1	-0.740641	0.070179	3.744621
6	1.449186	2.609831	4.404209
1	1.900525	4.237029	3.048648
1	0.783477	0.871491	5.509040
1	2.123281	2.958217	5.186122
14	-3.349342	3.801081	0.720997
14	-1.361983	3.218721	-1.769377
14	-5.524647	-1.263292	-0.768993
14	-3.236597	-2.339756	-2.766371
6	-2.278241	5.329122	1.100999
1	-1.344262	5.063658	1.608359
1	-2.033783	5.916379	0.207499
1	-2.844039	5.984070	1.779368
6	-4.941539	4.435053	-0.127938
1	-5.705761	3.652333	-0.214294
1	-5.367551	5.237646	0.493088
1	-4.767272	4.849944	-1.127193
6	-3.900747	3.097173	2.404787
1	-3.049969	2.906762	3.071270
1	-4.549248	3.832420	2.903581
1	-4.475005	2.166816	2.307537
6	0.202973	4.107266	-1.152408
1	0.651985	4.626340	-2.011702
1	0.011660	4.857680	-0.379207
1	0.944773	3.388353	-0.782722
6	-2.399313	4.519419	-2.721432

1	-2.665050	5.391047	-2.110840
1	-1.804919	4.885817	-3.571706
1	-3.327087	4.099976	-3.132666
6	-0.713627	2.033222	-3.112396
1	-0.140107	1.193180	-2.700053
1	-1.507505	1.633163	-3.753634
1	-0.033358	2.611483	-3.755941
6	-5.939757	-0.588722	0.962663
1	-5.353453	-1.091207	1.739190
1	-5.775127	0.491712	1.051982
1	-7.003439	-0.777114	1.170383
6	-6.647267	-0.303459	-1.992077
1	-6.585932	-0.685526	-3.017636
1	-7.694569	-0.400868	-1.667524
1	-6.413498	0.769116	-2.017435
6	-6.123540	-3.073605	-0.755137
1	-7.172204	-3.098273	-0.424612
1	-6.082039	-3.551822	-1.741296
1	-5.543245	-3.683724	-0.051571
6	-1.608554	-1.844714	-3.621074
1	-1.694590	-0.897823	-4.168935
1	-0.778556	-1.750725	-2.909352
1	-1.339586	-2.621833	-4.351683
6	-4.558561	-2.294892	-4.158550
1	-4.183420	-2.892821	-5.003435
1	-5.525285	-2.721169	-3.863590
1	-4.739997	-1.280734	-4.539209
6	-3.038061	-4.156241	-2.238076
1	-3.875680	-4.526104	-1.637860
1	-2.969846	-4.783829	-3.138608
1	-2.109670	-4.299432	-1.669891
46	1.587215	-0.510705	-0.339481
15	3.995540	-0.288707	-0.295665
6	4.775331	-1.590210	-1.509748
6	6.297514	-1.621486	-1.813634
6	4.273425	-3.005525	-1.120487
1	4.267331	-1.317562	-2.448697
6	6.592632	-2.647899	-2.943395
1	6.867184	-1.903891	-0.918218
1	6.659668	-0.633464	-2.126539

6	4.568487	-4.030463	-2.238544
1	4.769497	-3.331904	-0.192856
1	3.194998	-2.964570	-0.915078
6	6.071854	-4.061835	-2.594423
1	7.673956	-2.682757	-3.143470
1	6.108794	-2.307160	-3.872917
1	4.228242	-5.028857	-1.927880
1	3.986343	-3.759324	-3.133625
1	6.248391	-4.748113	-3.435596
1	6.639212	-4.457449	-1.736603
6	4.683838	1.449394	-0.829810
6	6.133151	1.834919	-0.433165
6	4.446993	1.680449	-2.344339
1	4.008766	2.127562	-0.283477
6	6.440875	3.300733	-0.838791
1	6.857871	1.170260	-0.924382
1	6.279250	1.727313	0.649553
6	4.766672	3.139168	-2.751133
1	5.089540	1.002504	-2.927233
1	3.405812	1.435799	-2.596561
6	6.204055	3.539613	-2.347445
1	7.478296	3.551578	-0.572225
1	5.791433	3.978599	-0.261645
1	4.628070	3.260832	-3.835322
1	4.050732	3.816866	-2.259668
1	6.389226	4.594004	-2.599515
1	6.925910	2.942500	-2.927976
6	4.712310	-0.535201	1.496418
6	3.740181	-1.411319	2.329219
6	6.165750	-1.054360	1.660586
1	4.672189	0.487715	1.909303
6	4.144960	-1.452299	3.820402
1	3.739326	-2.435320	1.924974
1	2.717207	-1.029914	2.214552
6	6.576010	-1.078214	3.157861
1	6.238075	-2.077465	1.264252
1	6.877460	-0.440419	1.096080
6	5.602758	-1.931366	4.002985
1	3.456372	-2.110411	4.369923
1	4.034825	-0.444556	4.252175

1	7.601734	-1.464031	3.256194
1	6.585236	-0.047735	3.548754
1	5.886879	-1.893113	5.064896
1	5.680209	-2.985417	3.690831

	1
	A
Frequencies --	-44.4581
Red. masses --	10.7563
Frc consts --	0.0099
IR Inten --	0.4336

Atom	AN	X	Y	Z
1	32	0.11	0.00	-0.04
2	32	0.11	0.00	-0.03
3	6	0.08	0.00	-0.01
4	6	0.06	0.00	-0.01
5	6	0.06	-0.01	0.00
6	6	0.06	0.00	-0.01
7	1	0.06	0.01	-0.03
8	1	0.04	0.00	0.00
9	1	0.05	0.00	0.01
10	1	0.07	-0.01	0.01
11	6	0.10	0.01	-0.02
12	6	0.09	0.01	-0.03
13	6	0.09	0.01	-0.02
14	6	0.07	0.02	-0.03
15	1	0.10	0.01	-0.03
16	6	0.07	0.01	-0.02
17	1	0.10	0.00	-0.02
18	6	0.06	0.02	-0.03
19	1	0.06	0.02	-0.03
20	1	0.06	0.01	-0.02
21	1	0.04	0.02	-0.03
22	6	0.07	0.02	-0.01
23	6	0.07	0.02	0.00
24	6	0.04	0.03	0.00
25	6	0.05	0.03	0.01
26	1	0.08	0.01	-0.01
27	6	0.03	0.04	0.01

28	1	0.04	0.03	0.00
29	6	0.03	0.03	0.02
30	1	0.05	0.03	0.02
31	1	0.01	0.04	0.02
32	1	0.02	0.04	0.03
33	14	0.06	-0.02	0.01
34	14	0.04	0.02	-0.01
35	14	0.08	-0.01	0.01
36	14	0.06	0.00	-0.02
37	6	0.04	-0.01	0.01
38	1	0.05	0.00	0.01
39	1	0.03	0.00	0.02
40	1	0.04	-0.02	0.02
41	6	0.05	-0.02	0.02
42	1	0.05	-0.02	0.02
43	1	0.05	-0.03	0.02
44	1	0.04	-0.01	0.02
45	6	0.07	-0.04	0.00
46	1	0.07	-0.03	0.00
47	1	0.06	-0.05	0.01
48	1	0.08	-0.04	-0.01
49	6	0.04	0.02	-0.01
50	1	0.04	0.03	-0.01
51	1	0.04	0.02	-0.01
52	1	0.04	0.03	-0.02
53	6	0.03	0.02	0.00
54	1	0.03	0.01	0.00
55	1	0.02	0.02	0.00
56	1	0.03	0.01	0.00
57	6	0.04	0.03	-0.02
58	1	0.04	0.02	-0.03
59	1	0.04	0.03	-0.02
60	1	0.04	0.03	-0.02
61	6	0.09	0.00	0.01
62	1	0.12	0.03	0.01
63	1	0.04	0.00	-0.01
64	1	0.10	-0.04	0.03
65	6	0.07	-0.01	0.02
66	1	0.06	-0.01	0.02
67	1	0.07	-0.02	0.03

68	1	0.07	-0.01	0.01
69	6	0.09	-0.01	0.01
70	1	0.09	-0.01	0.02
71	1	0.08	-0.01	0.01
72	1	0.09	-0.01	0.01
73	6	0.05	0.01	-0.04
74	1	0.04	0.01	-0.04
75	1	0.05	0.02	-0.04
76	1	0.05	0.01	-0.04
77	6	0.05	0.00	0.00
78	1	0.04	0.00	-0.01
79	1	0.05	-0.01	0.01
80	1	0.04	0.00	0.00
81	6	0.07	0.00	-0.02
82	1	0.08	0.00	-0.01
83	1	0.06	0.00	-0.02
84	1	0.08	0.00	-0.03
85	46	-0.17	-0.03	0.04
86	15	-0.13	0.00	0.02
87	6	-0.12	0.01	0.01
88	6	-0.12	0.03	0.01
89	6	-0.10	0.00	0.02
90	1	-0.13	0.00	0.02
91	6	-0.11	0.03	0.01
92	1	-0.11	0.04	0.00
93	1	-0.14	0.03	0.00
94	6	-0.09	0.00	0.02
95	1	-0.09	0.01	0.02
96	1	-0.10	-0.01	0.02
97	6	-0.09	0.02	0.02
98	1	-0.11	0.04	0.01
99	1	-0.12	0.02	0.01
100	1	-0.07	0.00	0.03
101	1	-0.09	-0.01	0.02
102	1	-0.08	0.02	0.02
103	1	-0.08	0.04	0.02
104	6	-0.13	0.00	0.01
105	6	-0.13	0.00	0.02
106	6	-0.11	0.00	0.01
107	1	-0.13	0.01	0.00

108	6	-0.11	0.00	0.01
109	1	-0.12	0.00	0.04
110	1	-0.14	0.01	0.03
111	6	-0.10	-0.01	0.00
112	1	-0.11	-0.01	0.02
113	1	-0.11	0.00	0.00
114	6	-0.10	-0.01	0.01
115	1	-0.12	-0.01	0.02
116	1	-0.12	0.01	0.00
117	1	-0.09	-0.02	0.00
118	1	-0.10	0.00	-0.01
119	1	-0.09	-0.02	0.00
120	1	-0.10	-0.03	0.02
121	6	-0.11	0.01	0.01
122	6	-0.09	-0.01	0.02
123	6	-0.10	0.02	-0.01
124	1	-0.11	0.00	0.01
125	6	-0.07	-0.01	0.01
126	1	-0.08	-0.01	0.02
127	1	-0.09	-0.02	0.03
128	6	-0.08	0.02	-0.01
129	1	-0.09	0.02	-0.01
130	1	-0.11	0.03	-0.01
131	6	-0.06	0.00	0.00
132	1	-0.06	-0.02	0.02
133	1	-0.08	-0.01	0.02
134	1	-0.08	0.03	-0.02
135	1	-0.09	0.02	-0.01
136	1	-0.05	0.00	-0.01
137	1	-0.06	0.01	-0.01

TS-PdPCy$_3$-Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	-1.677073	1.089108	1.005696
50	-2.029165	-1.515284	0.145699

6	-3.622589	-1.090338	-1.402314
6	-3.260788	0.355616	-1.954911
6	-3.647551	1.643465	-1.137035
6	-2.475485	2.506776	-0.470227
1	-2.183516	0.382438	-2.145628
1	-3.730065	0.465445	-2.947082
1	-4.199639	2.307684	-1.819248
1	-4.371233	1.367422	-0.359312
6	-2.764206	-2.763817	1.783559
6	-3.131437	-2.260529	3.062383
6	-2.777528	-4.175698	1.620372
6	-3.474013	-3.122129	4.125034
1	-3.163086	-1.187073	3.237262
6	-3.130265	-5.041092	2.675699
1	-2.504229	-4.620187	0.664934
6	-3.470849	-4.517502	3.937361
1	-3.744397	-2.703919	5.093147
1	-3.128050	-6.117436	2.514341
1	-3.728031	-5.184052	4.758136
6	-0.230396	1.782842	2.424410
6	0.533857	2.967710	2.290688
6	-0.043360	1.000377	3.595646
6	1.456518	3.355547	3.280059
1	0.428343	3.585388	1.406125
6	0.873322	1.388104	4.591704
1	-0.608745	0.079503	3.737290
6	1.627995	2.567325	4.434659
1	2.038782	4.264631	3.145213
1	0.998415	0.773394	5.480822
1	2.339758	2.867318	5.200685
14	-3.375033	3.903397	0.580914
14	-1.300299	3.259684	-1.827082
14	-5.478149	-1.244456	-0.849556
14	-3.194993	-2.320681	-2.857011
6	-2.283831	5.405907	0.998523
1	-1.385816	5.121403	1.559949
1	-1.973161	5.968395	0.109973
1	-2.864117	6.088916	1.635445
6	-4.935460	4.545064	-0.307875
1	-5.698187	3.762863	-0.410353

1	-5.375768	5.355308	0.291543
1	-4.724153	4.945775	-1.305770
6	-3.979343	3.221197	2.263840
1	-3.156439	3.036907	2.968483
1	-4.631567	3.974910	2.730379
1	-4.568208	2.298983	2.173326
6	0.256009	4.112324	-1.137491
1	0.751587	4.627907	-1.972997
1	0.055903	4.858774	-0.363051
1	0.967545	3.372472	-0.747638
6	-2.277244	4.546839	-2.846342
1	-2.542498	5.434994	-2.259177
1	-1.666204	4.881916	-3.696310
1	-3.204347	4.122751	-3.254480
6	-0.590719	2.020654	-3.089690
1	-0.055364	1.187568	-2.613895
1	-1.347407	1.607430	-3.766184
1	0.140035	2.565382	-3.706321
6	-5.900948	-0.568594	0.884525
1	-5.362589	-1.104714	1.674205
1	-5.696642	0.503085	0.995655
1	-6.977960	-0.714559	1.058428
6	-6.602824	-0.290074	-2.071398
1	-6.518203	-0.667310	-3.097292
1	-7.653422	-0.398324	-1.763694
1	-6.374684	0.783849	-2.087568
6	-6.079652	-3.053457	-0.819269
1	-7.130724	-3.071494	-0.496232
1	-6.031914	-3.541009	-1.800535
1	-5.506867	-3.658435	-0.104777
6	-1.537824	-1.837102	-3.663027
1	-1.600026	-0.888846	-4.211204
1	-0.731901	-1.746372	-2.923452
1	-1.243837	-2.616023	-4.381169
6	-4.489938	-2.296959	-4.262588
1	-4.111642	-2.895620	-5.103843
1	-5.456496	-2.719870	-3.962846
1	-4.667904	-1.280525	-4.638346
6	-2.993319	-4.124140	-2.271298
1	-3.835009	-4.480722	-1.668591

1	-2.909063	-4.780077	-3.149649
1	-2.070626	-4.251537	-1.687799
46	1.795529	-0.462860	-0.374623
15	4.216275	-0.282631	-0.331777
6	5.016437	-1.587137	-1.532829
6	6.546548	-1.600711	-1.796925
6	4.525517	-3.009374	-1.154870
1	4.526887	-1.319999	-2.483188
6	6.894369	-2.624644	-2.912335
1	7.092574	-1.873845	-0.884711
1	6.904033	-0.609145	-2.101183
6	4.867579	-4.030781	-2.264417
1	5.003887	-3.327601	-0.215123
1	3.441829	-2.988909	-0.976605
6	6.381008	-4.044116	-2.577274
1	7.983221	-2.644743	-3.070055
1	6.442387	-2.292711	-3.860686
1	4.532074	-5.033783	-1.963694
1	4.308973	-3.767699	-3.176687
1	6.589903	-4.728130	-3.412920
1	6.928983	-4.433038	-1.703825
6	4.932823	1.449307	-0.855715
6	6.388018	1.814680	-0.458298
6	4.702827	1.699390	-2.368164
1	4.267415	2.133141	-0.304661
6	6.708002	3.284274	-0.839098
1	7.104094	1.153393	-0.965394
1	6.540563	1.686957	0.621002
6	5.023545	3.165153	-2.748593
1	5.349775	1.030653	-2.957305
1	3.663442	1.458345	-2.630482
6	6.462115	3.557694	-2.340565
1	7.751055	3.516776	-0.577450
1	6.072618	3.957606	-0.241804
1	4.883040	3.308678	-3.829783
1	4.308743	3.832746	-2.241981
1	6.644236	4.618466	-2.566933
1	7.182272	2.977062	-2.939530
6	4.919442	-0.528657	1.465365
6	3.941081	-1.391684	2.303754

6	6.368135	-1.057754	1.638490
1	4.885535	0.497095	1.871579
6	4.341814	-1.409892	3.796924
1	3.940893	-2.421648	1.914402
1	2.919016	-1.010430	2.180059
6	6.777870	-1.062093	3.135263
1	6.430934	-2.087591	1.258369
1	7.085697	-0.459656	1.065273
6	5.796679	-1.893321	3.992620
1	3.648717	-2.054165	4.356924
1	4.236394	-0.393744	4.209806
1	7.799855	-1.456302	3.238945
1	6.797418	-0.025711	3.509673
1	6.077977	-1.836639	5.054411
1	5.869342	-2.953435	3.700526

	1
	A
Frequencies --	-42.9041
Red. masses --	11.3796
Frc consts --	0.0096
IR Inten --	0.1947

Atom	AN	X	Y	Z
1	50	0.09	0.01	-0.03
2	50	0.11	0.00	-0.02
3	6	0.08	0.00	0.00
4	6	0.06	0.00	-0.01
5	6	0.05	0.00	0.00
6	6	0.05	0.01	-0.01
7	1	0.06	0.01	-0.02
8	1	0.05	0.00	0.00
9	1	0.05	-0.01	0.00
10	1	0.06	-0.01	0.00
11	6	0.10	0.01	-0.02
12	6	0.10	0.02	-0.02
13	6	0.08	0.01	-0.02
14	6	0.07	0.02	-0.02
15	1	0.12	0.02	-0.02
16	6	0.05	0.02	-0.02

17	1	0.08	0.01	−0.02
18	6	0.05	0.02	−0.03
19	1	0.07	0.03	−0.03
20	1	0.03	0.02	−0.02
21	1	0.02	0.03	−0.03
22	6	0.04	0.03	0.01
23	6	0.04	0.03	0.02
24	6	0.02	0.04	0.02
25	6	0.02	0.04	0.04
26	1	0.05	0.03	0.02
27	6	0.00	0.04	0.03
28	1	0.01	0.03	0.01
29	6	0.00	0.04	0.04
30	1	0.02	0.04	0.04
31	1	−0.02	0.04	0.04
32	1	−0.01	0.04	0.05
33	14	0.04	−0.01	0.01
34	14	0.03	0.02	−0.01
35	14	0.08	−0.01	0.01
36	14	0.07	0.00	−0.01
37	6	0.02	0.00	0.01
38	1	0.02	0.01	0.01
39	1	0.01	0.01	0.01
40	1	0.01	−0.01	0.02
41	6	0.03	−0.02	0.01
42	1	0.03	−0.03	0.01
43	1	0.02	−0.03	0.02
44	1	0.02	−0.01	0.01
45	6	0.05	−0.03	0.00
46	1	0.05	−0.03	0.00
47	1	0.04	−0.04	0.01
48	1	0.05	−0.03	−0.01
49	6	0.03	0.03	0.00
50	1	0.03	0.03	0.00
51	1	0.02	0.03	0.00
52	1	0.02	0.03	0.00
53	6	0.02	0.02	0.01
54	1	0.01	0.01	0.02
55	1	0.02	0.04	0.01
56	1	0.02	0.02	0.00

57	6	0.04	0.04	-0.02
58	1	0.05	0.04	-0.02
59	1	0.04	0.03	-0.01
60	1	0.03	0.04	-0.02
61	6	0.09	-0.02	0.02
62	1	0.10	-0.01	0.01
63	1	0.08	-0.01	0.01
64	1	0.09	-0.03	0.02
65	6	0.07	-0.02	0.02
66	1	0.06	-0.01	0.02
67	1	0.07	-0.02	0.03
68	1	0.06	-0.01	0.02
69	6	0.09	-0.01	0.01
70	1	0.09	-0.01	0.02
71	1	0.08	-0.01	0.01
72	1	0.09	-0.01	0.01
73	6	0.05	0.01	-0.03
74	1	0.04	0.01	-0.03
75	1	0.06	0.02	-0.04
76	1	0.05	0.01	-0.04
77	6	0.05	0.00	0.00
78	1	0.04	0.00	0.00
79	1	0.06	-0.01	0.01
80	1	0.04	0.00	0.01
81	6	0.08	0.00	-0.01
82	1	0.09	0.00	0.00
83	1	0.07	0.00	-0.02
84	1	0.09	0.01	-0.03
85	46	-0.17	-0.05	0.03
86	15	-0.13	0.00	0.01
87	6	-0.13	0.00	0.01
88	6	-0.13	0.02	0.00
89	6	-0.10	-0.01	0.02
90	1	-0.14	-0.01	0.01
91	6	-0.12	0.02	0.00
92	1	-0.12	0.04	0.00
93	1	-0.14	0.02	-0.01
94	6	-0.09	-0.01	0.02
95	1	-0.09	0.01	0.02
96	1	-0.10	-0.02	0.02

97	6	−0.09	0.01	0.02
98	1	−0.12	0.04	0.00
99	1	−0.13	0.01	0.00
100	1	−0.07	−0.01	0.03
101	1	−0.10	−0.02	0.02
102	1	−0.08	0.01	0.02
103	1	−0.08	0.03	0.02
104	6	−0.13	0.00	0.01
105	6	−0.13	0.00	0.02
106	6	−0.12	−0.01	0.01
107	1	−0.13	0.00	0.00
108	6	−0.12	−0.01	0.01
109	1	−0.13	−0.01	0.03
110	1	−0.14	0.01	0.02
111	6	−0.10	−0.02	0.00
112	1	−0.12	−0.02	0.01
113	1	−0.11	0.00	0.00
114	6	−0.10	−0.02	0.00
115	1	−0.12	−0.01	0.02
116	1	−0.12	0.00	0.00
117	1	−0.09	−0.02	−0.01
118	1	−0.10	−0.01	−0.01
119	1	−0.09	−0.02	0.00
120	1	−0.10	−0.03	0.02
121	6	−0.11	0.00	0.01
122	6	−0.09	−0.02	0.01
123	6	−0.10	0.01	−0.01
124	1	−0.12	−0.01	0.01
125	6	−0.08	−0.02	0.01
126	1	−0.09	−0.02	0.01
127	1	−0.10	−0.03	0.03
128	6	−0.09	0.01	−0.01
129	1	−0.10	0.01	−0.01
130	1	−0.12	0.02	−0.01
131	6	−0.07	0.00	−0.01
132	1	−0.07	−0.02	0.02
133	1	−0.08	−0.02	0.01
134	1	−0.08	0.02	−0.03
135	1	−0.09	0.01	−0.01
136	1	−0.06	0.00	−0.01

137	1	-0.06	0.00	-0.01

TS-PdPCy$_3$-Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-1.475877	1.164681	0.948987
82	-1.872063	-1.621168	0.068319
6	-3.535021	-0.999903	-1.509326
6	-3.049342	0.419186	-2.020876
6	-3.440256	1.727175	-1.236216
6	-2.263987	2.617362	-0.623781
1	-1.956036	0.390672	-2.112914
1	-3.410203	0.557399	-3.055538
1	-4.021739	2.362933	-1.922117
1	-4.140559	1.464824	-0.432245
6	-2.791229	-2.725434	1.821481
6	-3.144441	-2.161290	3.077085
6	-2.828561	-4.141751	1.715871
6	-3.494772	-2.972884	4.176843
1	-3.152283	-1.080766	3.210517
6	-3.186501	-4.958104	2.808102
1	-2.567608	-4.629868	0.776391
6	-3.510482	-4.375281	4.048121
1	-3.751074	-2.511613	5.129294
1	-3.199687	-6.040319	2.692267
1	-3.767936	-5.002889	4.898766
6	0.018455	1.945732	2.379901
6	0.835325	3.089726	2.214859
6	0.170334	1.180559	3.566407
6	1.774931	3.457383	3.196480
1	0.757517	3.690134	1.315114
6	1.101161	1.550800	4.556877
1	-0.431395	0.284636	3.725202
6	1.907547	2.690624	4.371014
1	2.399157	4.334823	3.041462
1	1.198622	0.952161	5.460173

1	2.631379	2.977045	5.130700
14	-3.116797	4.040038	0.408633
14	-1.058441	3.291744	-1.983236
14	-5.384526	-1.074790	-0.960270
14	-3.122076	-2.266774	-2.926340
6	-1.985546	5.516087	0.811933
1	-1.096190	5.211513	1.376637
1	-1.657762	6.057070	-0.083829
1	-2.544702	6.224552	1.439572
6	-4.664253	4.710196	-0.481667
1	-5.443633	3.943361	-0.576342
1	-5.087555	5.538927	0.104197
1	-4.439705	5.090628	-1.485021
6	-3.728113	3.381549	2.101704
1	-2.905453	3.187451	2.805228
1	-4.358568	4.153145	2.568161
1	-4.344456	2.475357	2.024552
6	0.517438	4.108685	-1.293196
1	1.040678	4.593716	-2.130157
1	0.331125	4.873370	-0.533297
1	1.200349	3.354070	-0.880054
6	-1.982136	4.582384	-3.047330
1	-2.225856	5.490826	-2.481821
1	-1.355589	4.879571	-3.900008
1	-2.918998	4.175096	-3.450841
6	-0.370930	1.998206	-3.204489
1	0.160812	1.178459	-2.701744
1	-1.136962	1.564897	-3.857001
1	0.360596	2.510563	-3.847083
6	-5.790537	-0.359215	0.763501
1	-5.258077	-0.895113	1.558012
1	-5.568348	0.710888	0.856390
1	-6.869029	-0.482676	0.944882
6	-6.477114	-0.111859	-2.205568
1	-6.397504	-0.517885	-3.221385
1	-7.532951	-0.175086	-1.903642
1	-6.209023	0.952390	-2.246992
6	-6.037165	-2.865254	-0.894077
1	-7.090653	-2.848722	-0.579264
1	-5.994374	-3.377617	-1.862990

1	-5.485587	-3.466747	-0.159922
6	-1.430014	-1.853593	-3.705812
1	-1.445882	-0.907538	-4.261025
1	-0.630816	-1.786583	-2.955890
1	-1.151924	-2.648715	-4.412355
6	-4.383985	-2.249472	-4.359723
1	-4.009194	-2.879612	-5.179148
1	-5.366827	-2.636315	-4.063795
1	-4.526765	-1.237112	-4.760861
6	-2.974989	-4.061682	-2.287990
1	-3.833345	-4.377446	-1.685836
1	-2.897533	-4.745239	-3.145566
1	-2.063390	-4.205288	-1.689087
46	2.065576	-0.442416	-0.448864
15	4.464464	-0.320699	-0.348664
6	5.220024	-1.680818	-1.511048
6	6.750054	-1.761004	-1.757301
6	4.666869	-3.073217	-1.108364
1	4.750332	-1.414165	-2.471469
6	7.065609	-2.820558	-2.848396
1	7.274594	-2.036997	-0.833355
1	7.149728	-0.790624	-2.077147
6	4.977159	-4.130575	-2.192879
1	5.121731	-3.390811	-0.156855
1	3.583075	-3.003962	-0.942776
6	6.491489	-4.210933	-2.490538
1	8.153904	-2.888047	-2.995068
1	6.635865	-2.489172	-3.807241
1	4.598933	-5.112656	-1.874345
1	4.437262	-3.864939	-3.115641
1	6.679832	-4.919289	-3.310476
1	7.015021	-4.604248	-1.604214
6	5.226017	1.377123	-0.906024
6	6.689593	1.710827	-0.514163
6	5.003064	1.601810	-2.423356
1	4.578305	2.089348	-0.370052
6	7.043971	3.165606	-0.920108
1	7.388165	1.023228	-1.010846
1	6.839165	1.596864	0.567173
6	5.358519	3.052050	-2.830633

1	5.634589	0.906196	-2.998079
1	3.958365	1.380196	-2.681870
6	6.805106	3.418484	-2.426399
1	8.091895	3.378465	-0.661784
1	6.423894	3.863402	-0.334969
1	5.223582	3.178186	-3.914626
1	4.657929	3.745159	-2.338758
1	7.011375	4.470756	-2.670539
1	7.512385	2.811470	-3.014349
6	5.125865	-0.547575	1.463727
6	4.106591	-1.361658	2.302951
6	6.553654	-1.119191	1.668658
1	5.118237	0.487194	1.847649
6	4.484711	-1.366433	3.802034
1	4.076511	-2.397893	1.931993
1	3.100122	-0.947963	2.157946
6	6.940006	-1.108776	3.171336
1	6.588443	-2.157317	1.308005
1	7.297982	-0.554734	1.095122
6	5.920019	-1.893243	4.027466
1	3.762848	-1.978219	4.362054
1	4.406072	-0.340577	4.196120
1	7.947314	-1.532587	3.297955
1	6.986126	-0.066837	3.527360
1	6.187518	-1.827367	5.092165
1	5.962405	-2.959989	3.754244

	1
	A
Frequencies --	-41.8692
Red. masses --	11.4128
Frc consts --	0.0068
IR Inten --	0.1337

Atom	AN	X	Y	Z
1	82	0.06	0.01	-0.02
2	82	0.08	0.01	-0.02
3	6	0.06	0.00	0.00
4	6	0.04	0.00	-0.01
5	6	0.04	0.00	0.00

6	6	0.03	0.01	0.00
7	1	0.04	0.01	-0.02
8	1	0.03	0.00	0.00
9	1	0.03	0.00	0.00
10	1	0.04	-0.01	0.00
11	6	0.09	0.01	-0.01
12	6	0.08	0.01	-0.01
13	6	0.07	0.01	-0.02
14	6	0.07	0.01	-0.02
15	1	0.09	0.01	-0.01
16	6	0.05	0.01	-0.02
17	1	0.07	0.01	-0.01
18	6	0.05	0.01	-0.02
19	1	0.06	0.01	-0.02
20	1	0.04	0.01	-0.02
21	1	0.04	0.01	-0.02
22	6	0.02	0.03	0.01
23	6	0.02	0.03	0.02
24	6	0.02	0.03	0.01
25	6	0.00	0.04	0.03
26	1	0.02	0.03	0.02
27	6	0.00	0.04	0.02
28	1	0.02	0.02	0.01
29	6	-0.01	0.04	0.03
30	1	0.00	0.05	0.04
31	1	-0.01	0.04	0.03
32	1	-0.02	0.05	0.04
33	14	0.02	0.00	0.01
34	14	0.02	0.02	0.00
35	14	0.06	-0.01	0.01
36	14	0.06	0.00	-0.01
37	6	0.01	0.01	0.01
38	1	0.01	0.01	0.01
39	1	0.01	0.01	0.01
40	1	0.00	0.00	0.01
41	6	0.02	-0.01	0.01
42	1	0.02	-0.02	0.01
43	1	0.01	-0.02	0.01
44	1	0.01	-0.01	0.01
45	6	0.03	-0.01	0.00

46	1	0.03	-0.01	0.00
47	1	0.02	-0.02	0.01
48	1	0.04	-0.02	0.00
49	6	0.02	0.03	0.00
50	1	0.02	0.03	0.00
51	1	0.01	0.03	0.00
52	1	0.02	0.03	0.01
53	6	0.01	0.02	0.01
54	1	0.00	0.01	0.01
55	1	0.01	0.03	0.01
56	1	0.02	0.01	0.00
57	6	0.03	0.03	-0.01
58	1	0.04	0.03	-0.01
59	1	0.03	0.03	-0.01
60	1	0.02	0.04	-0.01
61	6	0.07	-0.01	0.01
62	1	0.07	-0.01	0.01
63	1	0.06	-0.01	0.01
64	1	0.07	-0.02	0.02
65	6	0.05	-0.02	0.02
66	1	0.05	-0.02	0.02
67	1	0.05	-0.02	0.02
68	1	0.05	-0.01	0.01
69	6	0.07	-0.01	0.01
70	1	0.07	-0.02	0.02
71	1	0.07	-0.01	0.01
72	1	0.08	-0.01	0.01
73	6	0.05	0.01	-0.02
74	1	0.03	0.02	-0.02
75	1	0.05	0.02	-0.03
76	1	0.04	0.02	-0.03
77	6	0.04	0.00	0.00
78	1	0.04	0.00	0.00
79	1	0.05	-0.01	0.01
80	1	0.03	0.00	0.00
81	6	0.07	0.00	-0.01
82	1	0.08	0.00	0.00
83	1	0.06	0.01	-0.01
84	1	0.08	0.01	-0.02
85	46	-0.16	-0.06	0.04

86	15	−0.14	−0.01	0.02
87	6	−0.13	0.00	0.01
88	6	−0.13	0.03	−0.01
89	6	−0.10	−0.01	0.03
90	1	−0.15	−0.02	0.02
91	6	−0.12	0.03	−0.01
92	1	−0.11	0.04	−0.01
93	1	−0.16	0.03	−0.02
94	6	−0.09	−0.01	0.03
95	1	−0.08	0.00	0.02
96	1	−0.10	−0.03	0.04
97	6	−0.09	0.02	0.01
98	1	−0.12	0.05	−0.02
99	1	−0.14	0.01	0.00
100	1	−0.07	−0.02	0.04
101	1	−0.10	−0.03	0.03
102	1	−0.09	0.01	0.02
103	1	−0.07	0.03	0.01
104	6	−0.14	−0.01	0.01
105	6	−0.15	0.00	0.02
106	6	−0.13	−0.01	0.01
107	1	−0.15	0.00	0.00
108	6	−0.14	0.00	0.01
109	1	−0.14	−0.01	0.03
110	1	−0.16	0.01	0.02
111	6	−0.13	−0.02	0.00
112	1	−0.13	−0.02	0.02
113	1	−0.13	−0.01	0.00
114	6	−0.13	−0.02	0.01
115	1	−0.14	0.00	0.02
116	1	−0.14	0.00	0.00
117	1	−0.12	−0.02	0.00
118	1	−0.13	−0.01	−0.01
119	1	−0.12	−0.02	0.00
120	1	−0.12	−0.02	0.02
121	6	−0.12	−0.01	0.01
122	6	−0.10	−0.02	0.02
123	6	−0.11	0.01	−0.01
124	1	−0.12	−0.01	0.01
125	6	−0.08	−0.02	0.01

126	1	-0.09	-0.02	0.01
127	1	-0.11	-0.03	0.03
128	6	-0.09	0.01	-0.01
129	1	-0.10	0.01	-0.01
130	1	-0.12	0.01	-0.01
131	6	-0.08	-0.01	0.00
132	1	-0.07	-0.03	0.02
133	1	-0.09	-0.02	0.02
134	1	-0.09	0.02	-0.02
135	1	-0.10	0.01	-0.01
136	1	-0.07	-0.01	0.00
137	1	-0.07	-0.01	-0.01

Pro-PdPCy$_3$-C

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.854132	-0.666317	0.370726
6	1.973077	0.757606	0.293606
6	2.487505	1.518989	-0.972737
6	2.408821	0.535873	-2.185248
6	3.066660	-0.827255	-1.893254
6	2.319367	-1.658274	-0.783802
1	1.358628	0.371393	-2.435115
1	2.878340	0.979734	-3.071773
1	3.123126	-1.408334	-2.824382
1	4.109107	-0.650692	-1.591371
6	1.848944	1.589821	1.578168
6	2.993395	2.058999	2.269222
6	0.593437	1.920312	2.140215
6	2.891188	2.804864	3.457342
1	3.985297	1.816884	1.910007
6	0.477808	2.670834	3.322806
1	-0.302574	1.561843	1.634291
6	1.629241	3.120725	3.994736
1	3.798988	3.125012	3.966241
1	-0.511474	2.900675	3.715890

1	1.546940	3.697027	4.913469
6	1.697205	-1.306582	1.754386
6	0.611790	-2.152338	2.078543
6	2.671758	-1.111848	2.762640
6	0.504686	-2.776990	3.333076
1	-0.172110	-2.296768	1.349600
6	2.576374	-1.732720	4.020378
1	3.515019	-0.460045	2.572287
6	1.491372	-2.577415	4.315689
1	-0.351962	-3.414450	3.541210
1	3.350156	-1.554351	4.764099
1	1.412827	-3.061313	5.286454
14	3.652043	-3.035251	-0.190211
14	0.877267	-2.644713	-1.760410
14	4.376050	2.159098	-0.865747
14	1.383385	3.078443	-1.535582
6	2.876348	-4.519679	0.714194
1	2.358660	-4.220186	1.631299
1	2.166885	-5.073968	0.087579
1	3.679726	-5.216722	0.994187
6	4.627928	-3.724839	-1.687422
1	5.002905	-2.929435	-2.344231
1	5.506221	-4.250185	-1.283849
1	4.074264	-4.438092	-2.300870
6	5.107466	-2.424450	0.882321
1	5.682952	-3.323080	1.151426
1	5.778105	-1.769260	0.316390
1	4.828754	-1.924989	1.809770
6	-0.463244	-3.573945	-0.769470
1	-1.001629	-4.216241	-1.483155
1	-0.050496	-4.219738	0.013241
1	-1.191467	-2.893900	-0.315297
6	1.596213	-4.025591	-2.876906
1	1.944264	-4.906213	-2.325509
1	0.771533	-4.353019	-3.528156
1	2.406775	-3.682008	-3.529452
6	-0.023786	-1.575093	-3.054274
1	-0.509302	-0.700481	-2.611241
1	0.654366	-1.243731	-3.851075
1	-0.795918	-2.204042	-3.519987

6	5.577185	1.018483	0.088530
1	5.135414	0.457655	0.916732
1	6.018642	0.286742	-0.600827
1	6.402469	1.625115	0.492056
6	5.157430	2.216238	-2.606899
1	4.637631	2.879397	-3.304030
1	6.187919	2.587211	-2.501558
1	5.215947	1.219281	-3.062443
6	4.570487	3.913215	-0.138809
1	5.643228	4.112918	-0.001154
1	4.177657	4.687183	-0.808504
1	4.080425	4.027549	0.833325
6	-0.307384	2.532349	-2.210016
1	-0.220506	2.045902	-3.190841
1	-0.803036	1.831334	-1.523243
1	-0.944468	3.421497	-2.331665
6	2.179287	3.957416	-3.037375
1	1.435946	4.670334	-3.424114
1	3.085918	4.526230	-2.804299
1	2.409866	3.259424	-3.852522
6	1.052630	4.428861	-0.238957
1	1.964932	4.821599	0.222158
1	0.549816	5.265225	-0.749731
1	0.397000	4.079996	0.565141
46	-0.381618	-0.004461	-0.031261
15	-2.840027	-0.038689	-0.116187
6	-3.704203	1.696450	-0.121337
6	-5.229813	1.765305	-0.385438
6	-3.347771	2.506078	1.152999
1	-3.201285	2.191497	-0.966674
6	-5.686473	3.238980	-0.534434
1	-5.777871	1.307332	0.446766
1	-5.498336	1.207581	-1.290125
6	-3.809343	3.978115	1.025937
1	-3.837864	2.052544	2.028007
1	-2.266921	2.470198	1.333863
6	-5.319221	4.075444	0.712349
1	-6.771471	3.275696	-0.709641
1	-5.204347	3.679822	-1.421603
1	-3.577812	4.521024	1.953715

1	-3.236912	4.465988	0.221448
1	-5.608105	5.125647	0.563508
1	-5.893642	3.706786	1.577560
6	-3.422705	-0.915180	-1.753843
6	-4.759097	-1.697222	-1.763182
6	-3.344007	0.058572	-2.960668
1	-2.626892	-1.660768	-1.887183
6	-4.928433	-2.455583	-3.104117
1	-5.610536	-1.015301	-1.626834
1	-4.784732	-2.419866	-0.937446
6	-3.543330	-0.684768	-4.303235
1	-4.122188	0.829304	-2.868655
1	-2.379207	0.579618	-2.968706
6	-4.856526	-1.497969	-4.314952
1	-5.883379	-3.000577	-3.104891
1	-4.130528	-3.210514	-3.192728
1	-3.537368	0.040847	-5.129527
1	-2.693919	-1.362482	-4.472604
1	-4.940734	-2.065906	-5.252511
1	-5.714182	-0.806983	-4.282031
6	-3.573604	-1.101521	1.329769
6	-2.812215	-0.838449	2.657403
6	-5.097533	-1.054663	1.609703
1	-3.323721	-2.127049	1.005627
6	-3.180528	-1.897564	3.723236
1	-3.079983	0.159402	3.037128
1	-1.731272	-0.829982	2.485725
6	-5.484895	-2.135571	2.650691
1	-5.359228	-0.068361	2.018684
1	-5.684295	-1.190693	0.696440
6	-4.704574	-1.954476	3.973065
1	-2.647804	-1.680563	4.659890
1	-2.832463	-2.885863	3.381939
1	-6.567312	-2.097380	2.841567
1	-5.270580	-3.132731	2.233077
1	-4.945417	-2.770111	4.670015
1	-5.027308	-1.017965	4.455736

Pro-PdPCy$_3$-Si

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.475228	-1.039892	0.702433
14	1.609376	1.181483	0.480140
6	2.729438	1.690881	-1.016420
6	2.924843	0.356136	-1.858507
6	3.619765	-0.867571	-1.166930
6	2.717755	-1.981177	-0.466073
1	1.946911	0.034346	-2.224234
1	3.519369	0.602079	-2.750996
1	4.226077	-1.370844	-1.935617
1	4.334441	-0.478993	-0.429184
6	1.204387	2.416664	1.871524
6	2.164332	3.273926	2.469920
6	-0.119007	2.472836	2.384911
6	1.819388	4.148612	3.517886
1	3.197003	3.256215	2.137588
6	-0.468958	3.341281	3.434931
1	-0.875334	1.820153	1.954367
6	0.499118	4.189678	4.005327
1	2.581558	4.790805	3.954729
1	-1.493095	3.356858	3.803294
1	0.231677	4.865845	4.814419
6	0.911948	-1.813961	2.347623
6	0.302512	-3.091461	2.441602
6	1.043600	-1.066772	3.548876
6	-0.140448	-3.607197	3.674905
1	0.159392	-3.691103	1.547944
6	0.595611	-1.573637	4.782656
1	1.503210	-0.081914	3.521317
6	0.004836	-2.850549	4.853358
1	-0.596406	-4.594751	3.713457
1	0.713600	-0.975121	5.683571
1	-0.333722	-3.248141	5.807803
14	3.984766	-3.033670	0.609390
14	1.867001	-3.088229	-1.824666
14	4.480134	2.411195	-0.534661

14	1.760959	2.916869	-2.195399
6	3.344030	-4.754991	1.113489
1	2.434173	-4.693389	1.720700
1	3.145803	-5.406236	0.253637
1	4.114162	-5.246121	1.725791
6	5.615145	-3.296076	-0.350005
1	6.124761	-2.345647	-0.553070
1	6.290887	-3.903985	0.269151
1	5.477482	-3.819005	-1.302004
6	4.472580	-2.125170	2.209196
1	5.347922	-2.623639	2.650948
1	4.743521	-1.078502	2.028522
1	3.667799	-2.140418	2.951988
6	0.474191	-4.175027	-1.111917
1	0.049500	-4.788543	-1.919490
1	0.831980	-4.857310	-0.332255
1	-0.338265	-3.564939	-0.696330
6	3.115071	-4.252480	-2.685350
1	3.524964	-5.022394	-2.021533
1	2.600905	-4.766258	-3.510758
1	3.955338	-3.695778	-3.121289
6	1.106393	-2.107362	-3.271573
1	0.416811	-1.323711	-2.943380
1	1.877155	-1.644215	-3.901061
1	0.541618	-2.809577	-3.902923
6	5.215566	1.651909	1.060257
1	5.882882	2.378018	1.546180
1	4.454258	1.353167	1.789990
1	5.815564	0.762287	0.828351
6	5.740087	2.045473	-1.919892
1	5.443971	2.481175	-2.881202
1	6.714244	2.475257	-1.644827
1	5.885426	0.967560	-2.066403
6	4.486124	4.303852	-0.283862
1	5.489781	4.607158	0.047732
1	4.268707	4.849522	-1.209517
1	3.770514	4.637659	0.475662
6	0.312003	2.024093	-3.052170
1	0.654396	1.356078	-3.853324
1	-0.266892	1.422294	-2.334594

1	-0.361702	2.768499	-3.501594
6	2.864406	3.556510	-3.618903
1	2.239813	4.124609	-4.323544
1	3.669332	4.220850	-3.283815
1	3.317943	2.728620	-4.180070
6	1.030505	4.411594	-1.273316
1	1.790691	5.007564	-0.757403
1	0.522174	5.068698	-1.994109
1	0.290847	4.098646	-0.525635
46	-0.510886	0.076170	-0.203755
15	-3.065157	-0.124311	-0.387956
6	-3.819147	1.582500	-0.947111
6	-5.357110	1.785748	-1.001105
6	-3.154473	2.738124	-0.142783
1	-3.439687	1.646722	-1.982592
6	-5.700368	3.172709	-1.605275
1	-5.783345	1.727842	0.010595
1	-5.839285	1.006331	-1.596509
6	-3.527023	4.132142	-0.700002
1	-3.483639	2.690133	0.903876
1	-2.062999	2.616319	-0.138104
6	-5.058440	4.318019	-0.791449
1	-6.792531	3.296203	-1.649296
1	-5.331685	3.216882	-2.643852
1	-3.086854	4.907207	-0.054983
1	-3.083393	4.260266	-1.700288
1	-5.296392	5.291052	-1.244478
1	-5.489744	4.325047	0.223708
6	-3.638138	-1.463553	-1.672576
6	-5.059724	-1.342660	-2.274727
6	-2.593313	-1.597563	-2.808021
1	-3.594885	-2.395511	-1.088441
6	-5.389310	-2.554459	-3.181508
1	-5.114431	-0.431392	-2.887989
1	-5.818903	-1.253717	-1.487871
6	-2.913822	-2.804340	-3.722435
1	-2.573543	-0.675832	-3.411864
1	-1.594631	-1.710814	-2.374130
6	-4.341828	-2.718381	-4.305653
1	-6.393219	-2.427468	-3.612641

1	-5.417662	-3.471101	-2.571231
1	-2.173246	-2.861361	-4.532749
1	-2.817174	-3.732894	-3.136486
1	-4.564251	-3.613211	-4.904205
1	-4.403643	-1.854754	-4.987258
6	-3.808566	-0.710854	1.329533
6	-4.259327	0.457172	2.245947
6	-4.894724	-1.815598	1.283809
1	-2.914426	-1.155792	1.792759
6	-4.637980	-0.034785	3.664613
1	-5.130619	0.960503	1.802941
1	-3.459063	1.202747	2.331770
6	-5.219596	-2.317059	2.713274
1	-5.814650	-1.429641	0.817372
1	-4.556660	-2.668159	0.680175
6	-5.694528	-1.160634	3.620361
1	-5.012152	0.815830	4.254241
1	-3.734104	-0.404007	4.173531
1	-5.982667	-3.107541	2.664237
1	-4.314742	-2.770915	3.149613
1	-5.897356	-1.529053	4.635957
1	-6.644753	-0.760354	3.229361

Pro-PdPCy$_3$-Ge

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-1.175464	1.086296	0.727110
32	-1.690913	-1.192125	0.288747
6	-2.953741	-1.255182	-1.302759
6	-2.786586	0.158662	-2.002834
6	-3.249082	1.450332	-1.244635
6	-2.155884	2.358681	-0.517250
1	-1.733778	0.280838	-2.270163
1	-3.339515	0.127718	-2.955114
1	-3.767474	2.088692	-1.975990
1	-4.011371	1.163320	-0.510366

6	-1.937729	-2.460677	1.801385
6	-2.649286	-2.086173	2.970907
6	-1.358148	-3.754928	1.778552
6	-2.790239	-2.968031	4.060475
1	-3.095256	-1.096061	3.037057
6	-1.498530	-4.642803	2.862949
1	-0.782471	-4.075746	0.914766
6	-2.218055	-4.253349	4.009126
1	-3.343943	-2.650806	4.941827
1	-1.044234	-5.630330	2.813138
1	-2.327005	-4.937383	4.848009
6	-0.311254	1.757232	2.377783
6	0.359713	3.001349	2.480191
6	-0.321536	0.922810	3.527210
6	0.981863	3.403051	3.678681
1	0.415703	3.662053	1.621628
6	0.301443	1.318230	4.725413
1	-0.814509	-0.045420	3.489655
6	0.953829	2.564338	4.808703
1	1.485223	4.366827	3.726786
1	0.274118	0.656767	5.588932
1	1.431079	2.874242	5.735827
14	-3.218134	3.614028	0.564908
14	-1.052637	3.283984	-1.819749
14	-4.803623	-1.637339	-0.843905
14	-2.251034	-2.544240	-2.597661
6	-2.315305	5.209377	1.084769
1	-1.446634	5.010023	1.721278
1	-1.990262	5.813123	0.228851
1	-3.016052	5.821848	1.670490
6	-4.774054	4.161751	-0.397567
1	-5.446487	3.319924	-0.603756
1	-5.330463	4.883256	0.218250
1	-4.537203	4.649698	-1.349447
6	-3.851196	2.788699	2.161900
1	-3.046177	2.617649	2.886435
1	-4.592906	3.448058	2.636140
1	-4.340312	1.826329	1.967153
6	0.441319	4.150579	-1.019612
1	0.998414	4.690750	-1.798249

1	0.155427	4.879636	-0.253852
1	1.124275	3.418351	-0.570067
6	-2.064659	4.609308	-2.753866
1	-2.377545	5.441073	-2.111274
1	-1.447883	5.028923	-3.561662
1	-2.964222	4.182194	-3.217004
6	-0.323330	2.171585	-3.183853
1	0.230500	1.319580	-2.771087
1	-1.090972	1.785452	-3.865792
1	0.375734	2.774954	-3.782397
6	-5.446931	-0.835433	0.762952
1	-4.838490	-1.102028	1.633054
1	-5.502498	0.257765	0.704490
1	-6.466363	-1.206241	0.946763
6	-5.964530	-1.006303	-2.222260
1	-5.761734	-1.468236	-3.194525
1	-7.006347	-1.234135	-1.954236
1	-5.887274	0.082760	-2.342254
6	-5.090666	-3.505034	-0.597021
1	-6.141690	-3.674176	-0.322639
1	-4.884172	-4.098481	-1.495385
1	-4.470438	-3.894608	0.221002
6	-0.675833	-1.872339	-3.432944
1	-0.894997	-1.080270	-4.160440
1	0.027391	-1.466717	-2.690815
1	-0.173640	-2.690073	-3.970650
6	-3.480277	-2.882248	-4.022760
1	-2.976196	-3.496440	-4.782999
1	-4.376006	-3.426170	-3.699064
1	-3.804176	-1.954943	-4.513485
6	-1.774932	-4.224476	-1.838045
1	-2.524754	-4.622293	-1.146660
1	-1.639954	-4.957661	-2.646470
1	-0.820048	-4.148806	-1.302028
46	0.639848	-0.464814	-0.240339
15	3.172213	-0.148248	-0.293956
6	3.888602	-1.455981	-1.529328
6	5.406779	-1.479431	-1.839819
6	3.385762	-2.874190	-1.145600
1	3.371444	-1.176416	-2.461852

6	5.716741	-2.501290	-2.963815
1	5.975281	-1.755663	-0.943342
1	5.754584	-0.486028	-2.147728
6	3.706165	-3.901752	-2.257229
1	3.866091	-3.197288	-0.209400
1	2.302367	-2.850421	-0.957091
6	5.213471	-3.916469	-2.599747
1	6.799130	-2.521173	-3.157462
1	5.231758	-2.173290	-3.897062
1	3.377616	-4.903006	-1.943486
1	3.130252	-3.645471	-3.160373
1	5.406467	-4.612582	-3.428399
1	5.779731	-4.289893	-1.731303
6	3.889051	1.569134	-0.834538
6	5.341799	1.916314	-0.421593
6	3.675380	1.796007	-2.354132
1	3.224887	2.267168	-0.299631
6	5.701717	3.365630	-0.834703
1	6.049934	1.224457	-0.898144
1	5.466943	1.810956	0.663401
6	4.048782	3.239937	-2.767065
1	4.300789	1.093707	-2.925494
1	2.631918	1.589591	-2.624185
6	5.492814	3.595992	-2.348587
1	6.743513	3.580570	-0.555929
1	5.068652	4.069573	-0.271508
1	3.927525	3.356018	-3.853779
1	3.350532	3.944358	-2.290569
1	5.715516	4.640914	-2.607443
1	6.201860	2.969541	-2.913554
6	3.898212	-0.436086	1.479483
6	2.935560	-1.312065	2.326357
6	5.345176	-0.978512	1.600136
1	3.877201	0.579684	1.909699
6	3.381821	-1.364725	3.806412
1	2.915224	-2.334168	1.916798
1	1.912754	-0.923138	2.251793
6	5.799609	-1.009982	3.081274
1	5.383847	-2.002870	1.201930
1	6.048531	-0.378365	1.012572

6	4.840328	-1.854073	3.950424
1	2.703724	-2.020615	4.370856
1	3.287126	-0.358738	4.244483
1	6.822546	-1.409159	3.145937
1	5.833744	0.019806	3.471769
1	5.152007	-1.817266	5.004248
1	4.903034	-2.908732	3.636639

Pro–PdPCy$_3$–Sn

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	-0.763448	1.150871	0.848798
50	-1.703999	-1.415846	0.220007
6	-3.269698	-0.905881	-1.282347
6	-2.814255	0.507110	-1.846291
6	-3.057349	1.787467	-0.969553
6	-1.798639	2.627195	-0.460464
1	-1.747650	0.446265	-2.090634
1	-3.323471	0.672815	-2.810421
1	-3.702062	2.466434	-1.547703
1	-3.649366	1.495558	-0.093873
6	-2.344487	-2.588234	1.923188
6	-2.583202	-2.017747	3.201487
6	-2.472947	-3.997420	1.803623
6	-2.935225	-2.816340	4.308310
1	-2.502716	-0.940930	3.337258
6	-2.833399	-4.799378	2.905108
1	-2.283983	-4.486661	0.849255
6	-3.064691	-4.210896	4.163194
1	-3.113458	-2.349286	5.275059
1	-2.927243	-5.876481	2.780542
1	-3.340988	-4.828367	5.015235
6	0.578842	1.953352	2.348276
6	1.399719	3.100548	2.199873
6	0.648994	1.256640	3.584484
6	2.248522	3.535691	3.237870

1	1.388170	3.665773	1.272800
6	1.492659	1.688126	4.626916
1	0.040274	0.366852	3.743286
6	2.296205	2.832226	4.456805
1	2.864409	4.421769	3.095448
1	1.518953	1.136078	5.564306
1	2.946723	3.170386	5.260574
14	-2.564482	3.993873	0.718126
14	-0.793974	3.396834	-1.920836
14	-5.089739	-0.930523	-0.618352
14	-2.998224	-2.168760	-2.746411
6	-1.437724	5.487868	1.074624
1	-0.485010	5.194303	1.529543
1	-1.226768	6.085295	0.179046
1	-1.954086	6.142363	1.791618
6	-4.183959	4.684156	-0.020812
1	-4.975895	3.925027	-0.046608
1	-4.541646	5.511026	0.609702
1	-4.053324	5.071859	-1.037574
6	-3.037184	3.265276	2.419541
1	-2.158943	3.033066	3.035360
1	-3.632524	4.009712	2.968657
1	-3.646096	2.355721	2.339582
6	0.828029	4.213755	-1.343834
1	1.299439	4.706508	-2.206145
1	0.676958	4.972722	-0.570020
1	1.537885	3.466462	-0.966245
6	-1.815116	4.736949	-2.825020
1	-2.012037	5.614224	-2.196115
1	-1.262446	5.081704	-3.710879
1	-2.781630	4.347468	-3.172357
6	-0.262338	2.167901	-3.278280
1	0.252259	1.288314	-2.871204
1	-1.108521	1.817138	-3.880962
1	0.434317	2.684986	-3.955212
6	-5.343663	-0.222459	1.135958
1	-4.721393	-0.734027	1.878554
1	-5.143054	0.853237	1.201920
1	-6.394421	-0.377241	1.423182
6	-6.226147	0.084225	-1.770565

1	-6.231870	-0.301644	-2.796559
1	-7.259098	0.051808	-1.394839
1	-5.922356	1.138895	-1.807922
6	-5.774544	-2.707123	-0.513647
1	-6.800437	-2.670459	-0.119868
1	-5.813363	-3.216163	-1.484124
1	-5.182463	-3.323980	0.175209
6	-1.381961	-1.780647	-3.679151
1	-1.444176	-0.845914	-4.250802
1	-0.530182	-1.700285	-2.990201
1	-1.169956	-2.592743	-4.390127
6	-4.389852	-2.083800	-4.053397
1	-4.113904	-2.710913	-4.913442
1	-5.354166	-2.444212	-3.675244
1	-4.534029	-1.060771	-4.425818
6	-2.849218	-3.977388	-2.157355
1	-3.665408	-4.285565	-1.495124
1	-2.858704	-4.644705	-3.031429
1	-1.896869	-4.143715	-1.634472
46	0.768580	-0.791207	-0.331841
15	3.250579	-0.472150	-0.406150
6	3.859814	-1.834974	-1.640417
6	5.361337	-1.923491	-2.015513
6	3.322402	-3.223073	-1.196379
1	3.311495	-1.557406	-2.555378
6	5.585320	-2.990274	-3.118239
1	5.959850	-2.191214	-1.136008
1	5.730262	-0.954169	-2.372195
6	3.556730	-4.291758	-2.289687
1	3.830321	-3.538839	-0.272595
1	2.249349	-3.154418	-0.963448
6	5.046704	-4.374590	-2.691186
1	6.657150	-3.055980	-3.355547
1	5.073485	-2.672183	-4.040438
1	3.203240	-5.269813	-1.933187
1	2.953938	-4.038554	-3.176093
1	5.180101	-5.100630	-3.505759
1	5.633900	-4.744241	-1.835156
6	4.013068	1.203275	-1.009989
6	5.491644	1.493676	-0.646866

6	3.763129	1.397875	−2.528873
1	3.398086	1.942525	−0.472171
6	5.911243	2.907706	−1.120150
1	6.152433	0.751064	−1.114906
1	5.639132	1.420476	0.437988
6	4.202259	2.804284	−3.002421
1	4.329657	0.645057	−3.096463
1	2.701186	1.240878	−2.760022
6	5.674600	3.095354	−2.635520
1	6.969268	3.079007	−0.874334
1	5.329097	3.661808	−0.567059
1	4.056434	2.887956	−4.089030
1	3.557951	3.563131	−2.535048
1	5.945255	4.116843	−2.938307
1	6.334054	2.411871	−3.194426
6	4.024810	−0.764541	1.346082
6	3.074380	−1.614702	2.232037
6	5.462594	−1.340819	1.417836
1	4.040345	0.253876	1.769924
6	3.573664	−1.669539	3.695087
1	3.013234	−2.637830	1.830559
1	2.059651	−1.200921	2.193382
6	5.969846	−1.374341	2.881432
1	5.461904	−2.367925	1.025594
1	6.157490	−0.761256	0.800778
6	5.024592	−2.192950	3.789001
1	2.901566	−2.305812	4.288737
1	3.520616	−0.658551	4.127710
1	6.985402	−1.795595	2.910766
1	6.039977	−0.343682	3.264393
1	5.374519	−2.158131	4.830764
1	5.051728	−3.250234	3.479375

Pro–PdPCy$_3$–Pb

Atomic Number	Coordinates (Angstroms) X	Y	Z

82	-0.672106	1.256544	0.870786
82	-1.537705	-1.552088	0.083469
6	-3.268331	-0.829328	-1.297598
6	-2.734085	0.548539	-1.871508
6	-2.963846	1.868073	-1.047353
6	-1.707478	2.741119	-0.597709
1	-1.660176	0.441311	-2.076387
1	-3.193922	0.709341	-2.863387
1	-3.625126	2.513787	-1.647654
1	-3.546607	1.620137	-0.150251
6	-2.183290	-2.733230	1.883483
6	-2.688936	-2.229608	3.109508
6	-1.950484	-4.131511	1.794663
6	-2.965106	-3.088887	4.193985
1	-2.865495	-1.162949	3.235491
6	-2.228421	-4.995406	2.873553
1	-1.537353	-4.563900	0.881852
6	-2.739563	-4.474856	4.078350
1	-3.354556	-2.676580	5.123471
1	-2.040697	-6.063177	2.773452
1	-2.953880	-5.137850	4.914095
6	0.751210	2.187423	2.342478
6	1.544789	3.352652	2.193932
6	0.842129	1.484992	3.573761
6	2.388677	3.800388	3.231662
1	1.517189	3.920253	1.268220
6	1.679857	1.929055	4.616833
1	0.255778	0.578388	3.730676
6	2.456214	3.091851	4.447710
1	2.985278	4.700246	3.092626
1	1.723608	1.372437	5.551159
1	3.102805	3.440443	5.250298
14	-2.449072	4.184076	0.484358
14	-0.629947	3.386652	-2.061189
14	-5.035976	-0.780832	-0.522856
14	-3.128795	-2.131128	-2.747408
6	-1.270522	5.641254	0.823799
1	-0.363317	5.327436	1.352600
1	-0.976180	6.172423	-0.089858
1	-1.792126	6.362722	1.469240

6	-4.010184	4.922686	-0.335213
1	-4.829528	4.194487	-0.393758
1	-4.366906	5.770274	0.268193
1	-3.814256	5.293911	-1.348457
6	-3.008350	3.548024	2.197948
1	-2.159785	3.296832	2.848517
1	-3.576846	4.342283	2.703681
1	-3.665906	2.671524	2.136537
6	1.018351	4.133480	-1.460255
1	1.558339	4.546254	-2.324635
1	0.880964	4.943734	-0.737160
1	1.661834	3.368620	-1.005621
6	-1.537295	4.749662	-3.051664
1	-1.692108	5.661232	-2.460570
1	-0.941434	5.023837	-3.934370
1	-2.518909	4.408972	-3.408218
6	-0.128319	2.072334	-3.349085
1	0.349897	1.197338	-2.888982
1	-0.978823	1.720741	-3.945709
1	0.595528	2.528936	-4.041061
6	-5.175117	-0.001657	1.214604
1	-4.479749	-0.459346	1.926513
1	-5.009814	1.081869	1.217102
1	-6.193812	-0.177008	1.592011
6	-6.228915	0.216626	-1.634737
1	-6.325815	-0.216558	-2.637069
1	-7.230346	0.236992	-1.180434
1	-5.896698	1.257404	-1.747272
6	-5.745265	-2.537292	-0.303548
1	-6.742986	-2.462808	0.152441
1	-5.855695	-3.085093	-1.246947
1	-5.121536	-3.137528	0.372146
6	-1.566449	-1.799543	-3.790939
1	-1.664954	-0.895329	-4.405888
1	-0.669978	-1.684239	-3.167075
1	-1.395908	-2.648257	-4.470231
6	-4.603078	-2.066484	-3.956945
1	-4.397471	-2.728179	-4.810958
1	-5.541895	-2.397840	-3.497162
1	-4.758458	-1.054160	-4.352927

6	-2.968731	-3.923612	-2.102850
1	-3.701671	-4.173310	-1.328157
1	-3.113441	-4.625204	-2.937143
1	-1.964700	-4.116994	-1.697726
46	0.946610	-0.761872	-0.391398
15	3.395621	-0.506919	-0.464924
6	3.986697	-1.918615	-1.655458
6	5.489348	-2.040720	-2.017734
6	3.425981	-3.285636	-1.177526
1	3.448259	-1.657607	-2.580947
6	5.701982	-3.138291	-3.092478
1	6.077284	-2.298125	-1.128123
1	5.877986	-1.087381	-2.395383
6	3.648824	-4.385667	-2.242078
1	3.924956	-3.585308	-0.243415
1	2.353788	-3.191080	-0.952533
6	5.138995	-4.502697	-2.634159
1	6.773992	-3.226996	-3.321308
1	5.200883	-2.835279	-4.025596
1	3.278184	-5.348668	-1.862569
1	3.054301	-4.145840	-3.137840
1	5.264469	-5.250832	-3.429795
1	5.716147	-4.860369	-1.766296
6	4.191204	1.134201	-1.118458
6	5.674467	1.403688	-0.756214
6	3.952278	1.285436	-2.643899
1	3.588931	1.902863	-0.608606
6	6.127021	2.792624	-1.271556
1	6.321433	0.632966	-1.197185
1	5.815206	1.361383	0.331200
6	4.423388	2.667160	-3.157631
1	4.505618	0.503890	-3.185105
1	2.888084	1.143981	-2.875123
6	5.900494	2.937376	-2.793161
1	7.187699	2.947590	-1.026178
1	5.559772	3.576307	-0.745074
1	4.284046	2.721096	-4.246974
1	3.793282	3.453077	-2.715785
1	6.195263	3.942498	-3.126546
1	6.546974	2.222255	-3.327272

6	4.154687	-0.756785	1.299575
6	3.178840	-1.546307	2.212756
6	5.574878	-1.371868	1.395252
1	4.200318	0.275318	1.685799
6	3.672747	-1.558560	3.678410
1	3.090806	-2.581562	1.849259
1	2.175779	-1.107028	2.153358
6	6.078267	-1.366140	2.860700
1	5.544966	-2.412137	1.040570
1	6.287776	-0.835375	0.759978
6	5.107334	-2.120541	3.796424
1	2.981108	-2.151543	4.293880
1	3.648224	-0.530457	4.071379
1	7.080400	-1.816832	2.908237
1	6.179581	-0.324440	3.204648
1	5.456559	-2.055578	4.836905
1	5.103364	-3.189385	3.528050
