

Supplementary Materials

A Mechanistic Analysis of the Tetrasilyl-Substituted Trimetallaallenes, $>\text{E}=\text{E}=\text{E}<$ ($\text{E} = \text{C}, \text{Si}, \text{Ge}, \text{Sn}, \text{and Pb}$)

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(All at the B3LYP/LANL2DZ level of theory)

>E=E=E<: (Singlet)
>C=C=C<

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.345298	-0.042620	-0.138644
6	-0.000153	-0.004143	-0.000123
6	1.344786	-0.042846	0.138585
14	-2.302387	-1.463447	0.925907
14	-2.374069	1.176731	-1.314869
14	2.373792	1.175667	1.315576
14	2.302026	-1.463048	-0.926677
6	-0.882628	-2.371853	1.803162
1	-0.267187	-2.913287	1.079105
1	-1.256487	-3.100905	2.529586
1	-0.230301	-1.669343	2.327067
6	-3.239715	-2.880094	-0.145668
6	-2.932071	-4.266827	0.508283
1	-3.469572	-5.048060	-0.051545
1	-3.257970	-4.327066	1.552627
1	-1.865263	-4.513892	0.472610
6	-4.791134	-2.758049	-0.204139
1	-5.129835	-1.823083	-0.656590
1	-5.257856	-2.845826	0.781870
1	-5.184528	-3.581587	-0.820855
6	-3.480689	-0.883598	2.429916
6	-3.919299	-2.150074	3.233798
1	-4.530347	-2.841381	2.646212
1	-4.526367	-1.826382	4.093333
1	-3.063055	-2.705650	3.634321
6	-4.776490	-0.109690	2.060109
1	-4.562960	0.855444	1.589097
1	-5.340635	0.102264	2.982430
1	-5.437102	-0.676319	1.397164
6	-2.735135	-2.967932	-1.610737
1	-2.983651	-2.077365	-2.190805
1	-3.212925	-3.828641	-2.105430
1	-1.653865	-3.113292	-1.671129
6	-2.686083	0.003388	3.425329
1	-2.403746	0.961493	2.983633
1	-1.776635	-0.491323	3.785068

1	-3.315248	0.215679	4.304483
6	-4.160817	0.531980	-1.428578
1	-4.751001	1.232204	-2.030383
1	-4.658136	0.443118	-0.461211
1	-4.208263	-0.439482	-1.925781
6	-2.531449	3.005639	-0.559035
6	-3.934149	3.604936	-0.882669
1	-4.131305	3.661939	-1.959671
1	-3.988261	4.629602	-0.482051
1	-4.744757	3.028618	-0.420740
6	-2.400548	2.962422	0.985262
1	-3.207378	2.377895	1.440867
1	-2.461720	3.982849	1.395523
1	-1.451593	2.522395	1.302201
6	-1.471336	4.002433	-1.104397
1	-1.631448	4.232093	-2.163699
1	-0.448019	3.636222	-0.991194
1	-1.545568	4.951116	-0.549706
6	-1.807920	1.235375	-3.201078
6	-1.928588	-0.168351	-3.859019
1	-1.593810	-0.106536	-4.906312
1	-2.963366	-0.533316	-3.870438
1	-1.309641	-0.918596	-3.357322
6	-2.729932	2.188335	-4.020631
1	-2.404786	2.180765	-5.073003
1	-2.682639	3.226475	-3.674367
1	-3.779839	1.869288	-4.002594
6	-0.343751	1.708446	-3.370721
1	-0.025340	1.581991	-4.417707
1	0.333921	1.122471	-2.747217
1	-0.216023	2.763991	-3.114585
6	3.238934	-2.880265	0.144428
6	0.882654	-2.370719	-1.805245
1	1.256725	-3.098857	-2.532474
1	0.230153	-1.667808	-2.328488
1	0.267103	-2.913161	-1.081995
6	3.481232	-0.882498	-2.429776
6	4.790341	-2.757979	0.203903
1	5.183448	-3.581355	0.820994
1	5.128252	-1.822798	0.656358
1	5.257771	-2.845817	-0.781766
6	2.931793	-4.266625	-0.510620
1	1.864984	-4.513798	-0.475701
1	3.469035	-5.048204	0.048984
1	3.258264	-4.326131	-1.554810
6	2.733800	-2.969291	1.609300

1	1.652595	-3.115023	1.669228
1	2.981953	-2.079145	2.190131
1	3.211640	-3.830311	2.103415
6	2.687093	0.004702	-3.425409
1	1.778058	-0.490182	-3.785909
1	3.316817	0.217375	-4.304070
1	2.404157	0.962598	-2.983715
6	3.920415	-2.148612	-3.234022
1	3.064471	-2.703949	-3.635519
1	4.531001	-2.840234	-2.646362
1	4.528134	-1.824466	-4.092929
6	4.776901	-0.108643	-2.059226
1	5.438145	-0.676247	-1.397755
1	4.563469	0.855612	-1.586465
1	5.340493	0.105040	-2.981491
6	1.807312	1.234393	3.201669
6	4.159769	0.529103	1.429644
1	4.654908	0.434474	0.461775
1	4.206526	-0.439894	1.931654
1	4.752302	1.231374	2.026687
6	2.532410	3.004471	0.559797
6	2.731419	2.184975	4.021700
1	3.780645	1.863754	4.003236
1	2.406413	2.177411	5.074117
1	2.686185	3.223448	3.676098
6	0.344138	1.710408	3.371838
1	-0.334853	1.126688	2.747630
1	0.218681	2.766544	3.117078
1	0.025446	1.583287	4.418663
6	1.925099	-0.169939	3.858938
1	1.305203	-0.918809	3.356426
1	1.589676	-0.108056	4.906029
1	2.959187	-0.536778	3.870955
6	3.935900	3.602512	0.882449
1	4.745607	3.025689	0.419591
1	4.134029	3.659007	1.959306
1	3.990524	4.627275	0.482142
6	2.400249	2.961831	-0.984404
1	1.450919	2.522205	-1.300724
1	3.206500	2.377261	-1.440863
1	2.461402	3.982411	-1.394287
6	1.473658	4.002151	1.106306
1	0.449886	3.636950	0.993903
1	1.548351	4.950892	0.551780
1	1.634944	4.231385	2.165520

>Si=Si=Si<

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-2.147672	-0.109043	0.087227
14	-0.006512	-0.013949	-0.190095
14	2.139938	0.055390	0.022973
14	-2.918222	1.660699	1.524380
14	-3.347181	-1.721438	-1.223077
14	3.325201	1.516279	-1.460427
14	2.936004	-1.429497	1.735495
6	-1.345014	2.463689	2.245508
1	-0.845750	1.789282	2.952157
1	-1.593647	3.391019	2.779938
1	-0.621140	2.705913	1.459874
6	-3.926696	0.935159	3.045809
6	-3.922510	1.960158	4.220467
1	-4.491349	1.544818	5.067233
1	-4.385955	2.915333	3.948676
1	-2.905467	2.165838	4.576545
6	-5.400820	0.598299	2.694925
1	-5.475892	-0.099190	1.851257
1	-5.979280	1.496161	2.442698
1	-5.889174	0.124903	3.561271
6	-3.860238	3.028597	0.483662
6	-4.467948	4.119276	1.413275
1	-5.283092	3.725429	2.032980
1	-4.885526	4.932073	0.798523
1	-3.716021	4.565369	2.078596
6	-4.998651	2.435248	-0.389715
1	-4.607394	1.712280	-1.115832
1	-5.489717	3.241648	-0.957141
1	-5.768577	1.935429	0.209897
6	-3.235203	-0.360886	3.555504
1	-3.293563	-1.169800	2.817505
1	-3.729029	-0.707467	4.476962
1	-2.173470	-0.199562	3.785545
6	-2.838980	3.722664	-0.464495
1	-2.351702	3.005399	-1.138060
1	-2.053948	4.248995	0.093249
1	-3.361593	4.466221	-1.086503
6	-5.203377	-1.517318	-0.816871
1	-5.791626	-2.301020	-1.313289
1	-5.587279	-0.547607	-1.155672

1	-5.392575	-1.594223	0.260008
6	-3.138927	-1.372539	-3.146255
6	-4.254300	-2.106412	-3.950040
1	-4.222587	-3.193923	-3.820184
1	-4.125207	-1.897533	-5.023516
1	-5.255996	-1.758886	-3.666384
6	-3.290940	0.149446	-3.425980
1	-4.258670	0.537025	-3.078995
1	-3.234387	0.331068	-4.510630
1	-2.497247	0.732328	-2.943812
6	-1.755419	-1.829015	-3.683296
1	-1.645592	-2.920412	-3.653884
1	-0.926436	-1.387228	-3.114593
1	-1.642903	-1.514314	-4.732755
6	-2.827947	-3.525961	-0.640555
6	-3.267559	-3.711469	0.841010
1	-2.980547	-4.716770	1.186728
1	-4.353842	-3.617053	0.967942
1	-2.777611	-2.982858	1.499965
6	-3.546253	-4.610570	-1.495425
1	-3.346101	-5.604686	-1.065836
1	-3.182739	-4.623343	-2.530396
1	-4.636182	-4.475444	-1.515599
6	-1.298247	-3.778114	-0.712609
1	-1.074390	-4.788049	-0.333476
1	-0.743232	-3.059531	-0.097795
1	-0.911069	-3.714733	-1.735460
6	3.935806	-0.445608	3.111994
6	1.390113	-2.145928	2.592057
1	1.675008	-2.933366	3.303653
1	0.690815	-2.580166	1.869894
1	0.845987	-1.371103	3.145774
6	3.900592	-2.927529	0.912175
6	5.392081	-0.117168	2.686601
1	5.874020	0.500171	3.461047
1	5.430543	0.444200	1.745279
1	5.999408	-1.023234	2.565120
6	3.983009	-1.274214	4.431324
1	2.978216	-1.466216	4.827784
1	4.536766	-0.707728	5.196509
1	4.488164	-2.238436	4.304884
6	3.203394	0.890154	3.425963
1	2.156555	0.728180	3.716100
1	3.206142	1.570193	2.566492
1	3.706039	1.400241	4.262986
6	2.882989	-3.788933	0.109527

1	2.131867	-4.250840	0.762817
1	3.415760	-4.600677	-0.410216
1	2.353276	-3.195847	-0.647665
6	4.554273	-3.834701	1.994057
1	3.824747	-4.190279	2.734075
1	5.361493	-3.320174	2.529860
1	4.992964	-4.722141	1.511463
6	5.006208	-2.454507	-0.069187
1	5.768116	-1.839843	0.424767
1	4.581071	-1.874576	-0.896869
1	5.515459	-3.328663	-0.504606
6	2.781205	3.375578	-1.121950
6	5.183589	1.407623	-1.021210
1	5.524955	0.371620	-0.921282
1	5.402952	1.926536	-0.079405
1	5.787838	1.882807	-1.806181
6	3.133610	0.905553	-3.318875
6	3.821149	4.362310	-1.732972
1	4.824562	4.210076	-1.314913
1	3.520943	5.396318	-1.500975
1	3.891084	4.277449	-2.823038
6	1.379790	3.705252	-1.703717
1	0.611902	3.002070	-1.354264
1	1.378374	3.693897	-2.800806
1	1.075277	4.715338	-1.386342
6	2.740559	3.634124	0.411771
1	1.968488	3.031186	0.904186
1	2.512976	4.695360	0.598903
1	3.703159	3.414940	0.894745
6	3.872803	1.868267	-4.294097
1	4.922279	2.028929	-4.012356
1	3.380576	2.846523	-4.354632
1	3.866976	1.435794	-5.306908
6	3.787464	-0.501227	-3.446299
1	3.288963	-1.239305	-2.804634
1	4.854797	-0.485474	-3.189316
1	3.702198	-0.853021	-4.486166
6	1.655445	0.788157	-3.777626
1	1.084862	0.101724	-3.140759
1	1.619299	0.396385	-4.806694
1	1.140533	1.755365	-3.773451

>Ge=Ge=Ge<

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

32	-2.197386	-0.128740	0.200181
32	-0.019420	-0.150936	-0.771558
32	2.175553	0.134920	0.102219
14	-2.696013	2.018966	1.438904
14	-3.915555	-1.444627	-1.114814
14	3.905216	1.022734	-1.511677
14	2.698116	-1.486049	1.966499
6	-1.035224	2.484285	2.259440
1	-0.815018	1.820716	3.104975
1	-1.066903	3.513597	2.641520
1	-0.197250	2.407043	1.558461
6	-3.954928	1.687417	2.916965
6	-3.773036	2.773271	4.021969
1	-4.472935	2.570678	4.848548
1	-3.982642	3.784255	3.655064
1	-2.759574	2.768069	4.440905
6	-5.441748	1.699417	2.470893
1	-5.637862	0.984359	1.663321
1	-5.757752	2.692174	2.126459
1	-6.086645	1.426802	3.321484
6	-3.203231	3.496452	0.249445
6	-3.599760	4.760122	1.069471
1	-4.527951	4.612611	1.635365
1	-3.767041	5.602539	0.379804
1	-2.813757	5.065467	1.773190
6	-4.384566	3.128190	-0.687266
1	-4.130521	2.281309	-1.335455
1	-4.625078	3.984526	-1.337344
1	-5.292838	2.870288	-0.129763
6	-3.646260	0.306913	3.564009
1	-3.865345	-0.523343	2.879711
1	-4.267952	0.170422	4.463109
1	-2.595269	0.219196	3.870975
6	-1.977443	3.867740	-0.632672
1	-1.632388	3.017065	-1.234585
1	-1.131157	4.218485	-0.028240
1	-2.252432	4.679316	-1.324572
6	-5.669005	-0.814032	-0.678580
1	-6.426912	-1.482856	-1.111562
1	-5.848628	0.193280	-1.074318

1	-5.839284	-0.782888	0.403156
6	-3.735192	-1.264384	-3.067812
6	-5.025030	-1.782713	-3.776725
1	-5.221527	-2.842025	-3.580021
1	-4.907973	-1.666238	-4.865809
1	-5.913739	-1.211046	-3.480664
6	-3.572035	0.232717	-3.452415
1	-4.417246	0.839733	-3.101012
1	-3.533234	0.327467	-4.548901
1	-2.648600	0.661321	-3.044686
6	-2.517434	-2.047990	-3.626066
1	-2.635700	-3.131741	-3.501214
1	-1.578360	-1.746876	-3.142183
1	-2.412766	-1.850143	-4.704522
6	-3.811176	-3.297188	-0.451749
6	-4.289043	-3.321105	1.029374
1	-4.200550	-4.343467	1.428999
1	-5.339566	-3.018082	1.128080
1	-3.680243	-2.665200	1.666909
6	-4.741377	-4.245977	-1.263451
1	-4.758376	-5.237622	-0.783603
1	-4.387312	-4.389542	-2.291754
1	-5.777942	-3.884295	-1.304154
6	-2.367929	-3.867560	-0.500706
1	-2.363126	-4.897920	-0.110735
1	-1.678857	-3.274140	0.113090
1	-1.968375	-3.897164	-1.520921
6	3.893937	-0.645994	3.285865
6	1.029573	-1.751590	2.854433
1	1.100340	-2.586229	3.565898
1	0.223469	-1.973347	2.146444
1	0.732968	-0.855683	3.415060
6	3.295246	-3.238361	1.311183
6	5.392760	-0.717693	2.888022
1	5.998082	-0.168493	3.626572
1	5.582485	-0.269919	1.905377
1	5.762398	-1.750579	2.866392
6	3.724852	-1.337598	4.673827
1	2.699921	-1.248901	5.054318
1	4.391272	-0.851765	5.404361
1	3.985465	-2.401631	4.648868
6	3.503294	0.849424	3.460421
1	2.439976	0.972571	3.706443
1	3.707358	1.433821	2.554478
1	4.088397	1.292665	4.281693
6	2.113950	-3.917199	0.560422

1	1.259404	-4.101908	1.223840
1	2.441760	-4.889717	0.160970
1	1.760903	-3.309876	-0.283156
6	3.702173	-4.163906	2.496251
1	2.902086	-4.265712	3.241838
1	4.603950	-3.806323	3.008044
1	3.921420	-5.172198	2.110824
6	4.495624	-3.138851	0.332345
1	5.379480	-2.690503	0.801227
1	4.240473	-2.546271	-0.554050
1	4.777758	-4.146609	-0.011916
6	3.837248	2.987015	-1.375495
6	5.649443	0.520659	-0.903351
1	5.732727	-0.554909	-0.714369
1	5.919065	1.045991	0.021132
1	6.401767	0.785458	-1.659760
6	3.717111	0.289627	-3.328750
6	5.086297	3.640604	-2.040120
1	6.025299	3.284658	-1.596693
1	5.046452	4.731647	-1.892497
1	5.131054	3.459589	-3.119594
6	2.560128	3.586603	-2.023629
1	1.644490	3.123250	-1.632259
1	2.561821	3.470187	-3.114431
1	2.505955	4.665683	-1.809335
6	3.849624	3.390426	0.128395
1	2.948830	3.041518	0.649770
1	3.879807	4.487932	0.214805
1	4.728689	2.997036	0.657678
6	4.799500	0.885190	-4.280100
1	5.819491	0.758621	-3.893834
1	4.635645	1.951845	-4.472645
1	4.750431	0.366480	-5.250318
6	3.938096	-1.249432	-3.266628
1	3.186236	-1.741705	-2.636912
1	4.933668	-1.507651	-2.882736
1	3.853713	-1.673583	-4.279186
6	2.326383	0.552796	-3.964285
1	1.512028	0.134520	-3.358788
1	2.279592	0.075819	-4.956221
1	2.130996	1.622208	-4.103740

>Sn=Sn=Sn<

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-2.326677	-0.042289	0.324439
50	-0.033921	-0.547583	-0.990810
50	2.287182	0.221395	0.118348
14	-2.719716	2.536450	0.848193
14	-4.117669	-1.731544	-0.671612
14	4.120312	0.539018	-1.773481
14	2.718473	-0.885997	2.499104
6	-1.030415	3.167678	1.483997
1	-0.796822	2.746320	2.470689
1	-1.028104	4.263019	1.577134
1	-0.216004	2.882795	0.807876
6	-3.972953	2.666827	2.353176
6	-3.797667	4.026575	3.091242
1	-4.499775	4.079860	3.938426
1	-3.999070	4.884222	2.439294
1	-2.783923	4.139876	3.496005
6	-5.450535	2.522610	1.902082
1	-5.616716	1.592601	1.341529
1	-5.768833	3.359904	1.268222
1	-6.111616	2.504289	2.782705
6	-3.175477	3.575036	-0.753234
6	-3.550752	5.036020	-0.371163
1	-4.480471	5.084300	0.209407
1	-3.702800	5.627670	-1.287634
1	-2.758170	5.527802	0.208909
6	-4.350651	2.947977	-1.550830
1	-4.096029	1.943164	-1.910544
1	-4.575845	3.568189	-2.432869
1	-5.267297	2.871644	-0.954078
6	-3.662785	1.534807	3.375214
1	-3.887643	0.541044	2.963367
1	-4.281641	1.663926	4.276908
1	-2.610760	1.536575	3.691755
6	-1.933858	3.628473	-1.690343
1	-1.602556	2.625924	-1.992747
1	-1.082815	4.136661	-1.218909
1	-2.188052	4.184636	-2.606211
6	-5.882640	-1.016788	-0.488642
1	-6.651629	-1.766751	-0.720343
1	-6.029578	-0.165576	-1.166601

1	-6.061340	-0.656482	0.531614
6	-3.841672	-2.107483	-2.588424
6	-5.108256	-2.805939	-3.167547
1	-5.319663	-3.762114	-2.675431
1	-4.951615	-3.010658	-4.238405
1	-5.998831	-2.171435	-3.079577
6	-3.642703	-0.778126	-3.372929
1	-4.477425	-0.079391	-3.223584
1	-3.580722	-0.993035	-4.451494
1	-2.715413	-0.269203	-3.083457
6	-2.615111	-3.017592	-2.867979
1	-2.742946	-4.023842	-2.450235
1	-1.683870	-2.595797	-2.465464
1	-2.476173	-3.125895	-3.955338
6	-3.964611	-3.295178	0.516730
6	-4.420622	-2.868360	1.942569
1	-4.316647	-3.716773	2.636552
1	-5.469822	-2.546682	1.963673
1	-3.803880	-2.047657	2.337649
6	-4.878530	-4.459315	0.040631
1	-4.864463	-5.269817	0.786492
1	-4.531850	-4.883818	-0.909977
1	-5.922865	-4.143334	-0.085193
6	-2.508994	-3.829768	0.626908
1	-2.483304	-4.696734	1.306113
1	-1.825935	-3.072924	1.032869
1	-2.108211	-4.154230	-0.339918
6	3.911347	0.292454	3.518138
6	1.024564	-0.852776	3.386190
1	1.056710	-1.441733	4.313781
1	0.228356	-1.261142	2.753440
1	0.734343	0.172881	3.649297
6	3.269913	-2.763526	2.351435
6	5.402676	0.102442	3.133628
1	6.021400	0.849921	3.654516
1	5.566868	0.229469	2.055099
1	5.776387	-0.889581	3.417784
6	3.745848	0.044188	5.046574
1	2.718374	0.238961	5.379220
1	4.408432	0.724637	5.604449
1	4.005633	-0.980962	5.334419
6	3.522151	1.773407	3.237434
1	2.456871	1.967676	3.422912
1	3.739448	2.061216	2.199564
1	4.101097	2.443205	3.892304
6	2.075161	-3.599949	1.809104

1	1.210729	-3.569741	2.484559
1	2.380018	-4.653005	1.704696
1	1.742826	-3.251548	0.822190
6	3.658385	-3.329190	3.748108
1	2.848905	-3.212115	4.481481
1	4.557850	-2.846786	4.150034
1	3.870958	-4.406331	3.661979
6	4.468571	-2.954375	1.383196
1	5.357826	-2.400342	1.706346
1	4.217336	-2.627901	0.365878
1	4.739661	-4.020581	1.330823
6	4.011287	2.457550	-2.204466
6	5.868075	0.210318	-1.065677
1	5.919139	-0.770150	-0.577039
1	6.139071	0.964633	-0.315766
1	6.633939	0.234604	-1.852762
6	3.858366	-0.711594	-3.276653
6	5.240850	2.910155	-3.042489
1	6.185841	2.713175	-2.519909
1	5.183734	3.994597	-3.226846
1	5.281797	2.411853	-4.018036
6	2.714875	2.828025	-2.976712
1	1.811533	2.481114	-2.456693
1	2.705837	2.408267	-3.989631
1	2.640182	3.922653	-3.073556
6	4.016746	3.272298	-0.876722
1	3.107766	3.089238	-0.285993
1	4.047019	4.349785	-1.101949
1	4.885841	3.042527	-0.245111
6	4.946822	-0.476885	-4.364787
1	5.965235	-0.524407	-3.958832
1	4.819460	0.491762	-4.863473
1	4.861760	-1.256973	-5.137482
6	4.012607	-2.163926	-2.737053
1	3.244980	-2.400565	-1.988192
1	4.998034	-2.335594	-2.284923
1	3.897087	-2.880518	-3.565170
6	2.473077	-0.609486	-3.968617
1	1.650217	-0.832636	-3.277493
1	2.415527	-1.347714	-4.784209
1	2.289784	0.379247	-4.403152

>Pb=Pb=Pb<

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-2.345943	0.264485	0.343381
82	-0.047440	-1.204445	-0.339675
82	2.319066	0.261417	-0.039561
14	-2.704599	2.593252	-1.034495
14	-4.272002	-1.660297	0.560405
14	4.223988	-0.738643	-1.699501
14	2.812278	1.014149	2.533295
6	-1.003004	3.465655	-0.915855
1	-0.793232	3.785680	0.113539
1	-0.972507	4.359780	-1.555430
1	-0.185764	2.802885	-1.223585
6	-3.969893	3.718319	-0.036284
6	-3.752567	5.221654	-0.380094
1	-4.459982	5.839416	0.195976
1	-3.916624	5.435080	-1.442495
1	-2.739277	5.553625	-0.121144
6	-5.447053	3.342763	-0.327829
1	-5.641913	2.277055	-0.145920
1	-5.726655	3.564271	-1.365655
1	-6.118371	3.921027	0.326408
6	-3.105036	2.334786	-2.939901
6	-3.424112	3.693992	-3.628782
1	-4.354744	4.137563	-3.253420
1	-3.547438	3.536039	-4.712031
1	-2.616345	4.426291	-3.494363
6	-4.299796	1.368937	-3.160858
1	-4.092112	0.377437	-2.739422
1	-4.484019	1.242057	-4.239545
1	-5.225289	1.741523	-2.706164
6	-3.713145	3.544410	1.488937
1	-3.963398	2.530648	1.831782
1	-4.341605	4.247825	2.057439
1	-2.667140	3.742780	1.760396
6	-1.855018	1.725737	-3.637585
1	-1.569401	0.760184	-3.198361
1	-0.985706	2.393220	-3.578963
1	-2.072934	1.555336	-4.703711
6	-6.020772	-0.959286	0.211800
1	-6.809096	-1.669234	0.499494
1	-6.142086	-0.738333	-0.857099

1	-6.193049	-0.025405	0.760856
6	-4.019143	-3.190423	-0.665222
6	-5.316560	-4.053213	-0.708401
1	-5.570855	-4.472446	0.271636
1	-5.169309	-4.895921	-1.402719
1	-6.177643	-3.476488	-1.067516
6	-3.754355	-2.674121	-2.108712
1	-4.558862	-2.016829	-2.465909
1	-3.691128	-3.527181	-2.803056
1	-2.810003	-2.120024	-2.175101
6	-2.841007	-4.116934	-0.260486
1	-3.022700	-4.623031	0.695543
1	-1.890189	-3.571623	-0.180443
1	-2.702687	-4.896253	-1.026639
6	-4.183001	-2.128325	2.474129
6	-4.631376	-0.886741	3.299405
1	-4.558728	-1.107921	4.375768
1	-5.669354	-0.601682	3.086217
1	-3.991337	-0.013951	3.102702
6	-5.134889	-3.308716	2.818797
1	-5.153387	-3.464124	3.909446
1	-4.799308	-4.247623	2.360877
1	-6.166399	-3.118620	2.493556
6	-2.748567	-2.508832	2.940011
1	-2.758722	-2.742538	4.016773
1	-2.037975	-1.685586	2.790234
1	-2.356439	-3.387788	2.415870
6	4.030506	2.550685	2.550982
6	1.119509	1.654193	3.156242
1	1.131402	1.804668	4.245474
1	0.309065	0.954466	2.920714
1	0.864674	2.614295	2.688043
6	3.319950	-0.516176	3.655361
6	5.512355	2.125741	2.374619
1	6.152204	3.018323	2.292135
1	5.658759	1.524674	1.466717
1	5.872394	1.539629	3.229670
6	3.885205	3.348790	3.880897
1	2.864845	3.729835	4.015102
1	4.563325	4.216812	3.866918
1	4.138747	2.744490	4.759436
6	3.652215	3.508007	1.383289
1	2.595021	3.805554	1.415648
1	3.843282	3.049562	0.403298
1	4.256651	4.426722	1.440821
6	2.097126	-1.468426	3.789498

1	1.245754	-0.978783	4.279252
1	2.374742	-2.342707	4.398828
1	1.756855	-1.838883	2.813103
6	3.717137	-0.043134	5.083992
1	2.924486	0.553080	5.556175
1	4.638517	0.552723	5.080619
1	3.894296	-0.920944	5.725377
6	4.497649	-1.326269	3.049158
1	5.404848	-0.720631	2.936944
1	4.238511	-1.732077	2.062388
1	4.741850	-2.177150	3.704548
6	4.123215	0.452218	-3.267513
6	5.981156	-0.553944	-0.962847
1	6.047484	-1.021945	0.026999
1	6.245596	0.504988	-0.844053
1	6.742065	-1.016863	-1.606864
6	3.940531	-2.659693	-2.047045
6	5.336509	0.236015	-4.216652
1	6.292281	0.404257	-3.703554
1	5.281217	0.947035	-5.056444
1	5.353020	-0.774119	-4.642288
6	2.813603	0.267607	-4.082608
1	1.918685	0.341629	-3.449545
1	2.784714	-0.699694	-4.598075
1	2.739382	1.051762	-4.852728
6	4.168460	1.928388	-2.772023
1	3.269412	2.191874	-2.196023
1	4.209781	2.609689	-3.636213
1	5.048018	2.134613	-2.146711
6	5.040119	-3.209476	-3.004104
1	6.054608	-3.004933	-2.639390
1	4.946806	-2.792116	-4.014269
1	4.933360	-4.302378	-3.090248
6	4.050786	-3.423506	-0.694166
1	3.264721	-3.116826	0.009204
1	5.023619	-3.269917	-0.209135
1	3.933004	-4.504529	-0.868879
6	2.562873	-3.005860	-2.673130
1	1.728315	-2.694344	-2.030659
1	2.478704	-4.097207	-2.797789
1	2.419707	-2.548565	-3.658203

Reactant:(Triplet)

>C=C=C<

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

6	1.429569	-0.001466	0.092595
6	-0.035890	0.294970	-0.137821
6	-1.356945	-0.007719	-0.132151
14	2.251570	-1.524778	-0.897185
14	2.497662	1.267092	1.141457
14	-2.549551	1.249163	-1.113687
14	-2.185142	-1.598817	0.871156
6	0.798907	-2.438902	-1.715749
1	0.236325	-3.039077	-0.998227
1	1.152306	-3.117374	-2.499923
1	0.103135	-1.726267	-2.166266
6	3.312051	-2.915956	0.080421
6	3.002765	-4.305076	-0.563801
1	3.594240	-5.076544	-0.046390
1	3.264987	-4.347530	-1.626978
1	1.946627	-4.580975	-0.466309
6	4.856373	-2.728306	0.023969
1	5.185791	-1.787590	0.472860
1	5.248843	-2.772483	-0.996546
1	5.331265	-3.545609	0.589449
6	3.292221	-0.899047	-2.500956
6	3.717078	-2.143772	-3.342184
1	4.396759	-2.812535	-2.806260
1	4.246289	-1.790727	-4.241098
1	2.857339	-2.730584	-3.685400
6	4.577545	-0.071591	-2.230158
1	4.354383	0.878222	-1.735433
1	5.055323	0.170818	-3.193102
1	5.314327	-0.611304	-1.627682
6	2.922350	-3.019426	1.579240
1	3.175589	-2.112241	2.132795
1	3.473640	-3.855047	2.039162
1	1.855021	-3.210331	1.720740
6	2.383182	-0.037977	-3.418992
1	2.112909	0.908956	-2.947779
1	1.460579	-0.557123	-3.702910
1	2.926964	0.197842	-4.348105
6	4.296141	0.644162	1.227264
1	4.889610	1.350986	1.818693

1	4.784259	0.548807	0.256651
1	4.350996	-0.323727	1.733609
6	2.561384	3.104367	0.394872
6	3.968565	3.726473	0.639529
1	4.222434	3.786271	1.704852
1	3.983739	4.752054	0.237815
1	4.762131	3.162529	0.134268
6	2.325294	3.070184	-1.137592
1	3.101770	2.497311	-1.656474
1	2.347447	4.094490	-1.542142
1	1.355695	2.628541	-1.384322
6	1.512723	4.069571	1.013420
1	1.725916	4.291081	2.064860
1	0.494543	3.676960	0.951119
1	1.534466	5.025810	0.467062
6	1.981804	1.300967	3.054338
6	2.133090	-0.110102	3.689662
1	1.833114	-0.063460	4.748326
1	3.169332	-0.469731	3.662835
1	1.501544	-0.857811	3.199221
6	2.923983	2.251565	3.852422
1	2.628564	2.237186	4.913583
1	2.865111	3.291722	3.513545
1	3.973454	1.934891	3.803492
6	0.519828	1.758637	3.275714
1	0.227167	1.584281	4.323292
1	-0.170372	1.197749	2.642543
1	0.381768	2.823485	3.069989
6	-3.175415	-3.024380	-0.129181
6	-0.674050	-2.445141	1.660697
1	-0.971414	-3.141066	2.453565
1	-0.005301	-1.697051	2.095421
1	-0.100772	-3.015343	0.927619
6	-3.249099	-1.059386	2.484314
6	-4.727102	-2.912099	-0.069045
1	-5.163313	-3.737723	-0.653406
1	-5.100636	-1.977657	-0.496721
1	-5.117132	-2.997612	0.949765
6	-2.797950	-4.410244	0.485226
1	-1.729230	-4.631155	0.383164
1	-3.350047	-5.199312	-0.049288
1	-3.058019	-4.488701	1.546962
6	-2.785978	-3.076927	-1.630953
1	-1.711041	-3.209092	-1.779021
1	-3.087571	-2.172510	-2.164659
1	-3.295123	-3.929828	-2.107566

6	-2.386992	-0.175019	3.424580
1	-1.440977	-0.654924	3.700337
1	-2.944236	0.013196	4.356658
1	-2.162456	0.794416	2.975363
6	-3.608502	-2.343626	3.298349
1	-2.719572	-2.901026	3.615606
1	-4.264547	-3.027452	2.752189
1	-4.141461	-2.038379	4.212421
6	-4.577367	-0.292745	2.239262
1	-5.283389	-0.848225	1.614764
1	-4.403958	0.685019	1.779850
1	-5.069164	-0.110250	3.208385
6	-2.050067	1.329266	-3.024916
6	-4.310800	0.526744	-1.187442
1	-4.786533	0.402674	-0.214106
1	-4.316394	-0.441572	-1.695794
1	-4.945646	1.201654	-1.773618
6	-2.704180	3.055359	-0.327295
6	-3.039286	2.247182	-3.805695
1	-4.074972	1.889523	-3.745309
1	-2.757619	2.251845	-4.870563
1	-3.015855	3.286583	-3.459365
6	-0.612077	1.850390	-3.256810
1	0.104764	1.300609	-2.642476
1	-0.511937	2.915197	-3.028588
1	-0.326160	1.708043	-4.311306
6	-2.141333	-0.081506	-3.672991
1	-1.475595	-0.802954	-3.187957
1	-1.845094	-0.013466	-4.731509
1	-3.160693	-0.486607	-3.647887
6	-4.134232	3.624455	-0.571213
1	-4.906821	3.018302	-0.082310
1	-4.383200	3.692587	-1.637198
1	-4.195771	4.640959	-0.151429
6	-2.481489	2.998034	1.206528
1	-1.497971	2.590171	1.455850
1	-3.238424	2.380985	1.704413
1	-2.551119	4.011438	1.632444
6	-1.689659	4.073123	-0.918676
1	-0.658647	3.713370	-0.865866
1	-1.744086	5.014924	-0.350015
1	-1.910377	4.311003	-1.965317

>Si=Si=Si<

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

14	-2.201015	-0.119521	0.089969
14	0.040780	0.306936	-0.614734
14	2.106756	0.032066	0.027675
14	-2.943126	1.615792	1.570403
14	-3.385469	-1.644715	-1.316730
14	3.452838	1.491880	-1.329997
14	2.809535	-1.528336	1.730759
6	-1.358855	2.345675	2.344933
1	-0.888649	1.636629	3.038283
1	-1.588500	3.262863	2.904792
1	-0.615558	2.590454	1.578114
6	-4.015578	0.888509	3.041096
6	-4.019683	1.882798	4.241176
1	-4.621602	1.461526	5.061537
1	-4.451852	2.855826	3.981002
1	-3.008033	2.054349	4.629691
6	-5.484832	0.601726	2.631431
1	-5.546739	-0.066762	1.763377
1	-6.030337	1.522479	2.388376
1	-6.015312	0.114860	3.464649
6	-3.801584	3.047609	0.536816
6	-4.390474	4.139995	1.476213
1	-5.241303	3.767143	2.060081
1	-4.754168	4.985204	0.870682
1	-3.641839	4.536941	2.175209
6	-4.939007	2.524762	-0.381618
1	-4.560123	1.800737	-1.113169
1	-5.377563	3.364967	-0.943128
1	-5.747011	2.046618	0.184362
6	-3.375262	-0.439681	3.535607
1	-3.430854	-1.224335	2.771508
1	-3.907000	-0.798889	4.430495
1	-2.317748	-0.312388	3.805028
6	-2.726416	3.722131	-0.365818
1	-2.250858	3.003705	-1.047481
1	-1.935636	4.201682	0.224537
1	-3.200967	4.502376	-0.981445
6	-5.251184	-1.427670	-0.967177
1	-5.834469	-2.180995	-1.513984

1	-5.607073	-0.438808	-1.280482
1	-5.476591	-1.542104	0.099191
6	-3.100369	-1.214335	-3.216987
6	-4.219678	-1.863659	-4.085394
1	-4.232333	-2.956714	-4.005204
1	-4.049947	-1.611910	-5.144064
1	-5.215600	-1.490933	-3.814544
6	-3.180821	0.324672	-3.425908
1	-4.140649	0.737365	-3.087287
1	-3.083817	0.556329	-4.498219
1	-2.376052	0.851844	-2.897172
6	-1.723614	-1.701898	-3.746270
1	-1.652124	-2.796811	-3.753947
1	-0.888435	-1.309430	-3.151590
1	-1.583837	-1.355723	-4.782629
6	-2.895733	-3.473906	-0.803276
6	-3.401894	-3.730659	0.645529
1	-3.125705	-4.749683	0.958189
1	-4.493351	-3.644565	0.725432
1	-2.949549	-3.029740	1.359888
6	-3.567286	-4.517502	-1.741928
1	-3.376157	-5.532444	-1.359477
1	-3.165022	-4.470789	-2.761675
1	-4.656914	-4.387857	-1.797044
6	-1.360291	-3.706229	-0.818801
1	-1.137398	-4.728340	-0.473507
1	-0.839483	-3.007318	-0.151174
1	-0.930483	-3.592954	-1.819979
6	3.794170	-0.633751	3.179290
6	1.209234	-2.223364	2.506082
1	1.438853	-3.046649	3.197181
1	0.525128	-2.608484	1.742042
1	0.672766	-1.451341	3.071903
6	3.761812	-3.029791	0.895015
6	5.272722	-0.334364	2.812545
1	5.747462	0.237608	3.625420
1	5.358592	0.260438	1.895444
1	5.856837	-1.253371	2.675274
6	3.776837	-1.514987	4.465060
1	2.755668	-1.697233	4.822531
1	4.319251	-0.993226	5.269337
1	4.263077	-2.485572	4.316375
6	3.092605	0.710471	3.525151
1	2.035222	0.567426	3.786311
1	3.135380	1.420965	2.691626
1	3.588962	1.175376	4.391751

6	2.751822	-3.838076	0.030418
1	1.966887	-4.300579	0.642514
1	3.281889	-4.647121	-0.496347
1	2.265326	-3.207707	-0.725761
6	4.354210	-3.990263	1.966895
1	3.593144	-4.346720	2.673993
1	5.161177	-3.519284	2.541806
1	4.780449	-4.875023	1.468044
6	4.915170	-2.557115	-0.030300
1	5.675654	-1.982571	0.511725
1	4.538053	-1.936371	-0.851247
1	5.415035	-3.431227	-0.476831
6	2.958791	3.360347	-0.941725
6	5.288889	1.312581	-0.823925
1	5.597991	0.263947	-0.755475
1	5.480673	1.784083	0.148306
1	5.938132	1.804469	-1.561232
6	3.331411	0.970599	-3.226822
6	4.056438	4.333101	-1.467908
1	5.036108	4.128281	-1.017791
1	3.781823	5.366907	-1.204997
1	4.166837	4.289706	-2.556969
6	1.598536	3.772098	-1.565561
1	0.788995	3.087427	-1.275645
1	1.640753	3.802287	-2.661545
1	1.320645	4.780249	-1.218511
6	2.861107	3.559264	0.598624
1	2.049202	2.963886	1.033231
1	2.660337	4.619394	0.820086
1	3.794459	3.287673	1.111366
6	4.157138	1.944468	-4.117927
1	5.193752	2.058300	-3.773733
1	3.699089	2.940074	-4.163554
1	4.192374	1.553810	-5.147051
6	3.934411	-0.455889	-3.381141
1	3.370922	-1.196865	-2.798881
1	4.985828	-0.497089	-3.067817
1	3.890514	-0.761154	-4.438250
6	1.882487	0.932024	-3.780592
1	1.252870	0.228693	-3.222741
1	1.899215	0.603336	-4.832281
1	1.395760	1.913290	-3.746464

>Ge=Ge=Ge<

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

32	-2.190359	0.069245	-0.034842
32	0.044306	-0.928985	-0.827981
32	2.140867	0.211994	0.078931
14	-2.594837	2.350269	1.028055
14	-4.012130	-1.575419	-0.722069
14	3.914046	0.668440	-1.699219
14	2.681294	-1.005105	2.246788
6	-0.894107	2.907012	1.697027
1	-0.658027	2.405310	2.643764
1	-0.887407	3.990073	1.885541
1	-0.083242	2.677173	0.996433
6	-3.828800	2.369946	2.560407
6	-3.609814	3.660020	3.409869
1	-4.293732	3.645832	4.273714
1	-3.816466	4.575788	2.844567
1	-2.587371	3.726583	3.801405
6	-5.321098	2.313211	2.138284
1	-5.534954	1.448370	1.498691
1	-5.628404	3.218340	1.599383
1	-5.958404	2.232723	3.033148
6	-3.086177	3.572589	-0.431618
6	-3.429092	4.993448	0.105248
1	-4.347109	4.998980	0.705358
1	-3.590540	5.673998	-0.745964
1	-2.619102	5.417701	0.713535
6	-4.299833	3.053886	-1.249988
1	-4.084181	2.084285	-1.715495
1	-4.535116	3.764082	-2.058265
1	-5.199596	2.942656	-0.633731
6	-3.527801	1.148743	3.474782
1	-3.747088	0.199552	2.969018
1	-4.152288	1.198599	4.380702
1	-2.478524	1.124418	3.799293
6	-1.870704	3.708608	-1.394125
1	-1.559643	2.737334	-1.802717
1	-1.002933	4.158880	-0.895691
1	-2.141060	4.356750	-2.242497
6	-5.752864	-0.858295	-0.377566
1	-6.524885	-1.592746	-0.649132

1	-5.941499	0.050763	-0.961916
1	-5.892199	-0.610829	0.680547
6	-3.902280	-1.840418	-2.674852
6	-5.227845	-2.449017	-3.226394
1	-5.444938	-3.435987	-2.803130
1	-5.139505	-2.571311	-4.317957
1	-6.091436	-1.799004	-3.038205
6	-3.704140	-0.462131	-3.368984
1	-4.512651	0.240117	-3.124626
1	-3.700648	-0.593964	-4.462373
1	-2.750147	0.003802	-3.088083
6	-2.732783	-2.771793	-3.094874
1	-2.885138	-3.800581	-2.744512
1	-1.764460	-2.423408	-2.713202
1	-2.664917	-2.805470	-4.194065
6	-3.869825	-3.231565	0.336401
6	-4.295255	-2.928063	1.802185
1	-4.174271	-3.833818	2.416607
1	-5.346365	-2.620800	1.871773
1	-3.677054	-2.139071	2.252249
6	-4.824997	-4.329342	-0.221052
1	-4.819469	-5.196655	0.458600
1	-4.507396	-4.688433	-1.207707
1	-5.864391	-3.983235	-0.300439
6	-2.431129	-3.814645	0.368312
1	-2.426620	-4.754185	0.943324
1	-1.727311	-3.126976	0.854871
1	-2.043061	-4.034942	-0.632229
6	3.908286	0.045568	3.372680
6	1.016587	-1.042369	3.196208
1	1.090501	-1.688421	4.083084
1	0.195398	-1.419053	2.574611
1	0.735586	-0.037111	3.536589
6	3.220406	-2.882468	1.985546
6	5.394719	-0.134792	2.963883
1	6.030142	0.544033	3.554538
1	5.558092	0.094016	1.903677
1	5.748297	-1.157343	3.148393
6	3.757032	-0.352384	4.873064
1	2.740001	-0.172180	5.243270
1	4.441853	0.259922	5.481622
1	4.003657	-1.403583	5.058213
6	3.545392	1.553237	3.255674
1	2.492991	1.743750	3.507630
1	3.720097	1.936834	2.243236
1	4.165609	2.139830	3.951909

6	2.009908	-3.684811	1.429330
1	1.171731	-3.706798	2.138007
1	2.311806	-4.727235	1.241565
1	1.642027	-3.273397	0.478861
6	3.640268	-3.543251	3.333104
1	2.857356	-3.464394	4.099631
1	4.561828	-3.107801	3.738340
1	3.830336	-4.616005	3.167957
6	4.396962	-3.024125	0.983295
1	5.298183	-2.503148	1.328002
1	4.130161	-2.626622	-0.003262
1	4.654494	-4.088047	0.857307
6	3.885903	2.618157	-2.001271
6	5.671314	0.263013	-1.052761
1	5.738537	-0.754687	-0.651625
1	5.975616	0.956447	-0.258531
1	6.406423	0.351774	-1.866078
6	3.668982	-0.423832	-3.325796
6	5.121392	3.093792	-2.823418
1	6.068449	2.829969	-2.335170
1	5.095117	4.191524	-2.917284
1	5.136934	2.680459	-3.837835
6	2.597689	3.084662	-2.732393
1	1.689802	2.721643	-2.231263
1	2.571880	2.743424	-3.774868
1	2.553224	4.185393	-2.747220
6	3.943390	3.340106	-0.623446
1	3.054773	3.125123	-0.015984
1	3.989266	4.429659	-0.779100
1	4.831025	3.053698	-0.042756
6	4.736863	-0.074189	-4.406702
1	5.763210	-0.134450	-4.021637
1	4.587057	0.927952	-4.825745
1	4.656423	-0.791239	-5.239386
6	3.856308	-1.921829	-2.947608
1	3.111200	-2.252042	-2.212328
1	4.855925	-2.121812	-2.539899
1	3.734323	-2.546898	-3.846216
6	2.269635	-0.267306	-3.978903
1	1.462081	-0.549574	-3.288679
1	2.193948	-0.932576	-4.853905
1	2.081974	0.755347	-4.324798

>Sn=Sn=Sn<

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

50	-2.275604	0.104059	-0.008335
50	0.057019	-1.351663	-0.701423
50	2.228552	0.316044	0.068039
14	-2.587063	2.697709	0.578916
14	-4.258611	-1.640751	-0.365321
14	4.063529	0.339276	-1.879980
14	2.786120	-0.537989	2.544086
6	-0.861382	3.323581	1.110557
1	-0.618769	2.993695	2.129116
1	-0.821388	4.422376	1.096458
1	-0.069885	2.944650	0.453360
6	-3.796563	3.024901	2.089408
6	-3.554130	4.452918	2.664774
1	-4.228478	4.623611	3.519040
1	-3.750959	5.240033	1.927952
1	-2.526346	4.577753	3.027692
6	-5.292464	2.894816	1.698196
1	-5.514998	1.921654	1.241871
1	-5.599043	3.677367	0.992575
1	-5.923705	2.994565	2.595149
6	-3.063903	3.595930	-1.101002
6	-3.378294	5.101960	-0.868284
1	-4.291920	5.245788	-0.278044
1	-3.532722	5.598473	-1.839422
1	-2.556232	5.624209	-0.360477
6	-4.287912	2.935464	-1.792036
1	-4.087602	1.886354	-2.047941
1	-4.519470	3.465026	-2.729638
1	-5.185975	2.962784	-1.164010
6	-3.491558	2.002313	3.221461
1	-3.733613	0.974642	2.918922
1	-4.097121	2.238625	4.110511
1	-2.436146	2.024033	3.526323
6	-1.849422	3.502264	-2.070023
1	-1.562133	2.460215	-2.269911
1	-0.968567	4.023238	-1.674345
1	-2.107261	3.966317	-3.034862
6	-5.973927	-0.816223	-0.174575
1	-6.781935	-1.554153	-0.277240

1	-6.127743	-0.043869	-0.939557
1	-6.082104	-0.336919	0.805348
6	-4.139329	-2.294272	-2.223417
6	-5.483856	-2.952253	-2.651778
1	-5.734678	-3.823236	-2.035203
1	-5.402702	-3.297392	-3.694842
1	-6.321360	-2.245316	-2.601960
6	-3.881774	-1.091124	-3.176895
1	-4.643182	-0.306206	-3.068632
1	-3.904517	-1.433578	-4.223290
1	-2.897207	-0.634984	-3.002847
6	-3.003236	-3.331003	-2.435873
1	-3.187241	-4.262548	-1.885730
1	-2.024108	-2.945324	-2.124498
1	-2.931172	-3.587249	-3.504929
6	-4.109882	-3.027691	1.022277
6	-4.507239	-2.402081	2.390777
1	-4.387466	-3.150245	3.189782
1	-5.551163	-2.064849	2.404108
1	-3.868585	-1.544125	2.646412
6	-5.077318	-4.209366	0.724234
1	-5.065233	-4.917358	1.567992
1	-4.775253	-4.764956	-0.172388
1	-6.114800	-3.875845	0.588429
6	-2.674303	-3.603295	1.168977
1	-2.673829	-4.411016	1.918125
1	-1.966984	-2.838358	1.515863
1	-2.284181	-4.017196	0.232510
6	4.032925	0.701425	3.418337
6	1.113715	-0.356743	3.469303
1	1.164021	-0.809908	4.469608
1	0.292861	-0.838791	2.923415
1	0.844718	0.700888	3.592491
6	3.277445	-2.441690	2.641536
6	5.506946	0.421383	3.021351
1	6.164190	1.198050	3.443350
1	5.642445	0.426154	1.931378
1	5.855466	-0.547448	3.401294
6	3.898831	0.622260	4.967868
1	2.887676	0.891133	5.299596
1	4.599134	1.332608	5.435534
1	4.128571	-0.375136	5.359051
6	3.681919	2.157105	2.993969
1	2.628960	2.402935	3.190035
1	3.867951	2.325772	1.925361
1	4.301979	2.871057	3.558779

6	2.043699	-3.308612	2.260143
1	1.203532	-3.157717	2.950062
1	2.314933	-4.375501	2.294111
1	1.689551	-3.097461	1.241048
6	3.697810	-2.837654	4.087215
1	2.921467	-2.594034	4.825405
1	4.628480	-2.345221	4.393817
1	3.868115	-3.925017	4.135671
6	4.433656	-2.800452	1.669404
1	5.352493	-2.246678	1.895393
1	4.159759	-2.589332	0.627894
1	4.664551	-3.875295	1.742030
6	4.022697	2.182520	-2.574101
6	5.821947	0.040991	-1.182107
1	5.863870	-0.879572	-0.588066
1	6.130639	0.867621	-0.529756
1	6.564952	-0.042833	-1.987625
6	3.741846	-1.077807	-3.217116
6	5.223663	2.462158	-3.522880
1	6.186194	2.284259	-3.025679
1	5.205564	3.516923	-3.840698
1	5.191139	1.845431	-4.428366
6	2.702052	2.500920	-3.327532
1	1.817337	2.245894	-2.726909
1	2.632335	1.961344	-4.279898
1	2.649884	3.577330	-3.555523
6	4.133697	3.168846	-1.373764
1	3.253986	3.107523	-0.718919
1	4.197383	4.203014	-1.747283
1	5.026092	2.982739	-0.760405
6	4.805964	-1.022186	-4.353737
1	5.832825	-1.050575	-3.967461
1	4.696700	-0.122667	-4.970984
1	4.678370	-1.893099	-5.016199
6	3.870945	-2.460641	-2.513349
1	3.114745	-2.591528	-1.728427
1	4.860923	-2.602602	-2.061370
1	3.722719	-3.266142	-3.249762
6	2.342140	-1.012604	-3.885523
1	1.529397	-1.090206	-3.149019
1	2.223353	-1.858759	-4.581119
1	2.192038	-0.089617	-4.456290

>Pb=Pb=Pb<

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

82	-2.360825	0.143380	0.041002
82	0.025300	-1.506471	-0.333099
82	2.281351	0.409405	0.004412
14	-2.629237	2.869882	0.170302
14	-4.505005	-1.543222	-0.077909
14	4.185339	0.036015	-1.957970
14	3.007941	-0.087237	2.615353
6	-0.872033	3.498117	0.588892
1	-0.630343	3.317046	1.644837
1	-0.784804	4.579498	0.406844
1	-0.104763	2.991513	-0.009031
6	-3.812110	3.491586	1.609177
6	-3.513399	4.986006	1.938444
1	-4.168188	5.317521	2.759973
1	-3.697092	5.646829	1.083656
1	-2.476326	5.134200	2.264512
6	-5.315730	3.353446	1.252134
1	-5.579588	2.324303	0.975048
1	-5.601862	4.011491	0.421614
1	-5.932246	3.634323	2.120513
6	-3.086706	3.500247	-1.632276
6	-3.347322	5.034955	-1.640632
1	-4.250049	5.302965	-1.077498
1	-3.493652	5.376352	-2.677799
1	-2.502951	5.601267	-1.224766
6	-4.339327	2.782255	-2.204752
1	-4.177602	1.699462	-2.291322
1	-4.561380	3.165019	-3.213448
1	-5.229542	2.940616	-1.584669
6	-3.532921	2.661173	2.895092
1	-3.804934	1.604513	2.766007
1	-4.128559	3.057739	3.732322
1	-2.476505	2.703522	3.193984
6	-1.886168	3.213560	-2.580147
1	-1.634901	2.144314	-2.615691
1	-0.984308	3.760517	-2.277915
1	-2.139673	3.528262	-3.604458
6	-6.176766	-0.612823	-0.032474
1	-7.020354	-1.317096	0.006995

1	-6.306574	0.012457	-0.925177
1	-6.247896	0.042035	0.843971
6	-4.410836	-2.462507	-1.820118
6	-5.774134	-3.135049	-2.160468
1	-6.050700	-3.907335	-1.433601
1	-5.704961	-3.619074	-3.147748
1	-6.590555	-2.403621	-2.208176
6	-4.116866	-1.416393	-2.935207
1	-4.860039	-0.607186	-2.949241
1	-4.141418	-1.905398	-3.921703
1	-3.122641	-0.961550	-2.820488
6	-3.304805	-3.550992	-1.873612
1	-3.513857	-4.383739	-1.190259
1	-2.312714	-3.150975	-1.622156
1	-3.242029	-3.967731	-2.891418
6	-4.447917	-2.729560	1.492601
6	-4.832946	-1.900141	2.752364
1	-4.762132	-2.534132	3.650046
1	-5.859714	-1.517223	2.696760
1	-4.157926	-1.044906	2.900627
6	-5.468786	-3.894909	1.347926
1	-5.499024	-4.477200	2.282676
1	-5.187753	-4.584672	0.542460
1	-6.487060	-3.534021	1.150621
6	-3.042580	-3.341900	1.741128
1	-3.077458	-4.011094	2.615474
1	-2.295973	-2.564982	1.952275
1	-2.681694	-3.927520	0.887849
6	4.291214	1.259728	3.260915
6	1.373767	0.259429	3.567046
1	1.454032	-0.034333	4.623911
1	0.525744	-0.284351	3.131439
1	1.123776	1.328740	3.536778
6	3.502167	-1.956588	3.008537
6	5.751632	0.914734	2.866309
1	6.425661	1.734485	3.162017
1	5.856009	0.772695	1.782482
1	6.105313	0.002337	3.363169
6	4.208471	1.412665	4.808368
1	3.206092	1.720627	5.131800
1	4.915785	2.189170	5.141988
1	4.463197	0.486142	5.334638
6	3.932730	2.638916	2.635682
1	2.898481	2.937467	2.856884
1	4.053688	2.634851	1.544266
1	4.596490	3.418365	3.042797

6	2.254962	-2.865610	2.818874
1	1.432880	-2.584160	3.489246
1	2.519562	-3.912484	3.036727
1	1.878596	-2.835429	1.786151
6	3.978492	-2.119918	4.481699
1	3.231668	-1.757468	5.201096
1	4.919462	-1.589223	4.669046
1	4.152242	-3.186706	4.696648
6	4.620709	-2.473233	2.064033
1	5.547050	-1.895426	2.165618
1	4.308675	-2.426431	1.012648
1	4.855406	-3.524431	2.297628
6	4.205472	1.742366	-2.948052
6	5.950156	-0.203840	-1.248479
1	5.985473	-1.031169	-0.529856
1	6.293243	0.698843	-0.726789
1	6.674294	-0.420928	-2.047440
6	3.806337	-1.568882	-3.048411
6	5.396817	1.816004	-3.946322
1	6.361524	1.671890	-3.442522
1	5.419179	2.808830	-4.424297
1	5.316978	1.069603	-4.744590
6	2.883838	1.987498	-3.725804
1	2.002418	1.879177	-3.078008
1	2.770674	1.295103	-4.568904
1	2.871756	3.009996	-4.135971
6	4.381525	2.903076	-1.924997
1	3.523244	2.978584	-1.243546
1	4.464554	3.862073	-2.460372
1	5.287668	2.784868	-1.315740
6	4.840685	-1.729806	-4.201893
1	5.875483	-1.728353	-3.835765
1	4.743303	-0.938454	-4.954211
1	4.673654	-2.690962	-4.714101
6	3.922680	-2.822678	-2.132990
1	3.195605	-2.797172	-1.309840
1	4.924846	-2.923390	-1.696345
1	3.724220	-3.732626	-2.721506
6	2.388163	-1.567517	-3.679926
1	1.600335	-1.469473	-2.918920
1	2.213929	-2.517004	-4.210912
1	2.254484	-0.754549	-4.402510

TS1-C=C-C-1MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.616579	-1.884035	-1.327776
6	0.006089	-0.296173	-0.254582
6	-1.478703	-0.030207	-0.089427
1	-1.812142	-0.732250	-0.891040
6	-0.567769	-2.759715	-2.479873
1	-1.611300	-3.071571	-2.663000
1	0.006626	-3.685516	-2.324125
1	-0.206555	-2.276133	-3.397086
6	1.328113	-0.056854	-0.105220
14	2.728775	-1.249784	-0.894884
6	4.467049	-0.574994	-0.493000
1	4.634868	-0.380776	0.565419
1	4.723956	0.323550	-1.053124
1	5.190147	-1.344740	-0.797451
6	2.787054	-2.991605	0.052768
6	3.843751	-3.941094	-0.585787
1	4.838102	-3.483393	-0.668260
1	3.539353	-4.285242	-1.577905
1	3.948466	-4.832892	0.051719
6	3.233509	-2.739856	1.524589
1	2.572642	-2.034422	2.040564
1	4.262767	-2.369639	1.591242
1	3.191715	-3.691519	2.076568
6	1.443480	-3.747459	0.119468
1	0.651268	-3.118609	0.523599
1	1.551342	-4.636800	0.761487
1	1.118363	-4.092808	-0.864959
6	2.720442	-1.284882	-2.899068
6	4.087052	-0.806847	-3.487382
1	4.323345	0.236834	-3.252918
1	4.036523	-0.887287	-4.584829
1	4.925332	-1.430036	-3.152322
6	2.529635	-2.718685	-3.484238
1	1.765186	-3.303414	-2.978228
1	3.467832	-3.284130	-3.436061
1	2.246942	-2.644281	-4.545577
6	1.634065	-0.325731	-3.463548
1	1.891523	0.718703	-3.260517

1	0.649815	-0.512458	-3.031599
1	1.568767	-0.439848	-4.557055
14	2.063176	1.602379	0.927095
6	0.538555	2.613905	1.410979
1	0.832818	3.489962	1.997214
1	-0.147868	2.024285	2.017770
1	-0.017749	2.980847	0.552585
6	2.925876	1.343553	2.732264
6	1.987809	0.558413	3.684449
1	1.000930	1.021493	3.777594
1	2.434649	0.532614	4.691330
1	1.851717	-0.474447	3.360434
6	3.103727	2.761437	3.375102
1	2.146639	3.254925	3.574848
1	3.720682	3.439090	2.778129
1	3.606390	2.635102	4.346222
6	4.311223	0.645830	2.804461
1	5.073106	1.130220	2.188594
1	4.251153	-0.409077	2.527740
1	4.664975	0.679804	3.847263
6	3.211889	2.852209	-0.178968
6	4.728113	2.861100	0.190139
1	5.249330	3.550425	-0.492919
1	5.207280	1.885598	0.093291
1	4.907811	3.224517	1.206966
6	2.713024	4.316538	0.053422
1	1.682927	4.467122	-0.287975
1	3.354601	4.997125	-0.528391
1	2.774620	4.628390	1.102283
6	3.106132	2.601725	-1.706535
1	2.077086	2.681639	-2.067761
1	3.490415	1.622630	-1.994357
1	3.705084	3.357502	-2.239477
14	-2.154658	1.638694	-1.054315
6	-0.649105	2.387070	-1.954212
1	0.022334	2.955214	-1.310492
1	-0.987970	3.068708	-2.741916
1	-0.061379	1.595239	-2.424366
6	-3.062373	3.098498	-0.034590
6	-2.613496	4.468328	-0.637055
1	-2.863085	4.563560	-1.700776
1	-3.126396	5.281980	-0.101060
1	-1.534820	4.632815	-0.528956
6	-4.615550	3.046832	-0.167609
1	-5.044872	2.120950	0.224690
1	-4.947802	3.161415	-1.203702

1	-5.048209	3.881114	0.405562
6	-3.271920	1.079656	-2.615481
6	-3.533853	2.303701	-3.549288
1	-4.017072	3.144509	-3.039759
1	-4.202916	1.989256	-4.365406
1	-2.611783	2.671209	-4.014994
6	-4.654665	0.456044	-2.274500
1	-4.580238	-0.343269	-1.535922
1	-5.089239	0.015212	-3.185975
1	-5.366991	1.196786	-1.901890
6	-2.494961	0.039733	-3.475633
1	-2.347890	-0.906135	-2.951178
1	-1.508319	0.404501	-3.785086
1	-3.070463	-0.170758	-4.391163
14	-2.590077	-1.075894	1.307344
6	-4.234158	-0.137273	1.542395
1	-4.816823	-0.637464	2.326416
1	-4.843185	-0.150554	0.631663
1	-4.105174	0.900824	1.849581
6	-3.220808	-2.860315	0.652854
6	-4.373095	-3.414842	1.553994
1	-4.037494	-3.687560	2.556864
1	-4.761954	-4.332928	1.085027
1	-5.215735	-2.719587	1.649198
6	-3.841512	-2.751845	-0.768792
1	-4.800377	-2.218328	-0.747928
1	-4.047928	-3.764573	-1.149904
1	-3.178970	-2.260747	-1.484994
6	-2.113768	-3.946771	0.610602
1	-1.713581	-4.171319	1.607530
1	-1.295295	-3.633261	-0.037286
1	-2.537753	-4.884359	0.214697
6	-1.794226	-1.231245	3.096418
6	-1.709568	0.182474	3.732059
1	-1.212793	0.123088	4.712488
1	-2.708440	0.608386	3.893301
1	-1.141202	0.881272	3.113835
6	-2.650484	-2.093157	4.071972
1	-2.255371	-1.967289	5.092554
1	-2.592737	-3.160628	3.835169
1	-3.707585	-1.799449	4.090837
6	-0.385231	-1.872745	3.037785
1	0.080043	-1.852193	4.035412
1	0.272692	-1.346914	2.342252
1	-0.436380	-2.918754	2.718192
6	-2.723551	3.138102	1.488449

1	-2.544960	2.150568	1.916447
1	-3.556146	3.595934	2.044066
1	-1.832391	3.742075	1.683608

Int-C=C=C-1MeOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

6	-1.336313	0.090124	0.218185
6	0.094015	-0.333054	-0.287689
6	1.412693	0.088492	-0.103566
14	-2.399621	1.462384	-0.943103
14	-2.410973	-1.335610	1.249731
14	2.781401	-1.093915	-0.985326
14	2.036871	1.712555	0.864921
6	-1.022796	2.331945	-1.936064
1	-0.305940	2.848345	-1.294819
1	-1.441405	3.076627	-2.621578
1	-0.455381	1.607942	-2.531486
6	-3.296259	2.873981	0.215786
6	-2.970688	4.278355	-0.392191
1	-3.446548	5.053424	0.228835
1	-3.342155	4.403731	-1.414575
1	-1.893219	4.481623	-0.400160
6	-4.851631	2.755176	0.293205
1	-5.176787	1.828370	0.775105
1	-5.344694	2.823313	-0.678407
1	-5.232143	3.589854	0.902036
6	-3.700282	0.986230	-2.420328
6	-4.145569	2.330977	-3.091851
1	-4.606939	3.039669	-2.402897
1	-4.893615	2.097772	-3.865035
1	-3.311121	2.836737	-3.591935
6	-4.986974	0.233834	-1.980596
1	-4.759378	-0.733629	-1.529657
1	-5.612293	0.040228	-2.867023
1	-5.594148	0.804368	-1.273724
6	-2.816493	2.942149	1.698358
1	-2.810373	1.974238	2.204817
1	-3.501235	3.596706	2.258782

1	-1.820001	3.373631	1.789859
6	-3.080378	0.167350	-3.595943
1	-3.022404	-0.903113	-3.381115
1	-2.085360	0.523689	-3.886705
1	-3.733450	0.272375	-4.475619
6	-4.103407	-0.541525	1.632101
1	-4.620401	-1.145821	2.388256
1	-4.750883	-0.498980	0.750313
1	-4.019902	0.468183	2.037660
6	-2.943912	-3.127834	0.511519
6	-3.906618	-3.841840	1.520079
1	-3.415361	-4.140149	2.446037
1	-4.279097	-4.761521	1.042356
1	-4.782665	-3.233250	1.772792
6	-3.792966	-3.048676	-0.793008
1	-4.756093	-2.557980	-0.608057
1	-4.017032	-4.073467	-1.127999
1	-3.305716	-2.540490	-1.624875
6	-1.746739	-4.089537	0.283664
1	-1.242345	-4.331232	1.227411
1	-0.994717	-3.677873	-0.390548
1	-2.112077	-5.038245	-0.140869
6	-1.532034	-1.525268	3.014510
6	-1.538271	-0.142461	3.728800
1	-0.996234	-0.223207	4.683206
1	-2.559237	0.189010	3.958001
1	-1.049406	0.642718	3.145954
6	-2.253803	-2.498996	3.992688
1	-1.838890	-2.354906	5.002696
1	-2.085331	-3.547532	3.726867
1	-3.335378	-2.324818	4.054308
6	-0.069618	-2.017847	2.872497
1	0.424456	-2.018460	3.856806
1	0.512516	-1.381040	2.202134
1	-0.027227	-3.041421	2.484042
6	2.943443	3.079863	-0.312442
6	0.494944	2.623571	1.494723
1	0.762074	3.593760	1.921867
1	-0.014803	2.058881	2.278868
1	-0.214310	2.809931	0.690546
6	3.048202	1.507283	2.590958
6	4.475151	3.244856	-0.082543
1	4.857805	4.002848	-0.784579
1	5.036132	2.324576	-0.259607
1	4.708685	3.595378	0.928341
6	2.316079	4.484475	-0.038126

1	1.248552	4.519730	-0.285715
1	2.824774	5.227933	-0.671332
1	2.433597	4.806137	1.003361
6	2.734888	2.798871	-1.824755
1	1.686139	2.630462	-2.083345
1	3.302455	1.927781	-2.156382
1	3.089792	3.663645	-2.408084
6	2.265891	0.588147	3.569748
1	1.228100	0.906837	3.713506
1	2.754994	0.610939	4.557007
1	2.257592	-0.450960	3.232306
6	3.116628	2.915467	3.267470
1	2.123939	3.303591	3.519060
1	3.629916	3.663169	2.653405
1	3.677726	2.826181	4.210521
6	4.502824	0.964813	2.544558
1	5.159595	1.553031	1.897619
1	4.540535	-0.079330	2.225187
1	4.926068	1.001999	3.561245
6	2.675140	-1.357137	-2.966923
6	4.470401	-0.225831	-0.775324
1	4.640558	0.142721	0.235043
1	4.595024	0.613663	-1.463107
1	5.274581	-0.935757	-1.000578
6	3.095710	-2.826360	-0.064377
6	4.111541	-1.398317	-3.581735
1	4.658039	-0.460240	-3.435654
1	4.030236	-1.564371	-4.667978
1	4.720371	-2.211383	-3.169454
6	1.999402	-2.693694	-3.388888
1	2.599255	-3.561189	-3.093500
1	1.906466	-2.723368	-4.486710
1	1.006512	-2.822046	-2.961980
6	1.935189	-0.181175	-3.667015
1	2.543345	0.729481	-3.667567
1	0.985062	0.066537	-3.185112
1	1.732626	-0.439573	-4.718796
6	4.280524	-3.601285	-0.719633
1	5.212483	-3.022432	-0.725597
1	4.065762	-3.911064	-1.747811
1	4.470567	-4.516303	-0.136313
6	3.510762	-2.564142	1.411290
1	2.746425	-2.005327	1.960505
1	4.457822	-2.016023	1.478592
1	3.653269	-3.526432	1.928488
6	1.873307	-3.776745	-0.035676

1	1.028038	-3.315229	0.474456
1	2.141032	-4.701949	0.502069
1	1.539333	-4.057347	-1.039124
8	0.044661	-1.557274	-1.051134
6	-0.949126	-1.656126	-2.103401
1	-1.898638	-1.266919	-1.752240
1	-1.057333	-2.714381	-2.350501
1	-0.630813	-1.104236	-2.991130
1	-1.141686	0.774987	1.052571

TS2-C=C=C-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

8	0.377754	0.768585	-2.463913
6	0.066297	-0.294003	-0.538623
6	1.500308	0.257456	-0.264207
1	1.535176	0.760026	-1.290523
6	0.087047	0.764266	-3.873778
1	0.416704	1.715567	-4.333055
1	-0.986235	0.659825	-4.102772
1	0.603031	-0.055575	-4.412608
8	0.197467	-1.543153	-1.119437
6	-0.721839	-1.907255	-2.195045
1	-1.670035	-1.395005	-2.060273
1	-0.844514	-2.991138	-2.169096
1	-0.273680	-1.588255	-3.135760
6	-1.372848	0.012427	0.077202
1	-1.151250	0.697104	0.904652
14	-2.814236	1.350145	-0.861111
6	-1.866522	2.572011	-1.975605
1	-0.867814	2.816398	-1.609440
1	-2.448370	3.493193	-2.084815
1	-1.723397	2.152463	-2.971716
6	-3.762735	2.561373	0.506925
6	-3.773809	4.026169	-0.047053
1	-4.298084	4.665208	0.680661
1	-4.300060	4.122095	-1.003179
1	-2.763572	4.430463	-0.169806
6	-5.261241	2.221303	0.786825

1	-5.416331	1.229015	1.212602
1	-5.885395	2.308912	-0.106859
1	-5.646883	2.950843	1.516075
6	-4.229729	0.658923	-2.128305
6	-4.908965	1.925165	-2.753711
1	-5.395602	2.565798	-2.013649
1	-5.690226	1.587663	-3.452527
1	-4.200868	2.535991	-3.323696
6	-5.366378	-0.220158	-1.538856
1	-4.987607	-1.163070	-1.143445
1	-6.075046	-0.470847	-2.344554
1	-5.933390	0.281781	-0.752899
6	-3.056367	2.671317	1.888007
1	-2.866191	1.708938	2.365593
1	-3.696497	3.251380	2.570770
1	-2.107525	3.203720	1.807211
6	-3.654557	-0.130040	-3.339198
1	-3.327695	-1.138205	-3.068656
1	-2.823374	0.387132	-3.825830
1	-4.449711	-0.250158	-4.091818
14	-2.296381	-1.521751	1.182921
6	-4.010424	-0.885258	1.709641
1	-4.364925	-1.533371	2.521142
1	-4.758028	-0.920894	0.916049
1	-3.978990	0.127173	2.108384
6	-2.722607	-3.342463	0.457835
6	-3.719300	-4.070766	1.424384
1	-3.296719	-4.281589	2.406821
1	-3.982509	-5.038083	0.968426
1	-4.653377	-3.514526	1.560439
6	-3.489569	-3.331818	-0.900167
1	-4.540034	-3.057290	-0.749568
1	-3.484142	-4.349091	-1.322717
1	-3.079367	-2.663176	-1.654359
6	-1.478735	-4.264566	0.343132
1	-1.015265	-4.438181	1.321980
1	-0.707892	-3.866342	-0.317820
1	-1.786435	-5.246490	-0.049269
6	-1.374141	-1.652704	2.931791
6	-1.507013	-0.292275	3.673963
1	-0.924434	-0.329198	4.606560
1	-2.547119	-0.075947	3.945372
1	-1.123194	0.548306	3.089351
6	-1.982953	-2.717623	3.891915
1	-1.521771	-2.594075	4.884440
1	-1.767904	-3.740993	3.565663

1	-3.067034	-2.612393	4.021586
6	0.121183	-1.992990	2.778132
1	0.628630	-1.922828	3.752070
1	0.623868	-1.312320	2.086233
1	0.265688	-3.012344	2.411779
14	1.934161	1.909679	0.860263
6	2.904191	3.289450	-0.240364
6	4.413330	3.481001	0.094841
1	4.824937	4.255296	-0.571733
1	5.004118	2.575064	-0.059021
1	4.576612	3.822671	1.122691
6	2.230469	4.682250	-0.018768
1	1.192553	4.697770	-0.370619
1	2.784871	5.436096	-0.599442
1	2.241758	5.003170	1.029115
6	2.801269	2.999515	-1.761929
1	1.769799	2.832114	-2.092943
1	3.382291	2.119427	-2.046959
1	3.210188	3.857300	-2.320308
6	2.729444	1.856007	2.714503
6	1.845412	1.016009	3.674538
1	0.820447	1.394641	3.735530
1	2.269956	1.063679	4.690150
1	1.806383	-0.035585	3.386396
6	0.258547	2.717678	1.227292
1	0.388721	3.732629	1.612963
1	-0.288271	2.154889	1.986046
1	-0.356810	2.785326	0.329058
6	2.704304	3.315668	3.277021
1	1.694758	3.739806	3.303583
1	3.349610	3.999094	2.717034
1	3.073536	3.294763	4.314362
6	4.185625	1.344210	2.896556
1	4.911954	1.889358	2.286055
1	4.279906	0.276451	2.681916
1	4.476607	1.485237	3.949926
14	3.077498	-1.040225	-0.692617
6	3.492636	-1.436464	-2.613426
6	4.628142	-0.027565	-0.237795
1	4.514024	0.572794	0.659181
1	4.916668	0.638635	-1.057403
1	5.471833	-0.707679	-0.063036
6	3.242358	-2.684073	0.400311
6	4.491720	-3.537601	0.023774
1	4.365102	-4.049462	-0.935954
1	4.621213	-4.317169	0.791937

1	5.420272	-2.955108	-0.012789
6	3.447516	-2.279446	1.888506
1	2.694309	-1.575809	2.247614
1	4.434478	-1.823684	2.037113
1	3.400445	-3.175827	2.526899
6	2.022201	-3.627843	0.278816
1	1.093587	-3.116578	0.512423
1	2.137158	-4.481828	0.966867
1	1.925860	-4.030089	-0.737131
6	4.977097	-1.910458	-2.774709
1	5.694558	-1.225931	-2.309356
1	5.209037	-1.938402	-3.851571
1	5.157285	-2.913129	-2.381770
6	2.608775	-2.539294	-3.249294
1	2.661919	-3.481731	-2.690044
1	2.956975	-2.743456	-4.274760
1	1.562858	-2.236749	-3.308080
6	3.391540	-0.148930	-3.480843
1	4.212229	0.544961	-3.254370
1	2.446810	0.374215	-3.339335
1	3.490436	-0.419749	-4.544376

TS3-C=C=C-3MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

6	-1.442691	-0.144476	0.011949
6	0.002181	0.128193	0.125775
6	1.277943	0.354581	0.172314
14	-2.533209	1.247762	-1.231488
14	-2.471102	-0.938644	1.596425
14	2.959269	-1.348037	-0.339867
14	2.004499	2.199130	0.506854
6	-1.213153	1.890678	-2.441903
1	-0.206422	1.817988	-2.029485
1	-1.410433	2.924177	-2.749163
1	-1.214255	1.273357	-3.344098
6	-3.450172	2.856747	-0.392705
6	-3.233694	4.093967	-1.324868
1	-3.778718	4.949678	-0.895951

1	-3.614358	3.937041	-2.340652
1	-2.179193	4.382363	-1.394905
6	-4.998864	2.704774	-0.264084
1	-5.303280	1.874648	0.375809
1	-5.489931	2.585589	-1.233780
1	-5.397825	3.626983	0.185851
6	-3.834856	0.352994	-2.468418
6	-4.272743	1.413198	-3.534007
1	-4.870403	2.227619	-3.111464
1	-4.902917	0.907538	-4.283097
1	-3.421410	1.851650	-4.067890
6	-5.134316	-0.239004	-1.856404
1	-4.921333	-1.058302	-1.170536
1	-5.750139	-0.653820	-2.670455
1	-5.744990	0.500472	-1.334691
6	-2.913308	3.278071	1.007922
1	-2.654486	2.434028	1.647345
1	-3.678843	3.868459	1.535146
1	-2.027479	3.910978	0.915226
6	-3.143576	-0.796155	-3.256701
1	-2.714466	-1.560286	-2.605249
1	-2.339903	-0.425427	-3.901765
1	-3.888566	-1.277431	-3.910225
6	-4.156807	-0.064218	1.718867
1	-4.687433	-0.442818	2.600915
1	-4.792594	-0.260192	0.850933
1	-4.067436	1.014855	1.841236
6	-3.004448	-2.845865	1.358325
6	-4.049091	-3.256637	2.443973
1	-3.616348	-3.326778	3.445401
1	-4.434494	-4.255592	2.186753
1	-4.910511	-2.580113	2.486533
6	-3.711563	-3.047792	-0.011163
1	-4.699341	-2.572733	-0.028161
1	-3.873998	-4.125529	-0.171574
1	-3.108302	-2.680395	-0.845322
6	-1.843345	-3.868535	1.419589
1	-1.256657	-3.787539	2.342444
1	-1.181938	-3.751381	0.558356
1	-2.264548	-4.886780	1.390230
6	-1.627806	-0.574735	3.340254
6	-1.618358	0.958397	3.592266
1	-1.094792	1.168865	4.537413
1	-2.632314	1.366636	3.680700
1	-1.092538	1.504680	2.803503
6	-2.412021	-1.219399	4.518854

1	-2.022001	-0.813259	5.465444
1	-2.271574	-2.305128	4.550807
1	-3.488040	-1.010816	4.487256
6	-0.174855	-1.086318	3.428014
1	0.272174	-0.795391	4.392327
1	0.438188	-0.666401	2.630589
1	-0.119025	-2.176940	3.355671
6	3.062166	3.010400	-0.970452
6	0.406629	3.212979	0.557417
1	0.558467	4.205684	0.995858
1	-0.337650	2.692672	1.159665
1	-0.011400	3.351566	-0.443584
6	2.787810	2.509003	2.311258
6	4.604827	2.818714	-0.909008
1	5.078113	3.527119	-1.605676
1	4.904838	1.816202	-1.221406
1	5.025166	3.009376	0.086607
6	2.802923	4.555334	-0.944557
1	1.740827	4.805995	-1.035638
1	3.319881	5.002617	-1.807043
1	3.192941	5.040576	-0.044126
6	2.572953	2.503074	-2.355029
1	1.537437	2.801311	-2.556247
1	2.628190	1.414933	-2.445942
1	3.199990	2.950873	-3.142782
6	1.683390	2.245863	3.372952
1	0.805848	2.884226	3.225560
1	2.084942	2.465838	4.374058
1	1.350397	1.204864	3.370164
6	3.180788	4.016295	2.416586
1	2.363096	4.693732	2.144945
1	4.051088	4.258175	1.796240
1	3.451410	4.232906	3.461136
6	4.039982	1.702910	2.746876
1	4.914405	1.903273	2.117101
1	3.861557	0.625808	2.757774
1	4.306066	2.001553	3.772877
6	3.602949	-2.227006	-2.007652
6	4.497905	-0.341729	0.156429
1	4.295257	0.646728	0.551031
1	5.182152	-0.233519	-0.689542
1	5.026544	-0.898668	0.942036
6	2.689240	-2.621244	1.139635
6	4.961412	-2.962907	-1.718442
1	5.664398	-2.384259	-1.108059
1	5.446360	-3.142311	-2.689683

1	4.816141	-3.937942	-1.249698
6	2.635338	-3.282009	-2.594522
1	2.337050	-4.028424	-1.846109
1	3.132871	-3.816974	-3.418772
1	1.733306	-2.802485	-2.967883
6	3.933146	-1.144097	-3.071971
1	4.832880	-0.573251	-2.800921
1	3.106007	-0.451881	-3.214778
1	4.140938	-1.635761	-4.034723
6	3.720353	-3.792205	1.083862
1	4.761244	-3.451048	1.034629
1	3.530740	-4.472846	0.248804
1	3.610968	-4.374399	2.012160
6	2.928483	-1.932486	2.513765
1	2.398212	-0.985743	2.621518
1	3.996499	-1.746773	2.686847
1	2.582572	-2.601292	3.316268
6	1.287408	-3.251011	1.086363
1	0.503227	-2.498196	1.130834
1	1.153351	-3.939862	1.934655
1	1.127290	-3.812730	0.160596
8	0.858485	-0.849756	-2.367144
6	0.738150	-0.550562	-3.766418
1	1.369267	-1.194186	-4.410169
1	1.022862	0.496366	-3.975364
1	-0.301426	-0.679406	-4.119031
8	-0.706229	-2.574642	-1.610325
6	-1.013109	-3.600877	-2.578201
1	-0.232393	-4.380679	-2.618338
1	-1.129854	-3.188583	-3.596313
1	-1.959971	-4.086971	-2.301816
1	0.042134	-1.825645	-1.975761
1	-1.455022	-0.992304	-0.726998

TS4-C=C=C-3MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.440673	-0.020673	0.274013
6	-0.077075	-0.426895	-0.337091

6	1.430980	0.136615	-0.195437
14	-2.720838	1.550310	-0.648137
14	-2.592177	-1.639946	0.885004
14	3.124078	-1.161477	-0.427705
14	1.870006	1.827305	1.087835
6	-1.718967	2.767116	-1.724032
1	-0.651770	2.781363	-1.536546
1	-2.107935	3.784421	-1.606809
1	-1.829396	2.468335	-2.767940
6	-3.452789	2.623539	0.942049
6	-3.218372	4.143091	0.655536
1	-3.610427	4.725890	1.503882
1	-3.742115	4.484974	-0.244707
1	-2.156961	4.388556	0.545328
6	-4.986137	2.474898	1.198773
1	-5.278519	1.462586	1.483864
1	-5.596126	2.778231	0.344318
1	-5.258989	3.138917	2.034201
6	-4.259978	1.211385	-1.933471
6	-4.806472	2.632542	-2.317020
1	-5.223619	3.189470	-1.473993
1	-5.619338	2.493390	-3.047027
1	-4.043473	3.253769	-2.794806
6	-5.486120	0.383418	-1.462792
1	-5.233189	-0.660317	-1.263353
1	-6.239273	0.382381	-2.266633
1	-5.965198	0.798847	-0.573032
6	-2.773354	2.340221	2.313790
1	-2.854461	1.295591	2.624749
1	-3.273645	2.944728	3.086467
1	-1.719423	2.625146	2.324681
6	-3.781392	0.594810	-3.277745
1	-3.333187	-0.388252	-3.155968
1	-3.052011	1.232026	-3.783817
1	-4.650528	0.491882	-3.947882
6	-4.261791	-0.948867	1.488876
1	-4.808320	-1.770366	1.968009
1	-4.901139	-0.554806	0.703844
1	-4.130965	-0.171417	2.243333
6	-3.048933	-3.096198	-0.394759
6	-4.452086	-3.688667	-0.041206
1	-4.490051	-4.126741	0.961833
1	-4.690295	-4.489631	-0.758918
1	-5.248881	-2.939215	-0.113149
6	-3.144449	-2.592268	-1.858741
1	-4.076174	-2.046314	-2.029688

1	-3.148872	-3.449797	-2.550425
1	-2.315035	-1.935588	-2.126733
6	-2.043621	-4.283878	-0.363326
1	-2.070889	-4.826995	0.586608
1	-1.015585	-3.963349	-0.535788
1	-2.313979	-5.002711	-1.153129
6	-1.939907	-2.431396	2.580687
6	-2.040244	-1.373179	3.720582
1	-1.513861	-1.744401	4.613850
1	-3.083925	-1.194741	4.006112
1	-1.597071	-0.412324	3.457262
6	-2.812676	-3.631048	3.061228
1	-2.440394	-3.958831	4.045157
1	-2.761182	-4.495773	2.393211
1	-3.867603	-3.358692	3.189950
6	-0.483834	-2.928109	2.464299
1	-0.069671	-3.162807	3.457148
1	0.154841	-2.176577	2.000956
1	-0.413425	-3.833121	1.851990
6	3.377897	3.134438	0.650398
6	0.384758	2.958380	0.785814
1	0.298777	3.714996	1.572054
1	-0.554524	2.424176	0.723446
1	0.525497	3.479785	-0.162898
6	1.904725	1.474964	3.042285
6	4.676273	3.006757	1.503921
1	5.403883	3.748542	1.138502
1	5.158581	2.029894	1.452962
1	4.490613	3.237190	2.559544
6	2.852355	4.581933	0.959862
1	2.060554	4.895357	0.274181
1	3.693983	5.278227	0.821121
1	2.491280	4.708169	1.985127
6	3.753142	3.165499	-0.855322
1	2.862842	3.287481	-1.482110
1	4.261807	2.258176	-1.191306
1	4.441405	4.009728	-1.033631
6	0.657594	0.639384	3.404847
1	-0.263486	1.189973	3.185774
1	0.651444	0.406343	4.481102
1	0.627281	-0.310207	2.864207
6	1.790353	2.814222	3.836438
1	0.908079	3.401837	3.557514
1	2.676075	3.447603	3.723368
1	1.696035	2.574502	4.907297
6	3.148833	0.740085	3.608459

1	4.077711	1.292018	3.440704
1	3.260868	-0.260920	3.193117
1	3.027063	0.624101	4.697644
6	3.923221	-1.347856	-2.301530
6	4.532748	-0.197756	0.400514
1	4.412802	-0.123349	1.481866
1	4.630040	0.805374	-0.003903
1	5.484748	-0.708726	0.211897
6	3.209226	-2.877682	0.623162
6	5.121068	-2.347886	-2.252317
1	5.825328	-2.146378	-1.439470
1	5.682214	-2.263201	-3.196415
1	4.783554	-3.387484	-2.168151
6	3.055095	-1.822376	-3.498516
1	2.587372	-2.800181	-3.333166
1	3.709793	-1.927344	-4.377786
1	2.283557	-1.094166	-3.768795
6	4.515264	0.031528	-2.725677
1	5.340767	0.344540	-2.076772
1	3.757805	0.819377	-2.737864
1	4.926983	-0.058352	-3.743709
6	4.661547	-3.458365	0.702189
1	5.411788	-2.703250	0.959676
1	4.975102	-3.959989	-0.215427
1	4.674996	-4.212926	1.504508
6	2.846948	-2.555345	2.103999
1	2.028155	-1.844115	2.209229
1	3.716332	-2.146568	2.630858
1	2.554612	-3.478389	2.625381
6	2.318799	-4.044665	0.126773
1	1.253488	-3.829116	0.241638
1	2.535602	-4.944187	0.723216
1	2.527334	-4.298423	-0.921934
8	-0.202460	-1.744979	-0.699851
6	0.411999	-2.300072	-1.907390
1	1.045245	-1.551118	-2.357545
1	-0.409551	-2.539283	-2.585465
1	0.952070	-3.206055	-1.647579
1	-1.241224	0.550588	1.188827
8	-0.442860	0.337432	-2.516009
6	-0.611385	-0.174859	-3.858422
1	-0.961156	0.632959	-4.527295
1	-1.364008	-0.976659	-3.913173
1	0.323981	-0.570749	-4.298049
1	0.519535	1.328782	-2.597213
8	1.358376	2.012313	-2.588805

1	1.578142	0.738387	-1.118359
6	1.867674	2.336324	-3.898456
1	2.820247	2.871050	-3.779254
1	1.177042	2.987028	-4.461393
1	2.062719	1.433751	-4.504622

Pro-C=C=C-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

6	-1.429882	0.055383	0.089198
6	0.002859	-0.002714	-0.743615
6	1.465061	0.116503	-0.003484
14	-2.932237	1.377957	-0.813806
14	-2.207691	-1.553618	1.131531
14	2.986838	-1.108785	-0.722394
14	2.065027	2.003389	0.627832
6	-2.197078	2.781342	-1.904455
1	-1.339460	3.277807	-1.449234
1	-2.962446	3.540606	-2.085686
1	-1.878417	2.385162	-2.871916
6	-3.888849	2.449529	0.637889
6	-3.942899	3.958681	0.229704
1	-4.425717	4.520560	1.044938
1	-4.529691	4.136424	-0.678992
1	-2.945539	4.386713	0.081307
6	-5.367015	2.045730	0.926411
1	-5.472895	1.025992	1.300962
1	-6.009284	2.153483	0.046199
1	-5.767455	2.719825	1.700761
6	-4.310436	0.701610	-2.144250
6	-5.096277	1.954633	-2.664127
1	-5.537904	2.554927	-1.863482
1	-5.921955	1.602774	-3.301894
1	-4.471297	2.610802	-3.277609
6	-5.384137	-0.307011	-1.653623
1	-4.948399	-1.254100	-1.334440
1	-6.067092	-0.533426	-2.488719
1	-5.995044	0.089423	-0.837089
6	-3.134261	2.424620	1.993132

1	-3.062832	1.422047	2.413148
1	-3.674283	3.049679	2.722288
1	-2.122723	2.833359	1.903156
6	-3.657631	0.070216	-3.410674
1	-3.342438	-0.962731	-3.237755
1	-2.795298	0.640732	-3.775479
1	-4.403117	0.044707	-4.221266
6	-4.025099	-1.107347	1.501161
1	-4.549739	-2.002233	1.857474
1	-4.562177	-0.743702	0.629051
1	-4.107971	-0.354823	2.290210
6	-2.414777	-3.387235	0.331895
6	-2.935675	-4.382386	1.418037
1	-2.178454	-4.588755	2.180636
1	-3.167270	-5.339452	0.924574
1	-3.850467	-4.043862	1.917907
6	-3.519355	-3.379714	-0.766671
1	-4.490038	-3.068797	-0.365074
1	-3.640778	-4.403019	-1.154693
1	-3.285134	-2.739429	-1.621441
6	-1.141785	-4.054014	-0.253295
1	-0.488279	-4.413559	0.547180
1	-0.552232	-3.387542	-0.879521
1	-1.432760	-4.933907	-0.849485
6	-1.477455	-1.660651	2.994004
6	-1.296655	-0.234681	3.583573
1	-0.730406	-0.297356	4.525461
1	-2.262679	0.225557	3.819595
1	-0.751248	0.438509	2.920123
6	-2.460610	-2.373100	3.978709
1	-2.076783	-2.239457	5.002871
1	-2.542304	-3.447463	3.804130
1	-3.468244	-1.944243	3.952195
6	-0.122452	-2.400487	3.089154
1	0.201385	-2.453556	4.141004
1	0.663715	-1.884686	2.531373
1	-0.183180	-3.426846	2.709431
6	3.235550	3.272675	-0.470093
6	0.421387	2.923544	0.881624
1	0.571333	3.966242	1.173752
1	-0.148663	2.440583	1.680549
1	-0.182877	2.899309	-0.024152
6	2.788177	1.997255	2.509887
6	4.704662	3.383212	0.045742
1	5.218634	4.162217	-0.538595
1	5.268937	2.455788	-0.083389

1	4.766850	3.679810	1.094634
6	2.618060	4.703751	-0.336715
1	1.606002	4.756175	-0.754286
1	3.245841	5.413024	-0.898604
1	2.576162	5.053991	0.700255
6	3.349984	3.021721	-2.001105
1	2.417200	3.248037	-2.521522
1	3.655171	2.002218	-2.254684
1	4.115100	3.699892	-2.409557
6	1.823230	1.222470	3.449334
1	0.843920	1.706390	3.513116
1	2.242702	1.206820	4.467576
1	1.668337	0.181451	3.148757
6	2.795938	3.465513	3.050468
1	1.808724	3.937695	2.995245
1	3.512343	4.110984	2.533732
1	3.086638	3.445137	4.112560
6	4.210165	1.418913	2.758321
1	4.987430	1.905944	2.165568
1	4.255472	0.346031	2.567703
1	4.470248	1.566456	3.818972
6	3.184582	-1.845385	-2.584111
6	4.594291	-0.101037	-0.502104
1	4.610980	0.452800	0.436840
1	4.764248	0.608433	-1.317158
1	5.452482	-0.783451	-0.490055
6	3.258626	-2.623333	0.541659
6	4.708035	-2.067056	-2.867335
1	5.248532	-1.116468	-2.948248
1	4.810138	-2.585309	-3.833851
1	5.211027	-2.677199	-2.114620
6	2.467271	-3.213135	-2.771512
1	2.940464	-4.013804	-2.194650
1	2.516337	-3.506840	-3.832318
1	1.415575	-3.160884	-2.479715
6	2.696295	-0.933195	-3.738937
1	3.116252	0.079970	-3.690367
1	1.608740	-0.866536	-3.763425
1	3.024643	-1.370618	-4.695288
6	4.493382	-3.512704	0.202381
1	5.426512	-2.937176	0.149804
1	4.376690	-4.067143	-0.733318
1	4.616851	-4.257076	1.005341
6	3.538120	-2.081879	1.971125
1	2.779843	-1.378896	2.327454
1	4.514259	-1.585858	2.021617

1	3.561157	-2.922308	2.682455
6	2.021855	-3.546651	0.601387
1	1.107120	-2.975552	0.746295
1	2.117303	-4.256767	1.439057
1	1.899737	-4.127972	-0.316037
8	0.162089	-1.257686	-1.492223
6	-0.856948	-1.534256	-2.496147
1	-1.839523	-1.579956	-2.032781
1	-0.607068	-2.503867	-2.931991
1	-0.867968	-0.771863	-3.279170
1	-1.203465	0.716873	0.937493
8	-0.226751	1.078065	-1.680271
6	0.672011	1.370774	-2.774037
1	0.554994	2.437711	-2.979835
1	0.394881	0.807319	-3.672391
1	1.702540	1.152463	-2.515620
1	1.298141	-0.359223	0.979297

TS1-Si=Si=Si-1MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

8	-0.320626	-2.322758	-1.205181
14	0.041395	-0.701046	-0.048067
14	-2.229743	-0.363369	-0.322362
1	-1.333403	-2.015909	-1.320466
6	-0.022601	-3.768108	-1.347957
1	0.065526	-4.233323	-0.361662
1	0.900081	-3.880933	-1.913999
1	-0.858523	-4.212447	-1.898171
14	2.119062	0.032194	-0.100182
14	4.034013	-1.168758	-0.931739
6	5.537112	-0.035456	-0.603140
1	5.626727	0.219951	0.460359
1	5.464264	0.901417	-1.168120
1	6.469553	-0.533523	-0.906434
6	4.386420	-2.823436	0.078468
6	5.786174	-3.404096	-0.279140
1	6.592197	-2.685927	-0.083001

1	5.856639	-3.717793	-1.325694
1	5.979474	-4.290159	0.345621
6	4.394733	-2.506859	1.600527
1	3.451631	-2.054306	1.933637
1	5.216656	-1.831190	1.869411
1	4.537711	-3.439630	2.168703
6	3.319515	-3.918868	-0.166758
1	2.322875	-3.571383	0.128331
1	3.553863	-4.807007	0.440796
1	3.283309	-4.236998	-1.216263
6	3.880548	-1.348330	-2.885137
6	5.121262	-2.073043	-3.484026
1	6.068029	-1.613862	-3.169910
1	5.078956	-2.021383	-4.583248
1	5.147579	-3.134449	-3.209103
6	2.606497	-2.116351	-3.325228
1	2.643795	-3.168389	-3.015687
1	2.527811	-2.103383	-4.423726
1	1.692129	-1.666113	-2.919592
6	3.812889	0.075734	-3.511447
1	4.723369	0.657704	-3.318998
1	2.953091	0.646023	-3.137708
1	3.705003	-0.012179	-4.603629
14	2.274481	1.997262	1.316337
6	3.239873	3.468332	0.417461
6	2.646770	4.831398	0.890704
1	1.593642	4.943324	0.607662
1	3.206049	5.652469	0.415201
1	2.722168	4.967163	1.976740
6	3.041093	3.380994	-1.122446
1	1.981784	3.311580	-1.403404
1	3.554177	2.511760	-1.551839
1	3.455911	4.282597	-1.600806
6	4.764549	3.497063	0.711758
1	5.235686	4.298900	0.121364
1	5.261049	2.557582	0.447447
1	4.971141	3.707178	1.768344
6	0.475175	2.594316	1.507866
1	0.413298	3.423972	2.224760
1	-0.188775	1.795723	1.854559
1	0.081728	2.947933	0.547937
6	2.926441	1.586706	3.120562
6	1.967715	0.550298	3.772640
1	0.943132	0.933057	3.858309
1	2.319231	0.310304	4.788317
1	1.927681	-0.386413	3.201471

6	2.915180	2.871646	4.000362
1	1.919278	3.330593	4.049710
1	3.623426	3.627628	3.638722
1	3.208648	2.611491	5.029332
6	4.360299	0.994411	3.140194
1	5.105859	1.692987	2.745893
1	4.418020	0.067522	2.561300
1	4.646560	0.753537	4.176502
14	-2.714173	1.472185	-1.791810
6	-1.036334	2.156368	-2.400531
1	-0.575935	2.807875	-1.647810
1	-1.167745	2.746019	-3.318485
1	-0.326191	1.348981	-2.610473
6	-3.707206	3.005299	-1.052425
6	-3.410867	4.283685	-1.893793
1	-3.972551	5.134073	-1.475182
1	-3.709557	4.174526	-2.942897
1	-2.346714	4.549223	-1.871059
6	-5.246155	2.794045	-1.024909
1	-5.532559	1.893516	-0.470234
1	-5.671375	2.718775	-2.032907
1	-5.725566	3.653844	-0.529894
6	-3.236276	3.280316	0.401144
1	-3.499092	2.454357	1.070579
1	-3.717025	4.195778	0.782816
1	-2.150290	3.423701	0.464749
6	-3.585453	0.670168	-3.367426
6	-4.030097	1.759535	-4.385190
1	-4.819179	2.405915	-3.983720
1	-4.429367	1.275449	-5.290728
1	-3.192171	2.397852	-4.697545
6	-4.821078	-0.185958	-2.976123
1	-4.536885	-1.004512	-2.302577
1	-5.266594	-0.635597	-3.878040
1	-5.599692	0.408207	-2.483217
6	-2.568930	-0.258802	-4.091438
1	-2.197762	-1.047162	-3.424873
1	-1.703432	0.299083	-4.471875
1	-3.058254	-0.743148	-4.951712
14	-3.622063	-1.189316	1.458680
6	-5.342529	-0.377710	1.254201
1	-6.051383	-0.783624	1.988537
1	-5.754404	-0.566956	0.254476
1	-5.299300	0.707162	1.398691
6	-3.935950	-3.126633	1.196770
6	-5.170093	-3.616485	2.012715

1	-5.053041	-3.469186	3.091122
1	-5.315622	-4.695157	1.840355
1	-6.091310	-3.109627	1.698482
6	-4.251646	-3.415767	-0.298740
1	-5.122219	-2.846234	-0.651767
1	-4.481906	-4.485709	-0.427665
1	-3.407181	-3.163202	-0.951014
6	-2.707637	-3.983984	1.607705
1	-2.545894	-3.970949	2.692570
1	-1.784553	-3.634603	1.125431
1	-2.866264	-5.033916	1.312476
6	-2.990509	-0.731975	3.269695
6	-2.984842	0.816695	3.413946
1	-2.611420	1.092151	4.413002
1	-3.990648	1.243789	3.309754
1	-2.334969	1.291076	2.669331
6	-3.941038	-1.301843	4.363340
1	-3.658186	-0.889508	5.344916
1	-3.872613	-2.393692	4.437876
1	-4.991157	-1.034561	4.184883
6	-1.553392	-1.238767	3.564947
1	-1.233295	-0.887251	4.559459
1	-0.829092	-0.862903	2.831387
1	-1.489938	-2.332843	3.568377

Int-Si=Si=Si-1MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-2.090577	0.028966	0.116456
14	0.104765	-0.583024	-0.590394
14	2.106681	0.167930	-0.087815
14	-3.195618	1.607079	-1.387849
14	-3.206299	-1.656928	1.478343
14	3.982914	-1.156132	-0.840203
14	2.252580	2.258738	1.101449
6	-1.756894	2.694938	-2.024463
1	-1.393487	3.364730	-1.235508
1	-2.083721	3.322658	-2.864665
1	-0.906960	2.089721	-2.361364

6	-4.396771	2.804153	-0.382063
6	-4.497517	4.175807	-1.117658
1	-5.174832	4.838415	-0.556198
1	-4.897404	4.080326	-2.133375
1	-3.524792	4.678176	-1.182063
6	-5.833082	2.234443	-0.223374
1	-5.837413	1.247522	0.253118
1	-6.350252	2.147958	-1.186532
1	-6.429304	2.911095	0.408809
6	-4.031424	0.792149	-2.960388
6	-4.760141	1.859748	-3.827177
1	-5.634093	2.279277	-3.315506
1	-5.116916	1.391912	-4.758151
1	-4.097661	2.688644	-4.109675
6	-5.051058	-0.319259	-2.592143
1	-4.582113	-1.123176	-2.014480
1	-5.461372	-0.767704	-3.511111
1	-5.894274	0.068782	-2.009809
6	-3.830046	3.083404	1.039262
1	-3.859420	2.190790	1.675546
1	-4.437038	3.860507	1.529737
1	-2.792086	3.440418	1.013043
6	-2.915480	0.158215	-3.837938
1	-2.339153	-0.591110	-3.284396
1	-2.213768	0.912286	-4.215830
1	-3.366342	-0.343868	-4.708281
6	-5.057083	-1.184166	1.575235
1	-5.582102	-1.831201	2.291993
1	-5.551516	-1.293709	0.601770
1	-5.192435	-0.148612	1.906973
6	-3.130776	-3.468961	0.737393
6	-4.110033	-4.421901	1.487682
1	-3.837064	-4.564544	2.537661
1	-4.088993	-5.411459	1.004405
1	-5.146242	-4.061155	1.450211
6	-3.593019	-3.434293	-0.745567
1	-4.642265	-3.124112	-0.838615
1	-3.506353	-4.440217	-1.184990
1	-2.982704	-2.754616	-1.350036
6	-1.701424	-4.074472	0.799489
1	-1.353488	-4.190136	1.834141
1	-0.967921	-3.468698	0.253597
1	-1.706863	-5.077704	0.343342
6	-2.469046	-1.468139	3.292573
6	-2.945235	-0.114552	3.897109
1	-2.495193	0.019589	4.893216

1	-4.035409	-0.081737	4.021764
1	-2.644366	0.743528	3.282871
6	-2.978902	-2.602921	4.227928
1	-2.666158	-2.387851	5.261939
1	-2.556943	-3.577704	3.955136
1	-4.074086	-2.688690	4.226449
6	-0.916305	-1.487541	3.309108
1	-0.557190	-1.397483	4.346908
1	-0.489527	-0.654623	2.739175
1	-0.507173	-2.416438	2.894791
6	3.151529	3.626926	0.003363
6	0.485385	2.915280	1.391530
1	0.521041	3.830763	1.997282
1	-0.140617	2.188854	1.917790
1	-0.012077	3.157481	0.446181
6	3.019817	2.013544	2.896769
6	4.700892	3.555570	0.071951
1	5.133834	4.298153	-0.617052
1	5.087265	2.572536	-0.218034
1	5.078036	3.784306	1.076970
6	2.717314	5.051662	0.464279
1	1.641079	5.214606	0.329944
1	3.242660	5.804609	-0.144158
1	2.961868	5.247393	1.514599
6	2.717215	3.465730	-1.481121
1	1.624949	3.489503	-1.596223
1	3.070682	2.520678	-1.909202
1	3.134650	4.289599	-2.081656
6	2.032874	1.159455	3.744310
1	1.069376	1.664595	3.887956
1	2.464534	0.979428	4.741422
1	1.838205	0.182913	3.282436
6	3.197274	3.388045	3.605684
1	2.265664	3.968596	3.628678
1	3.971317	4.001068	3.127285
1	3.507889	3.223016	4.649351
6	4.390890	1.288016	2.895509
1	5.147432	1.825548	2.312252
1	4.304393	0.271480	2.496380
1	4.765674	1.204868	3.928188
6	4.067446	-1.363323	-2.797496
6	5.572846	-0.191176	-0.387699
1	5.552801	0.206862	0.630060
1	5.734387	0.648629	-1.075299
1	6.445225	-0.853445	-0.471703
6	4.038681	-2.843441	0.166662

6	5.535158	-1.643814	-3.241520
1	6.206398	-0.812243	-2.994310
1	5.562032	-1.775938	-4.334902
1	5.944050	-2.554988	-2.789308
6	3.174804	-2.521343	-3.315916
1	3.561041	-3.499985	-3.003538
1	3.155261	-2.511124	-4.417778
1	2.148946	-2.433225	-2.950060
6	3.616655	-0.045071	-3.487659
1	4.220464	0.814540	-3.164114
1	2.565428	0.186942	-3.277638
1	3.735763	-0.138818	-4.578945
6	5.236650	-3.722464	-0.299717
1	6.198473	-3.196821	-0.225282
1	5.114059	-4.068071	-1.333309
1	5.301455	-4.616961	0.339528
6	4.244318	-2.519533	1.674258
1	3.415832	-1.920921	2.075208
1	5.182227	-1.978954	1.857471
1	4.284687	-3.458133	2.249008
6	2.737103	-3.678418	0.032456
1	1.854061	-3.115323	0.352612
1	2.815924	-4.579592	0.662317
1	2.555522	-4.003568	-0.996961
8	0.156412	-2.084141	-1.445208
6	-0.415008	-2.468182	-2.717618
1	-0.107950	-1.782390	-3.520951
1	-1.511158	-2.497313	-2.674109
1	-0.050396	-3.474623	-2.946941
1	-1.685159	0.991342	1.176177

TS2-Si=Si=Si-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-2.026265	0.014424	0.104503
14	0.086219	-0.351332	-0.965409
14	2.193108	0.401003	-0.370686
14	-3.575205	1.610647	-0.882023
14	-2.806096	-1.932428	1.343456

14	3.945046	-1.205090	-0.449347
14	2.265940	2.485499	0.783903
6	-2.460745	2.897967	-1.748628
1	-1.895229	3.481983	-1.014174
1	-3.064740	3.599851	-2.339038
1	-1.729253	2.426076	-2.409535
6	-4.544425	2.605909	0.525521
6	-4.803034	4.063187	0.035024
1	-5.390200	4.602287	0.794690
1	-5.366262	4.097298	-0.905485
1	-3.867769	4.616361	-0.110945
6	-5.915496	1.978016	0.895097
1	-5.826891	0.929414	1.198040
1	-6.627719	2.033072	0.062538
1	-6.355821	2.531398	1.739150
6	-4.734151	0.843311	-2.266015
6	-5.622557	1.947702	-2.909025
1	-6.317506	2.389932	-2.184797
1	-6.225585	1.509726	-3.719836
1	-5.023617	2.758024	-3.345559
6	-5.659049	-0.283845	-1.735137
1	-5.080117	-1.089748	-1.273622
1	-6.228980	-0.721118	-2.570011
1	-6.380534	0.081974	-0.998203
6	-3.691128	2.700003	1.822340
1	-3.560135	1.722777	2.301572
1	-4.193853	3.360698	2.546002
1	-2.691897	3.113796	1.633261
6	-3.848931	0.235220	-3.391656
1	-3.198330	-0.563415	-3.010489
1	-3.222885	0.997850	-3.872321
1	-4.489474	-0.205718	-4.171593
6	-4.611345	-1.551857	1.843366
1	-4.986144	-2.325351	2.526905
1	-5.282125	-1.518659	0.977701
1	-4.683382	-0.589159	2.361945
6	-2.826480	-3.608922	0.315665
6	-3.839261	-4.609641	0.950090
1	-3.582336	-4.867879	1.983395
1	-3.840653	-5.543472	0.366289
1	-4.863811	-4.216094	0.943288
6	-3.289448	-3.356976	-1.146437
1	-4.330402	-3.014066	-1.195300
1	-3.229766	-4.298024	-1.716527
1	-2.656002	-2.621670	-1.654715
6	-1.429646	-4.285075	0.260966

1	-1.082246	-4.587073	1.256057
1	-0.675164	-3.631968	-0.192153
1	-1.491493	-5.198408	-0.352406
6	-1.799853	-2.025557	3.033049
6	-2.070376	-0.742435	3.872879
1	-1.513399	-0.806052	4.820807
1	-3.132455	-0.625806	4.124050
1	-1.734669	0.165726	3.358578
6	-2.270267	-3.246281	3.878202
1	-1.765011	-3.227043	4.856382
1	-2.018930	-4.200910	3.400367
1	-3.351931	-3.229988	4.067979
6	-0.268082	-2.142901	2.821940
1	0.244212	-2.111245	3.796421
1	0.129522	-1.319323	2.216953
1	0.013605	-3.080685	2.334170
6	3.666698	3.631888	-0.031674
6	0.606134	3.344714	0.370968
1	0.547909	4.334540	0.843906
1	-0.246532	2.751801	0.720233
1	0.499248	3.482088	-0.711863
6	2.358246	2.402516	2.744436
6	5.042492	3.519245	0.681318
1	5.792754	4.107498	0.128652
1	5.403248	2.486046	0.729180
1	5.006497	3.914313	1.704151
6	3.226273	5.126364	0.017085
1	2.322010	5.303087	-0.578250
1	4.026817	5.755336	-0.404724
1	3.033387	5.475725	1.038879
6	3.872780	3.267558	-1.529019
1	2.936622	3.337031	-2.099700
1	4.251176	2.246457	-1.652770
1	4.598991	3.961236	-1.983669
6	1.089855	1.666551	3.260550
1	0.168340	2.209776	3.014008
1	1.134481	1.568260	4.356954
1	1.011078	0.658231	2.836894
6	2.372013	3.825682	3.371666
1	1.493772	4.413279	3.071663
1	3.270692	4.391589	3.096852
1	2.355090	3.745918	4.470401
6	3.596095	1.616905	3.252756
1	4.538451	2.108250	2.987969
1	3.614569	0.599586	2.846126
1	3.561211	1.534458	4.351060

6	4.319830	-1.750280	-2.313967
6	5.503175	-0.275519	0.158488
1	5.344064	0.160473	1.150917
1	5.773262	0.538495	-0.525978
1	6.363179	-0.954853	0.221994
6	3.694608	-2.726866	0.775136
6	5.829975	-2.096442	-2.476548
1	6.467415	-1.221276	-2.297420
1	6.019579	-2.437176	-3.507046
1	6.154112	-2.894740	-1.797819
6	3.480715	-2.981703	-2.753695
1	3.794892	-3.894670	-2.232928
1	3.618200	-3.157475	-3.833157
1	2.411686	-2.833460	-2.561937
6	4.006732	-0.590929	-3.300885
1	4.540492	0.333136	-3.041902
1	2.936008	-0.354998	-3.310854
1	4.308524	-0.880570	-4.320865
6	4.910720	-3.695370	0.717946
1	5.853924	-3.189708	0.965381
1	5.020975	-4.162245	-0.268586
1	4.770128	-4.506138	1.450760
6	3.581171	-2.189233	2.229834
1	2.732290	-1.502901	2.336583
1	4.490545	-1.665416	2.551625
1	3.421669	-3.031322	2.922359
6	2.404010	-3.533804	0.475885
1	1.521176	-2.887204	0.456661
1	2.250657	-4.291722	1.261661
1	2.449811	-4.056334	-0.484035
8	0.113683	-1.875316	-1.758174
6	-0.269257	-2.225046	-3.107698
1	-1.264614	-1.831726	-3.365974
1	-0.293815	-3.316958	-3.174204
1	0.464374	-1.841245	-3.830533
1	-1.495921	0.858126	1.213434
8	0.368161	0.858548	-2.526347
6	-0.019646	1.094784	-3.936003
1	0.006219	2.171999	-4.126589
1	-1.028933	0.712084	-4.087611
1	0.686454	0.575106	-4.592630
1	1.389948	1.075823	-2.175388

TS3-Si=Si=Si-3MeOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

14	2.207023	-0.216123	-0.204372
14	-0.005499	0.208001	-0.873461
14	-2.094128	0.033332	-0.087149
14	2.324329	-1.795522	1.612100
14	3.708793	1.661079	-0.426424
14	-3.733703	-1.572746	-0.837407
14	-2.751376	2.002436	1.158394
6	0.981791	-3.072699	1.160838
1	-0.014607	-2.624869	1.192000
1	0.992866	-3.923810	1.854573
1	1.134041	-3.455455	0.145212
6	1.885930	-1.098504	3.397644
6	1.192617	-2.195389	4.258266
1	0.962894	-1.791733	5.257303
1	1.823212	-3.082228	4.394727
1	0.246529	-2.521667	3.808355
6	3.124988	-0.571019	4.168702
1	3.683271	0.172863	3.585737
1	3.816287	-1.378565	4.439138
1	2.801514	-0.086993	5.103899
6	4.010083	-2.828710	1.554431
6	3.997289	-3.920466	2.665164
1	3.982046	-3.488143	3.672689
1	4.908721	-4.534734	2.584219
1	3.137358	-4.596342	2.570003
6	5.285449	-1.964395	1.735622
1	5.385876	-1.235291	0.924954
1	6.178595	-2.609830	1.712001
1	5.292963	-1.420992	2.686301
6	0.886755	0.078266	3.239051
1	1.351489	0.924496	2.717308
1	0.553280	0.426408	4.230261
1	-0.001599	-0.215375	2.664085
6	4.132342	-3.562452	0.186447
1	4.157563	-2.853799	-0.650533
1	3.304068	-4.260955	0.015798
1	5.068723	-4.143269	0.163068
6	4.793478	1.783736	1.144576
1	5.419932	2.685956	1.116923

1	5.456387	0.918849	1.255830
1	4.168662	1.838789	2.043673
6	4.929966	1.292002	-1.933304
6	6.183633	2.213386	-1.893115
1	5.935922	3.270105	-2.029738
1	6.877081	1.927431	-2.700188
1	6.726220	2.111668	-0.944347
6	5.448175	-0.170866	-1.851088
1	6.062494	-0.334720	-0.956436
1	6.078463	-0.393255	-2.727125
1	4.624312	-0.893626	-1.830347
6	4.213894	1.468899	-3.299448
1	3.886536	2.503252	-3.462317
1	3.333343	0.814925	-3.374836
1	4.898293	1.205148	-4.121832
6	2.806460	3.411303	-0.568798
6	2.283504	3.787268	0.848290
1	1.657404	4.691521	0.789434
1	3.110281	4.001584	1.536663
1	1.674149	2.990930	1.289600
6	3.788511	4.533271	-1.014717
1	3.285590	5.509266	-0.924529
1	4.092348	4.418467	-2.062283
1	4.693320	4.570064	-0.394580
6	1.611437	3.424893	-1.556924
1	1.160671	4.430259	-1.585433
1	0.826585	2.720483	-1.253104
1	1.916027	3.169724	-2.580117
6	-3.702308	1.640905	2.852565
6	-1.141609	2.903833	1.629273
1	-1.361264	3.858125	2.124606
1	-0.538457	3.118310	0.743448
1	-0.531012	2.306827	2.314172
6	-3.702592	3.237082	-0.060137
6	-5.249548	1.603991	2.719873
1	-5.690897	1.313899	3.686687
1	-5.591796	0.882328	1.970689
1	-5.658364	2.587928	2.458764
6	-3.352607	2.749647	3.892371
1	-2.283602	2.764303	4.135022
1	-3.901943	2.555067	4.827132
1	-3.635164	3.752330	3.546847
6	-3.231880	0.281638	3.441773
1	-2.144154	0.247857	3.581461
1	-3.510503	-0.559493	2.795957
1	-3.700778	0.121808	4.425889

6	-2.837399	3.477856	-1.330658
1	-1.838700	3.862668	-1.087289
1	-3.334191	4.217808	-1.978377
1	-2.707541	2.555095	-1.909642
6	-3.907747	4.613327	0.639052
1	-2.954479	5.078830	0.919865
1	-4.529631	4.535656	1.539933
1	-4.417690	5.301433	-0.054004
6	-5.088506	2.718864	-0.530574
1	-5.814862	2.670766	0.286742
1	-5.018680	1.724528	-0.983798
1	-5.495788	3.399900	-1.295202
6	-3.164002	-3.327681	-0.146933
6	-5.388731	-1.209086	0.048912
1	-5.749574	-0.190595	-0.125739
1	-5.293918	-1.351371	1.132740
1	-6.163602	-1.902988	-0.306691
6	-4.055855	-1.509485	-2.768651
6	-4.305287	-4.383327	-0.246828
1	-5.193498	-4.080124	0.322686
1	-3.952058	-5.335241	0.181062
1	-4.611515	-4.581274	-1.278691
6	-1.926258	-3.859148	-0.918154
1	-2.178752	-4.117093	-1.955048
1	-1.541372	-4.769974	-0.433414
1	-1.107818	-3.130351	-0.938686
6	-2.813937	-3.203315	1.365077
1	-3.697155	-2.939971	1.963466
1	-2.041568	-2.450505	1.556697
1	-2.440318	-4.170113	1.737348
6	-4.858126	-2.742780	-3.266899
1	-5.795528	-2.889043	-2.713747
1	-4.268100	-3.664197	-3.193308
1	-5.116565	-2.602923	-4.328477
6	-4.873350	-0.229278	-3.099429
1	-4.336184	0.678785	-2.797215
1	-5.855938	-0.224538	-2.610864
1	-5.040453	-0.169225	-4.186208
6	-2.728790	-1.433197	-3.562750
1	-2.168645	-0.535434	-3.291189
1	-2.940465	-1.398726	-4.643880
1	-2.072741	-2.290722	-3.372332
8	0.141585	-0.315011	-2.679614
6	0.071132	0.663129	-3.775261
1	1.065513	1.089907	-3.961063
1	-0.619711	1.465134	-3.499479

1	-0.293358	0.155681	-4.673788
8	1.820840	-1.996639	-2.637855
6	2.764856	-2.535629	-3.612295
1	3.196720	-1.738191	-4.231638
1	2.244705	-3.263833	-4.243594
1	3.566274	-3.041937	-3.062896
1	0.931796	-1.226335	-2.854873
1	2.226136	-1.465720	-1.711659

TS4-Si=Si=Si-3MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-2.066238	0.005100	-0.157069
14	0.090784	0.418753	0.812342
14	2.122042	-0.263721	0.116970
14	-3.478609	-1.805207	0.680358
14	-3.037150	2.021961	-1.156028
14	3.900098	1.345188	0.302445
14	2.216499	-2.238941	-1.256715
6	-2.298129	-3.052699	1.510104
1	-1.635973	-3.525262	0.777695
1	-2.869949	-3.849802	2.003919
1	-1.668820	-2.551386	2.251747
6	-4.317399	-2.751887	-0.846960
6	-4.452031	-4.264646	-0.491648
1	-4.952462	-4.788023	-1.321686
1	-5.048210	-4.432863	0.413617
1	-3.473410	-4.736711	-0.345477
6	-5.733384	-2.222613	-1.205091
1	-5.736341	-1.150431	-1.428610
1	-6.454557	-2.404852	-0.399164
1	-6.103432	-2.747489	-2.099955
6	-4.757856	-1.258142	2.065502
6	-5.561235	-2.490587	2.576303
1	-6.184688	-2.932737	1.790070
1	-6.231511	-2.178159	3.392739
1	-4.904082	-3.275362	2.972766
6	-5.767008	-0.176841	1.599395
1	-5.251267	0.712925	1.227206

1	-6.394380	0.135084	2.449879
1	-6.434606	-0.538127	0.811142
6	-3.440174	-2.657727	-2.127761
1	-3.388082	-1.633774	-2.516100
1	-3.876075	-3.291218	-2.916330
1	-2.412051	-3.002251	-1.956549
6	-3.967095	-0.679427	3.272494
1	-3.378461	0.202339	2.987529
1	-3.281860	-1.419606	3.699380
1	-4.670399	-0.372124	4.062923
6	-4.781678	1.517254	-1.753262
1	-5.220997	2.320090	-2.360685
1	-5.464684	1.315561	-0.921220
1	-4.734169	0.617833	-2.377481
6	-3.247694	3.560933	0.049092
6	-4.349301	4.518272	-0.498924
1	-4.109109	4.910741	-1.492762
1	-4.454630	5.378534	0.180911
1	-5.327106	4.023425	-0.557037
6	-3.712218	3.104566	1.459822
1	-4.725358	2.685537	1.438880
1	-3.732208	3.970902	2.140132
1	-3.043624	2.353867	1.895083
6	-1.927035	4.365768	0.206724
1	-1.634070	4.852050	-0.731404
1	-1.094162	3.735581	0.538723
1	-2.070772	5.162808	0.953829
6	-2.022701	2.432656	-2.788418
6	-2.182389	1.265290	-3.806971
1	-1.583562	1.482684	-4.705407
1	-3.224365	1.139994	-4.128379
1	-1.828881	0.310111	-3.403725
6	-2.567038	3.719941	-3.475114
1	-2.045811	3.865620	-4.434316
1	-2.393326	4.618012	-2.870620
1	-3.641488	3.653253	-3.693437
6	-0.511486	2.629918	-2.509383
1	0.029015	2.770501	-3.458332
1	-0.070803	1.761650	-2.005259
1	-0.313671	3.507303	-1.885005
6	3.770688	-3.403002	-0.845705
6	0.672921	-3.249087	-0.760370
1	0.581214	-4.156122	-1.372931
1	-0.241116	-2.660008	-0.890964
1	0.730647	-3.555157	0.291457
6	2.055831	-1.855733	-3.179251

6	5.024808	-3.090286	-1.708161
1	5.867817	-3.711963	-1.366161
1	5.333657	-2.042680	-1.632668
1	4.860524	-3.320226	-2.767452
6	3.385706	-4.893813	-1.097973
1	2.583414	-5.226616	-0.428703
1	4.263847	-5.530556	-0.903712
1	3.065771	-5.078920	-2.130046
6	4.178832	-3.295043	0.649294
1	3.351702	-3.574007	1.313385
1	4.503313	-2.280266	0.912947
1	5.019805	-3.978714	0.851085
6	0.710223	-1.122187	-3.425234
1	-0.153637	-1.739978	-3.148832
1	0.611962	-0.869852	-4.493012
1	0.654092	-0.187734	-2.855710
6	2.041514	-3.163715	-4.020363
1	1.232866	-3.840743	-3.713318
1	2.989163	-3.711879	-3.957361
1	1.875848	-2.914573	-5.080738
6	3.191501	-0.934381	-3.699349
1	4.172414	-1.419695	-3.665314
1	3.246667	-0.008303	-3.116827
1	2.994302	-0.656220	-4.747286
6	4.412106	1.624765	2.184962
6	5.420567	0.552206	-0.546898
1	5.250873	0.408460	-1.620854
1	5.663714	-0.423475	-0.112903
1	6.303475	1.196308	-0.431110
6	3.530466	3.001246	-0.700875
6	5.344926	2.856223	2.363189
1	6.219071	2.821675	1.699666
1	5.717971	2.886318	3.399588
1	4.812669	3.797312	2.179818
6	3.177787	1.825452	3.101603
1	2.574465	2.684013	2.788525
1	3.507064	1.994394	4.140284
1	2.523104	0.944983	3.087785
6	5.188822	0.371173	2.678637
1	6.161575	0.273369	2.180683
1	4.624930	-0.553107	2.499902
1	5.376402	0.450796	3.761613
6	4.801676	3.889845	-0.849472
1	5.637005	3.343175	-1.306521
1	5.142470	4.302432	0.104745
1	4.566311	4.739702	-1.509960

6	3.079576	2.630115	-2.141534
1	2.221478	1.950918	-2.140295
1	3.892333	2.158082	-2.710372
1	2.786757	3.543261	-2.683833
6	2.411659	3.843801	-0.032567
1	1.481172	3.277830	0.083306
1	2.200928	4.734280	-0.647479
1	2.707140	4.194709	0.966101
8	0.163405	1.923132	1.618953
6	-0.302207	2.355946	2.913181
1	0.362001	1.981332	3.700383
1	-1.324725	2.010972	3.115630
1	-0.288678	3.450782	2.920646
1	-1.540676	-0.649212	-1.388019
8	-0.300616	-0.760168	2.995736
6	-0.617106	-0.606901	4.418542
1	-0.968134	-1.563511	4.832230
1	-1.412588	0.132668	4.519589
1	0.264026	-0.271248	4.985734
1	0.448599	-1.438202	2.911549
8	1.813643	-2.218435	2.795414
1	2.184146	-1.689848	2.022596
6	2.727777	-2.277909	3.934335
1	3.705037	-2.664863	3.621259
1	2.282949	-2.963685	4.659658
1	2.858500	-1.285201	4.388535

Pro-Si=Si=Si-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	-2.069547	-0.010352	0.187696
14	-0.005029	-0.051154	-1.108123
14	2.061158	0.192130	0.127719
14	-3.663232	1.640167	-0.686470
14	-2.816695	-2.102140	1.220673
14	3.967520	-1.202515	-0.509147
14	2.306119	2.489293	0.914406
6	-2.602632	3.150838	-1.170395
1	-2.225827	3.669431	-0.280270

1	-3.199551	3.869916	-1.748615
1	-1.742451	2.832331	-1.766219
6	-4.893293	2.290401	0.718081
6	-5.314935	3.756988	0.393502
1	-6.007692	4.113358	1.172416
1	-5.830306	3.842185	-0.570303
1	-4.456153	4.437919	0.378794
6	-6.191230	1.451033	0.863435
1	-5.986637	0.392700	1.051612
1	-6.825011	1.519672	-0.029194
1	-6.781683	1.831477	1.712299
6	-4.580813	1.043854	-2.311686
6	-5.610709	2.107539	-2.794420
1	-6.451521	2.217104	-2.098893
1	-6.026798	1.798224	-3.766435
1	-5.151514	3.095301	-2.933441
6	-5.323433	-0.305607	-2.124680
1	-4.631549	-1.106959	-1.844517
1	-5.806232	-0.600772	-3.070285
1	-6.105003	-0.247227	-1.358889
6	-4.169054	2.313327	2.093806
1	-3.947300	1.303429	2.457099
1	-4.811469	2.803690	2.842442
1	-3.222106	2.868829	2.054117
6	-3.527733	0.866574	-3.441805
1	-2.733650	0.167770	-3.153734
1	-3.044254	1.816649	-3.698826
1	-4.018391	0.477381	-4.348206
6	-4.703860	-1.995716	1.503089
1	-5.059428	-2.891838	2.030238
1	-5.253937	-1.923193	0.557510
1	-4.973363	-1.128448	2.114287
6	-2.537887	-3.686852	0.097251
6	-3.309777	-4.920025	0.655757
1	-2.939676	-5.239969	1.634587
1	-3.183379	-5.767071	-0.037056
1	-4.386641	-4.727830	0.744014
6	-3.110213	-3.410805	-1.322004
1	-4.196977	-3.257905	-1.298937
1	-2.915714	-4.277522	-1.973770
1	-2.651119	-2.533765	-1.790021
6	-1.038419	-4.063441	-0.038925
1	-0.597484	-4.342975	0.926334
1	-0.443881	-3.248219	-0.467903
1	-0.937087	-4.935518	-0.705612
6	-2.006921	-2.198142	3.014211

6	-2.600815	-1.067886	3.905304
1	-2.128879	-1.102974	4.899621
1	-3.682525	-1.181953	4.051078
1	-2.411107	-0.071029	3.488446
6	-2.325056	-3.556291	3.705549
1	-1.993147	-3.515481	4.755002
1	-1.796759	-4.391063	3.229341
1	-3.398992	-3.785294	3.708581
6	-0.467267	-2.019392	2.986092
1	-0.068739	-2.063754	4.012306
1	-0.179566	-1.050484	2.562471
1	0.030663	-2.804125	2.405634
6	3.400696	3.659825	-0.223428
6	0.542607	3.218043	0.872695
1	0.514884	4.201166	1.362232
1	-0.174321	2.567544	1.385935
1	0.190211	3.343668	-0.157061
6	2.856500	2.460638	2.800682
6	4.924353	3.544394	0.047699
1	5.476314	4.174430	-0.668003
1	5.287278	2.517927	-0.065532
1	5.188387	3.887402	1.055531
6	2.984428	5.148258	-0.017292
1	1.934389	5.319059	-0.283474
1	3.599874	5.790386	-0.667178
1	3.131584	5.486157	1.014727
6	3.138342	3.312510	-1.714334
1	2.073122	3.395369	-1.964847
1	3.470060	2.295909	-1.960222
1	3.689146	4.010989	-2.364099
6	1.721663	1.824784	3.655382
1	0.796153	2.411899	3.605867
1	2.034635	1.786209	4.710649
1	1.490428	0.799657	3.340787
6	3.084881	3.907836	3.328414
1	2.205065	4.548006	3.179981
1	3.944867	4.391793	2.850075
1	3.287401	3.873170	4.410548
6	4.155851	1.645251	3.039357
1	5.009505	2.055138	2.486633
1	4.033455	0.595044	2.750704
1	4.414386	1.664261	4.110107
6	4.067793	-1.691941	-2.410494
6	5.568760	-0.219616	-0.145197
1	5.547157	0.260514	0.838457
1	5.739061	0.559990	-0.897936

1	6.436478	-0.892861	-0.170276
6	3.987967	-2.753235	0.700932
6	5.541974	-1.999968	-2.809654
1	6.194071	-1.126895	-2.683222
1	5.575615	-2.287363	-3.872494
1	5.968902	-2.827322	-2.231339
6	3.191901	-2.925215	-2.763080
1	3.571071	-3.843038	-2.297345
1	3.206624	-3.084703	-3.853939
1	2.153987	-2.773887	-2.450041
6	3.584265	-0.501007	-3.281306
1	4.135546	0.425234	-3.065911
1	2.516456	-0.317708	-3.126307
1	3.736386	-0.732433	-4.347712
6	5.150863	-3.719373	0.328516
1	6.127441	-3.216579	0.334794
1	5.008833	-4.179167	-0.656446
1	5.197831	-4.534938	1.067457
6	4.228366	-2.273299	2.161209
1	3.418388	-1.624015	2.516025
1	5.178065	-1.733095	2.268882
1	4.267182	-3.146407	2.831437
6	2.654847	-3.546735	0.672260
1	1.806780	-2.914425	0.956376
1	2.705211	-4.380962	1.390486
1	2.440995	-3.967673	-0.315259
8	0.246808	-1.493550	-2.021758
6	-0.379820	-1.961923	-3.242142
1	-1.314927	-1.429910	-3.465544
1	-0.595276	-3.029844	-3.131777
1	0.315024	-1.823682	-4.081045
1	-1.560921	0.726220	1.385516
8	-0.270442	1.209826	-2.253345
6	0.377209	1.520164	-3.509489
1	-0.053912	2.458887	-3.874551
1	0.192209	0.732759	-4.253289
1	1.459775	1.648255	-3.390977
1	1.650550	-0.463095	1.404435

TS1-Ge=Ge=Ge-1MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

8	-0.343961	-2.311578	-1.146822
32	0.078069	-0.795589	0.135337
32	-2.382581	-0.438891	-0.441557
1	-1.453733	-1.908598	-1.271163
6	-0.028463	-3.730021	-1.353628
1	0.104619	-4.241717	-0.393387
1	0.876078	-3.819830	-1.956825
1	-0.875174	-4.174081	-1.889660
32	2.226489	0.139916	-0.189323
14	4.187289	-1.171020	-0.964483
6	5.737946	-0.097939	-0.651846
1	5.909245	0.056821	0.420915
1	5.644266	0.889389	-1.118962
1	6.635002	-0.578018	-1.068318
6	4.467422	-2.851057	0.022578
6	5.842943	-3.476118	-0.353431
1	6.676149	-2.789932	-0.156327
1	5.890170	-3.776283	-1.405894
1	6.009526	-4.378514	0.255474
6	4.485451	-2.556246	1.549018
1	3.537288	-2.121581	1.890647
1	5.298507	-1.873934	1.827103
1	4.641267	-3.495549	2.102248
6	3.359300	-3.902504	-0.235119
1	2.372869	-3.516347	0.046588
1	3.550915	-4.798810	0.375656
1	3.322099	-4.220069	-1.284360
6	3.969457	-1.314675	-2.913480
6	5.181996	-2.035362	-3.569482
1	6.138916	-1.569442	-3.299057
1	5.088919	-1.985387	-4.665705
1	5.227154	-3.096122	-3.294265
6	2.671420	-2.063702	-3.318336
1	2.714310	-3.124368	-3.041686
1	2.542350	-2.016380	-4.411096
1	1.777617	-1.623193	-2.858210
6	3.890564	0.123316	-3.507290
1	4.801453	0.704887	-3.314043
1	3.033300	0.681858	-3.108701
1	3.764611	0.061499	-4.599287
14	2.370459	2.046372	1.416335
6	3.329414	3.531818	0.544825

6	2.777214	4.892044	1.067988
1	1.715771	5.022851	0.825081
1	3.329414	5.716959	0.590856
1	2.891959	5.001677	2.153403
6	3.089928	3.489026	-0.992200
1	2.022508	3.460401	-1.249520
1	3.566490	2.615363	-1.456030
1	3.521513	4.387922	-1.460167
6	4.860738	3.502495	0.797622
1	5.347073	4.301147	0.215578
1	5.312749	2.550108	0.496051
1	5.101911	3.674201	1.853829
6	0.559063	2.624650	1.602202
1	0.484480	3.448028	2.325224
1	-0.099372	1.818574	1.944496
1	0.165749	2.981996	0.643545
6	3.006931	1.589650	3.213053
6	2.026997	0.561714	3.847506
1	1.011171	0.964916	3.946144
1	2.377086	0.294005	4.856708
1	1.966224	-0.363589	3.258995
6	3.027468	2.857096	4.117121
1	2.043475	3.341294	4.171751
1	3.756194	3.600518	3.770366
1	3.310769	2.571531	5.142247
6	4.424283	0.959311	3.208592
1	5.186626	1.649804	2.831911
1	4.451164	0.051955	2.596425
1	4.708786	0.676589	4.234579
14	-2.766165	1.616963	-1.794088
6	-1.052982	2.274331	-2.333278
1	-0.588937	2.870024	-1.537229
1	-1.145453	2.915368	-3.221568
1	-0.362627	1.457408	-2.571098
6	-3.720418	3.137872	-0.992741
6	-3.423522	4.438998	-1.797770
1	-3.962407	5.283746	-1.339510
1	-3.745960	4.368841	-2.842893
1	-2.354804	4.687304	-1.789321
6	-5.258718	2.931507	-0.945980
1	-5.535155	2.007741	-0.423732
1	-5.699544	2.896855	-1.949789
1	-5.728565	3.771117	-0.409169
6	-3.218347	3.361315	0.459783
1	-3.463577	2.511875	1.106282
1	-3.693961	4.259685	0.885235

1	-2.131800	3.511021	0.502819
6	-3.628501	0.897990	-3.413382
6	-4.048084	2.032875	-4.390511
1	-4.831359	2.674045	-3.968898
1	-4.446536	1.590926	-5.317815
1	-3.198116	2.670426	-4.670486
6	-4.882141	0.046290	-3.069194
1	-4.621643	-0.810394	-2.432956
1	-5.329179	-0.353744	-3.993192
1	-5.652913	0.631280	-2.553406
6	-2.613936	-0.016444	-4.160294
1	-2.263097	-0.838772	-3.524789
1	-1.735417	0.544531	-4.504635
1	-3.097133	-0.456472	-5.047384
14	-3.776630	-1.161654	1.493300
6	-5.484423	-0.309237	1.348567
1	-6.181057	-0.691751	2.107205
1	-5.934028	-0.490488	0.363229
1	-5.406231	0.775695	1.482951
6	-4.114145	-3.088327	1.205211
6	-5.318550	-3.587113	2.056968
1	-5.154232	-3.471286	3.133464
1	-5.484874	-4.658535	1.860370
1	-6.244919	-3.059320	1.795239
6	-4.487300	-3.339881	-0.285948
1	-5.350780	-2.737456	-0.601470
1	-4.756300	-4.399483	-0.423605
1	-3.654864	-3.111395	-0.961762
6	-2.873655	-3.960005	1.545556
1	-2.660492	-3.964308	2.621851
1	-1.971872	-3.612931	1.022828
1	-3.054655	-5.003986	1.242605
6	-3.078397	-0.723975	3.287773
6	-3.032941	0.823092	3.445284
1	-2.652348	1.078683	4.446984
1	-4.025999	1.279249	3.344673
1	-2.367255	1.288893	2.708485
6	-4.015013	-1.284194	4.398845
1	-3.693824	-0.894830	5.378040
1	-3.972742	-2.378432	4.454291
1	-5.062153	-0.987693	4.253755
6	-1.647306	-1.262164	3.552428
1	-1.304873	-0.932749	4.546925
1	-0.928132	-0.885506	2.814361
1	-1.600709	-2.356883	3.534951

Int-Ge=Ge=Ge-1MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-2.237201	0.092356	0.228522
32	0.049009	-0.211599	-0.856196
32	2.166469	0.117406	0.155694
14	-3.604252	1.705545	-1.103812
14	-3.072503	-1.902983	1.491236
14	4.094362	-1.136774	-0.835968
14	2.362941	2.407857	1.129493
6	-2.462935	3.236858	-1.206116
1	-2.334792	3.693425	-0.216531
1	-2.883890	3.998836	-1.877059
1	-1.466722	2.971985	-1.580871
6	-5.198814	2.264066	-0.104632
6	-5.669159	3.672429	-0.579262
1	-6.555844	3.973260	0.000821
1	-5.947893	3.688466	-1.638817
1	-4.897303	4.435537	-0.419063
6	-6.381834	1.271173	-0.265726
1	-6.104324	0.249289	0.016641
1	-6.758384	1.247393	-1.295826
1	-7.217588	1.579340	0.382132
6	-3.952456	1.105245	-2.932987
6	-4.941955	2.056613	-3.667014
1	-5.949610	2.016888	-3.236374
1	-5.023268	1.756102	-4.723472
1	-4.602626	3.101110	-3.647956
6	-4.532494	-0.334922	-2.971493
1	-3.845342	-1.061296	-2.521065
1	-4.704712	-0.642436	-4.015206
1	-5.490744	-0.408188	-2.442850
6	-4.850879	2.380488	1.407327
1	-4.585581	1.411105	1.845596
1	-5.721548	2.768819	1.958555

1	-4.012434	3.067364	1.584944
6	-2.614896	1.124109	-3.728239
1	-1.829390	0.535961	-3.237967
1	-2.234713	2.145287	-3.855473
1	-2.773226	0.699814	-4.732074
6	-4.973747	-1.769558	1.658701
1	-5.340618	-2.517082	2.376005
1	-5.475659	-1.956796	0.700899
1	-5.290741	-0.784644	2.016881
6	-2.724777	-3.599310	0.575518
6	-3.613767	-4.729859	1.176364
1	-3.402031	-4.914363	2.235144
1	-3.418523	-5.667268	0.632363
1	-4.684386	-4.510016	1.076034
6	-3.108596	-3.450834	-0.922805
1	-4.151714	-3.131547	-1.055286
1	-2.992488	-4.419882	-1.433200
1	-2.452355	-2.733066	-1.424255
6	-1.237539	-4.036684	0.653701
1	-0.913298	-4.206721	1.688120
1	-0.570618	-3.302859	0.186521
1	-1.106693	-4.985645	0.109466
6	-2.327876	-1.755986	3.304378
6	-2.976419	-0.536184	4.022050
1	-2.546092	-0.432867	5.030361
1	-4.061397	-0.656792	4.137934
1	-2.790198	0.403383	3.486384
6	-2.659753	-3.027989	4.138415
1	-2.335214	-2.875158	5.179643
1	-2.137399	-3.914861	3.759805
1	-3.736276	-3.245767	4.159401
6	-0.787327	-1.557826	3.307628
1	-0.427945	-1.484947	4.346611
1	-0.488709	-0.638717	2.790350
1	-0.259183	-2.391010	2.831017
6	3.222033	3.718283	-0.060605
6	0.588717	3.049674	1.423769
1	0.612435	3.945537	2.060312
1	-0.040608	2.302636	1.918032
1	0.098093	3.323133	0.482389
6	3.184239	2.236922	2.906793
6	4.771015	3.625651	-0.052671
1	5.187546	4.326008	-0.793942
1	5.126111	2.621371	-0.309777
1	5.193338	3.894763	0.924063
6	2.816922	5.163646	0.359649

1	1.734497	5.323148	0.283023
1	3.305421	5.886833	-0.312434
1	3.124174	5.404951	1.383468
6	2.723813	3.497661	-1.516741
1	1.627370	3.520733	-1.585551
1	3.058151	2.535107	-1.920950
1	3.116159	4.294678	-2.168084
6	2.208407	1.450570	3.830209
1	1.263058	1.987243	3.978627
1	2.670208	1.309804	4.820090
1	1.972265	0.456471	3.427354
6	3.421247	3.637391	3.542147
1	2.503493	4.239578	3.573442
1	4.187357	4.208488	3.003466
1	3.770287	3.515414	4.579665
6	4.536647	1.476148	2.881690
1	5.279604	1.968309	2.243122
1	4.410351	0.445035	2.529883
1	4.953750	1.426119	3.899965
6	4.038419	-1.386428	-2.784227
6	5.698859	-0.160208	-0.471054
1	5.718284	0.242455	0.546302
1	5.818704	0.678949	-1.167496
1	6.574091	-0.813941	-0.590354
6	4.193823	-2.803948	0.199552
6	5.475235	-1.670152	-3.319332
1	6.155012	-0.827194	-3.143391
1	5.427691	-1.834935	-4.407361
1	5.921009	-2.565310	-2.869917
6	3.116799	-2.563857	-3.202414
1	3.540678	-3.532467	-2.907726
1	3.008572	-2.575423	-4.299179
1	2.120956	-2.477287	-2.756707
6	3.529829	-0.090498	-3.475268
1	4.136999	0.785831	-3.207211
1	2.488218	0.128351	-3.210648
1	3.585652	-0.207994	-4.569128
6	5.338990	-3.718049	-0.326158
1	6.314082	-3.211516	-0.322174
1	5.143744	-4.076552	-1.344036
1	5.426685	-4.603742	0.322687
6	4.508170	-2.451481	1.682025
1	3.712929	-1.840087	2.130138
1	5.458755	-1.912353	1.787509
1	4.583809	-3.377229	2.273515
6	2.864453	-3.606636	0.170451

1	2.025866	-3.015732	0.558397
1	2.964196	-4.504993	0.800708
1	2.596988	-3.933621	-0.839217
8	0.032994	-1.792134	-1.792256
6	-0.445978	-2.010401	-3.144308
1	0.088410	-1.381841	-3.873238
1	-1.523888	-1.811628	-3.237936
1	-0.265528	-3.063193	-3.388738
1	-1.808499	1.062758	1.372984

TS2-Ge=Ge=Ge-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-2.158892	0.011096	0.164290
32	0.070436	-0.422953	-0.922670
32	2.355599	0.488440	-0.505208
14	-3.653188	1.680093	-0.900335
14	-2.935962	-1.963448	1.447897
14	4.055001	-1.280626	-0.364362
14	2.327617	2.542398	0.859283
6	-2.463999	2.918627	-1.738784
1	-1.918546	3.502839	-0.988461
1	-3.016239	3.625441	-2.372969
1	-1.713919	2.411757	-2.352024
6	-4.621067	2.695898	0.483208
6	-4.877835	4.144413	-0.030912
1	-5.456874	4.700705	0.722482
1	-5.446573	4.163998	-0.968551
1	-3.939741	4.688637	-0.193600
6	-5.985480	2.061812	0.862895
1	-5.881358	1.018171	1.181836
1	-6.698617	2.094121	0.029774
1	-6.431619	2.622379	1.699101
6	-4.779756	0.902290	-2.297701
6	-5.656451	1.999323	-2.967834
1	-6.372613	2.441194	-2.264039
1	-6.234813	1.556403	-3.793607
1	-5.048774	2.810985	-3.389925
6	-5.708751	-0.222824	-1.768366

1	-5.134014	-1.023543	-1.290115
1	-6.266395	-0.670296	-2.606067
1	-6.440143	0.147846	-1.043205
6	-3.765193	2.806366	1.777567
1	-3.647817	1.836394	2.275250
1	-4.259376	3.487681	2.487644
1	-2.759780	3.201150	1.581282
6	-3.867597	0.286914	-3.397816
1	-3.221881	-0.506901	-2.998013
1	-3.231741	1.047255	-3.868803
1	-4.489887	-0.161088	-4.188092
6	-4.751251	-1.590492	1.917826
1	-5.140497	-2.350562	2.608419
1	-5.400229	-1.577398	1.034039
1	-4.839397	-0.615703	2.411738
6	-2.918170	-3.633197	0.413266
6	-3.929979	-4.642863	1.032079
1	-3.674895	-4.908976	2.064516
1	-3.926344	-5.571075	0.439707
1	-4.954818	-4.250418	1.025516
6	-3.361499	-3.364682	-1.051800
1	-4.384923	-2.973074	-1.110106
1	-3.338317	-4.307568	-1.620877
1	-2.687859	-2.660731	-1.553359
6	-1.514796	-4.296275	0.366319
1	-1.163261	-4.586787	1.363440
1	-0.767925	-3.641690	-0.097650
1	-1.568635	-5.214943	-0.239839
6	-1.915530	-2.016417	3.125575
6	-2.205361	-0.728216	3.950622
1	-1.651656	-0.773694	4.901407
1	-3.270256	-0.621757	4.194763
1	-1.878872	0.177303	3.425259
6	-2.360196	-3.238514	3.982045
1	-1.848327	-3.207453	4.956419
1	-2.101432	-4.192136	3.505787
1	-3.440900	-3.234225	4.178754
6	-0.382049	-2.104631	2.902671
1	0.134696	-2.069804	3.874774
1	-0.003517	-1.266538	2.303385
1	-0.084508	-3.032738	2.405453
6	3.733273	3.699735	0.081738
6	0.657596	3.365452	0.410830
1	0.563237	4.349645	0.889737
1	-0.188369	2.748708	0.735521
1	0.570611	3.507063	-0.673416

6	2.373136	2.434248	2.819221
6	5.099362	3.549627	0.804792
1	5.863357	4.143438	0.277936
1	5.444312	2.508329	0.821378
1	5.058007	3.910525	1.839635
6	3.296741	5.192875	0.154600
1	2.394488	5.377628	-0.441848
1	4.098463	5.828558	-0.254358
1	3.098168	5.524512	1.180764
6	3.956832	3.363946	-1.421184
1	3.026646	3.416257	-2.001814
1	4.365657	2.355161	-1.558312
1	4.671798	4.080423	-1.857072
6	1.085858	1.710551	3.306869
1	0.175482	2.261086	3.037881
1	1.105567	1.616809	4.404403
1	1.003831	0.699732	2.888729
6	2.385730	3.856820	3.451514
1	1.525107	4.457301	3.126863
1	3.300316	4.411232	3.206662
1	2.334194	3.773907	4.548931
6	3.594216	1.639797	3.354625
1	4.545934	2.121914	3.106566
1	3.615182	0.620291	2.953886
1	3.536223	1.563861	4.452468
6	4.429925	-1.878618	-2.208416
6	5.618929	-0.370081	0.260459
1	5.437710	0.093425	1.237326
1	5.914558	0.426262	-0.435151
1	6.469610	-1.056522	0.362342
6	3.711308	-2.752059	0.894976
6	5.925284	-2.291674	-2.339180
1	6.594400	-1.438959	-2.165455
1	6.116587	-2.658922	-3.359988
1	6.205538	-3.089022	-1.640221
6	3.536027	-3.076062	-2.634274
1	3.799896	-3.993565	-2.093504
1	3.676098	-3.277304	-3.708867
1	2.472095	-2.873971	-2.458638
6	4.181903	-0.725508	-3.222862
1	4.720197	0.194109	-2.954610
1	3.117784	-0.470506	-3.285918
1	4.522473	-1.035990	-4.223854
6	4.901929	-3.754926	0.884771
1	5.855186	-3.268338	1.131662
1	5.012495	-4.251236	-0.087244

1	4.728071	-4.540841	1.637014
6	3.582615	-2.173960	2.332562
1	2.739710	-1.475565	2.409480
1	4.492755	-1.652906	2.656275
1	3.400884	-2.995952	3.043348
6	2.405700	-3.534363	0.591500
1	1.536083	-2.870540	0.541924
1	2.223878	-4.269005	1.393189
1	2.452680	-4.081007	-0.354585
8	0.092435	-2.035332	-1.752410
6	-0.298685	-2.361839	-3.106247
1	-1.295779	-1.964949	-3.356508
1	-0.324765	-3.453484	-3.190929
1	0.429566	-1.967719	-3.829654
1	-1.546001	0.896566	1.288382
8	0.356354	0.794657	-2.539190
6	-0.037558	1.006769	-3.939711
1	-0.016086	2.081795	-4.149902
1	-1.046944	0.621706	-4.093319
1	0.665074	0.483503	-4.599193
1	1.442162	1.004731	-2.181224

TS3-Ge=Ge=Ge-3MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-2.402054	0.378791	-0.227778
32	0.015786	-0.228114	-0.940243
32	2.202647	-0.016054	0.043135
14	-2.351524	1.585893	1.962993
14	-3.996578	-1.516362	-0.654216
14	3.999735	1.613645	-0.644941
14	2.769719	-2.266016	0.993142
6	-0.879387	2.784036	1.736393
1	0.078344	2.258659	1.822074
1	-0.896428	3.584070	2.489509
1	-0.907438	3.249432	0.743638
6	-2.016717	0.569162	3.610696
6	-1.343098	1.477455	4.683289
1	-1.147609	0.888788	5.594197

1	-1.974468	2.327063	4.968373
1	-0.381220	1.873973	4.334660
6	-3.301956	-0.047076	4.224893
1	-3.840228	-0.674669	3.502930
1	-3.995258	0.721462	4.588974
1	-3.034923	-0.682230	5.084734
6	-3.952796	2.736681	2.053792
6	-3.939649	3.589060	3.355883
1	-4.043410	2.970986	4.256253
1	-4.786409	4.294445	3.342139
1	-3.020197	4.181886	3.452249
6	-5.280451	1.934150	2.004981
1	-5.371242	1.374091	1.066850
1	-6.137047	2.625213	2.062505
1	-5.370075	1.223060	2.833748
6	-1.034461	-0.589354	3.291884
1	-1.486146	-1.318842	2.607737
1	-0.759258	-1.115618	4.220466
1	-0.111096	-0.221823	2.824699
6	-3.945534	3.719299	0.846511
1	-3.955695	3.184262	-0.111815
1	-3.065473	4.374187	0.856082
1	-4.841157	4.360035	0.886003
6	-5.163893	-1.752198	0.846135
1	-5.817683	-2.623416	0.696783
1	-5.806439	-0.878168	1.003059
1	-4.597708	-1.914847	1.770128
6	-5.143815	-0.909635	-2.143020
6	-6.411154	-1.802225	-2.291869
1	-6.169939	-2.834282	-2.564175
1	-7.056811	-1.392402	-3.085196
1	-7.001795	-1.824102	-1.366954
6	-5.644201	0.536538	-1.861996
1	-6.227605	0.595293	-0.933730
1	-6.300618	0.866829	-2.682952
1	-4.813831	1.249420	-1.786855
6	-4.379771	-0.897745	-3.495135
1	-4.090814	-1.907887	-3.811482
1	-3.469906	-0.283166	-3.439128
1	-5.021347	-0.475812	-4.285594
6	-3.162190	-3.277998	-0.948812
6	-2.588147	-3.761629	0.415003
1	-2.037315	-4.705093	0.274640
1	-3.385622	-3.949411	1.144977
1	-1.893900	-3.033602	0.852140
6	-4.203066	-4.335858	-1.421764

1	-3.740559	-5.335400	-1.395720
1	-4.528757	-4.155153	-2.453348
1	-5.093871	-4.369059	-0.781265
6	-2.010504	-3.263762	-1.988704
1	-1.592814	-4.278007	-2.095734
1	-1.190122	-2.601227	-1.683288
1	-2.351605	-2.940671	-2.980242
6	3.690739	-2.127877	2.729066
6	1.090713	-3.107845	1.336808
1	1.240643	-4.140289	1.680217
1	0.468790	-3.145593	0.436816
1	0.524780	-2.579632	2.111138
6	3.684182	-3.409828	-0.324767
6	5.233996	-2.020773	2.601226
1	5.676280	-1.863117	3.597667
1	5.539840	-1.181811	1.965835
1	5.674649	-2.937672	2.190557
6	3.364919	-3.378442	3.601329
1	2.293031	-3.456505	3.819125
1	3.893379	-3.297868	4.564399
1	3.683166	-4.314791	3.127268
6	3.179867	-0.875850	3.497258
1	2.088538	-0.879205	3.616076
1	3.458749	0.055482	2.988479
1	3.623952	-0.852143	4.505156
6	2.761000	-3.616257	-1.560098
1	1.811719	-4.098133	-1.292997
1	3.268420	-4.263908	-2.292339
1	2.524720	-2.666497	-2.057006
6	3.969166	-4.811525	0.291824
1	3.054041	-5.298820	0.653769
1	4.682959	-4.762778	1.123577
1	4.406866	-5.466603	-0.477970
6	5.023901	-2.811812	-0.831101
1	5.762534	-2.702285	-0.029045
1	4.873496	-1.829788	-1.293942
1	5.459992	-3.475303	-1.595157
6	3.522817	3.277678	0.294791
6	5.649266	1.028015	0.129820
1	5.918700	0.014701	-0.186985
1	5.601817	1.033733	1.225713
1	6.468308	1.698609	-0.165775
6	4.314775	1.792941	-2.575408
6	4.711657	4.283301	0.297612
1	5.610277	3.857470	0.762973
1	4.430465	5.174668	0.880665

1	4.977712	4.621587	-0.709712
6	2.283904	3.971942	-0.333108
1	2.507736	4.375955	-1.327959
1	1.966849	4.813628	0.302414
1	1.429819	3.290289	-0.428277
6	3.201593	2.947963	1.781775
1	4.056959	2.489596	2.296912
1	2.344046	2.270447	1.875411
1	2.951318	3.875880	2.319227
6	5.435855	2.834401	-2.868882
1	6.361952	2.630854	-2.313686
1	5.112607	3.856398	-2.634438
1	5.682105	2.808460	-3.942247
6	4.787308	0.416429	-3.127596
1	4.031955	-0.366654	-2.973733
1	5.724496	0.083608	-2.660785
1	4.969823	0.497271	-4.210640
6	3.041850	2.220385	-3.352239
1	2.182305	1.587782	-3.109821
1	3.232091	2.155415	-4.436325
1	2.756183	3.256671	-3.129114
8	0.016185	0.863535	-2.598868
6	0.175844	0.158095	-3.874671
1	-0.755352	-0.356737	-4.151882
1	0.981152	-0.580033	-3.786646
1	0.440740	0.888605	-4.647331
8	-1.749392	2.458712	-2.368859
6	-2.506342	3.193503	-3.373800
1	-2.948715	2.516741	-4.118093
1	-1.838821	3.906287	-3.870177
1	-3.303054	3.745392	-2.864805
1	-0.842779	1.794968	-2.614970
1	-2.280441	1.761199	-1.551113

TS4-Ge=Ge=Ge-3MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-2.201588	-0.005982	0.233109
32	0.114304	-0.466477	-0.655122

32	2.298411	0.364982	-0.176627
14	-3.554389	1.891685	-0.664540
14	-3.167017	-2.095729	1.200965
14	4.024257	-1.411599	-0.264123
14	2.264353	2.274360	1.403982
6	-2.292790	3.069408	-1.472471
1	-1.630227	3.529131	-0.731195
1	-2.808280	3.880992	-2.004942
1	-1.667811	2.521519	-2.186577
6	-4.400111	2.844880	0.844077
6	-4.550621	4.349191	0.464098
1	-5.053309	4.883361	1.285787
1	-5.148908	4.496080	-0.443355
1	-3.575172	4.825429	0.307738
6	-5.804256	2.287361	1.202674
1	-5.779666	1.213658	1.424283
1	-6.529310	2.451304	0.396389
1	-6.185933	2.802883	2.097808
6	-4.795897	1.340853	-2.075211
6	-5.591805	2.570243	-2.603919
1	-6.249960	2.996531	-1.836521
1	-6.228291	2.260285	-3.447679
1	-4.929417	3.366902	-2.967213
6	-5.810231	0.256598	-1.626750
1	-5.298381	-0.630520	-1.240283
1	-6.417828	-0.060555	-2.489165
1	-6.495853	0.617581	-0.853334
6	-3.522196	2.778837	2.126300
1	-3.475652	1.765073	2.541348
1	-3.954492	3.434587	2.898344
1	-2.491989	3.112384	1.945263
6	-3.966134	0.762146	-3.256714
1	-3.377199	-0.112167	-2.950416
1	-3.268616	1.499922	-3.667430
1	-4.645104	0.446971	-4.065027
6	-4.930847	-1.616166	1.762871
1	-5.373229	-2.417788	2.370082
1	-5.597070	-1.435038	0.911244
1	-4.916476	-0.706042	2.374156
6	-3.322156	-3.594440	-0.055366
6	-4.416191	-4.588336	0.439307
1	-4.181282	-5.016915	1.419684
1	-4.499023	-5.422153	-0.275334
1	-5.402617	-4.111632	0.504464
6	-3.766387	-3.090346	-1.456965
1	-4.764085	-2.635702	-1.432955

1	-3.812356	-3.941109	-2.155117
1	-3.066555	-2.357831	-1.874209
6	-1.985361	-4.369169	-0.226447
1	-1.680173	-4.871232	0.699873
1	-1.167441	-3.715080	-0.550061
1	-2.114886	-5.152367	-0.990786
6	-2.154456	-2.509848	2.833297
6	-2.347841	-1.364630	3.870234
1	-1.764149	-1.591885	4.775724
1	-3.397268	-1.255069	4.172094
1	-1.996664	-0.399357	3.488016
6	-2.681280	-3.824245	3.479635
1	-2.170768	-3.985907	4.441968
1	-2.481817	-4.701097	2.852350
1	-3.759874	-3.784346	3.683221
6	-0.633649	-2.667637	2.572439
1	-0.111116	-2.861546	3.522132
1	-0.198361	-1.757050	2.142717
1	-0.405571	-3.496989	1.894551
6	3.804985	3.443981	0.997428
6	0.704860	3.250470	0.887064
1	0.573935	4.146396	1.508805
1	-0.196536	2.636158	0.988908
1	0.775348	3.571210	-0.159803
6	2.079481	1.850821	3.310759
6	5.069180	3.095582	1.829368
1	5.914506	3.716357	1.492740
1	5.363652	2.045286	1.716494
1	4.923827	3.293085	2.898514
6	3.426406	4.928940	1.280738
1	2.611437	5.269547	0.630064
1	4.298651	5.571420	1.081309
1	3.122352	5.096875	2.320895
6	4.178065	3.349561	-0.508210
1	3.326321	3.594559	-1.156167
1	4.526132	2.343856	-0.776701
1	4.990884	4.058771	-0.733364
6	0.719313	1.136241	3.537254
1	-0.132827	1.764349	3.248971
1	0.604266	0.887363	4.604038
1	0.658875	0.200634	2.968832
6	2.082531	3.151864	4.165231
1	1.292831	3.849466	3.854228
1	3.042927	3.678869	4.115973
1	1.899017	2.898085	5.221314
6	3.197280	0.904680	3.824442

1	4.190897	1.361542	3.766791
1	3.217048	-0.030393	3.252124
1	3.009760	0.646143	4.878975
6	4.501438	-1.652663	-2.156846
6	5.555122	-0.663003	0.607357
1	5.392921	-0.573626	1.689144
1	5.794456	0.334228	0.220560
1	6.437886	-1.299416	0.452389
6	3.589712	-3.064337	0.706122
6	5.429406	-2.882021	-2.366492
1	6.319582	-2.850428	-1.723544
1	5.776770	-2.904373	-3.411738
1	4.901799	-3.824379	-2.176237
6	3.249285	-1.830938	-3.055591
1	2.641044	-2.689580	-2.752570
1	3.562253	-1.981910	-4.101869
1	2.602913	-0.944981	-3.017413
6	5.267633	-0.388705	-2.641541
1	6.231487	-0.270887	-2.130121
1	4.682541	0.526182	-2.479452
1	5.471175	-0.469794	-3.721283
6	4.862561	-3.944945	0.890012
1	5.666942	-3.406081	1.408094
1	5.256108	-4.315627	-0.061894
1	4.606228	-4.822531	1.504747
6	3.077630	-2.706424	2.129775
1	2.193700	-2.060355	2.098712
1	3.850584	-2.199189	2.723793
1	2.805418	-3.629649	2.665333
6	2.505208	-3.904948	-0.019721
1	1.594336	-3.331740	-0.223466
1	2.234997	-4.774350	0.601693
1	2.869911	-4.290415	-0.981799
8	0.167006	-2.002702	-1.600774
6	-0.311947	-2.289499	-2.936647
1	0.374079	-1.869063	-3.681206
1	-1.312564	-1.871596	-3.112457
1	-0.350373	-3.379669	-3.047003
1	-1.641736	0.653167	1.526692
8	-0.373050	0.838389	-3.294216
6	-0.650081	0.649464	-4.711534
1	-0.979708	1.588530	-5.183741
1	-1.455509	-0.084158	-4.800448
1	0.231696	0.270997	-5.253935
1	0.399443	1.473940	-3.180992
8	1.804757	2.281751	-2.933940

1	2.138492	1.761901	-2.140877
6	2.815874	2.409029	-3.981296
1	3.737079	2.849670	-3.578881
1	2.400687	3.077413	-4.739835
1	3.047188	1.433610	-4.433579

Pro-Ge=Ge=Ge-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-2.176461	-0.012292	0.244663
32	-0.004053	-0.053551	-1.093832
32	2.173085	0.185241	0.188048
14	-3.763572	1.704503	-0.653865
14	-2.912137	-2.179412	1.262427
14	4.096920	-1.268165	-0.466560
14	2.376757	2.548683	0.965648
6	-2.663600	3.194237	-1.114221
1	-2.271668	3.687160	-0.215451
1	-3.242114	3.939119	-1.678990
1	-1.811260	2.867466	-1.719391
6	-4.984837	2.336262	0.761206
6	-5.417714	3.801709	0.450822
1	-6.102648	4.152046	1.239223
1	-5.943491	3.890462	-0.507082
1	-4.560312	4.484858	0.430167
6	-6.268224	1.475760	0.907452
1	-6.041273	0.419237	1.087075
1	-6.908335	1.538408	0.018883
1	-6.860127	1.838520	1.762888
6	-4.666835	1.110737	-2.285987
6	-5.697111	2.175691	-2.765295
1	-6.540915	2.278376	-2.071966
1	-6.108442	1.873506	-3.741390
1	-5.238518	3.165274	-2.894625
6	-5.405154	-0.243005	-2.108083
1	-4.709759	-1.046743	-1.840618
1	-5.891179	-0.529446	-3.054535
1	-6.183040	-0.195658	-1.337711
6	-4.251261	2.350159	2.132623

1	-4.023392	1.337043	2.484858
1	-4.891825	2.829742	2.889612
1	-3.306872	2.909634	2.093591
6	-3.608209	0.940367	-3.412500
1	-2.823133	0.227437	-3.133833
1	-3.111925	1.887822	-3.653285
1	-4.099150	0.570175	-4.326625
6	-4.800192	-2.078662	1.543173
1	-5.158211	-2.972751	2.072283
1	-5.346400	-2.009218	0.594698
1	-5.072166	-1.207456	2.148419
6	-2.613487	-3.727609	0.095973
6	-3.379244	-4.977195	0.625938
1	-3.013771	-5.311251	1.602210
1	-3.241188	-5.810826	-0.080529
1	-4.458189	-4.794196	0.709799
6	-3.181074	-3.420338	-1.319045
1	-4.264063	-3.241574	-1.294817
1	-3.006227	-4.283139	-1.981246
1	-2.699773	-2.550022	-1.778086
6	-1.110201	-4.089801	-0.044950
1	-0.667842	-4.387415	0.914264
1	-0.519440	-3.263055	-0.457941
1	-1.001688	-4.945510	-0.731003
6	-2.083854	-2.291470	3.043470
6	-2.682936	-1.178541	3.953166
1	-2.199192	-1.216670	4.941579
1	-3.761391	-1.309808	4.109332
1	-2.512519	-0.174752	3.543774
6	-2.382543	-3.662981	3.716437
1	-2.037013	-3.637667	4.761826
1	-1.855236	-4.485863	3.218721
1	-3.454997	-3.899121	3.729575
6	-0.545430	-2.095908	3.001156
1	-0.135118	-2.157866	4.021713
1	-0.270377	-1.115049	2.596322
1	-0.045085	-2.862718	2.398650
6	3.465349	3.691223	-0.198708
6	0.602501	3.251427	0.899005
1	0.558698	4.242482	1.372085
1	-0.110453	2.600827	1.418271
1	0.256840	3.354788	-0.136189
6	2.922472	2.531988	2.850886
6	4.989854	3.547962	0.053304
1	5.546116	4.154927	-0.678593
1	5.327961	2.510920	-0.050261

1	5.275131	3.898474	1.053032
6	3.073207	5.187077	-0.003673
1	2.021050	5.367859	-0.255667
1	3.685865	5.814271	-0.670396
1	3.240586	5.534528	1.022265
6	3.173566	3.325209	-1.680456
1	2.105038	3.412687	-1.916014
1	3.491756	2.301692	-1.916831
1	3.720433	4.008454	-2.349265
6	1.780004	1.912151	3.707564
1	0.860946	2.509090	3.655183
1	2.092027	1.873912	4.763048
1	1.538209	0.888467	3.395602
6	3.165944	3.980567	3.365751
1	2.291798	4.627120	3.210423
1	4.030166	4.451142	2.881367
1	3.368269	3.954801	4.448091
6	4.211970	1.701003	3.090264
1	5.068847	2.094318	2.530136
1	4.071936	0.650416	2.808511
1	4.475599	1.723009	4.159566
6	4.163433	-1.743244	-2.370415
6	5.699367	-0.287622	-0.100892
1	5.677647	0.183975	0.887548
1	5.860995	0.501291	-0.846201
1	6.570882	-0.955697	-0.135233
6	4.078599	-2.809888	0.751958
6	5.628018	-2.079925	-2.781923
1	6.300401	-1.222847	-2.650476
1	5.648616	-2.357131	-3.847636
1	6.039045	-2.923221	-2.214339
6	3.255683	-2.953128	-2.724482
1	3.604922	-3.879402	-2.251254
1	3.277510	-3.117435	-3.814447
1	2.216915	-2.770919	-2.427555
6	3.696681	-0.532770	-3.225501
1	4.261732	0.383096	-3.000019
1	2.630893	-0.335775	-3.069598
1	3.843705	-0.754299	-4.294555
6	5.222591	-3.799525	0.383707
1	6.208497	-3.315018	0.392008
1	5.073226	-4.255803	-0.601924
1	5.251933	-4.615557	1.122878
6	4.324628	-2.324935	2.209985
1	3.526738	-1.656778	2.557670
1	5.284708	-1.803086	2.316882

1	4.343479	-3.193922	2.886251
6	2.728076	-3.575497	0.722703
1	1.893356	-2.928777	1.016815
1	2.765046	-4.415726	1.434619
1	2.501293	-3.984552	-0.267146
8	0.273929	-1.542957	-2.100323
6	-0.402992	-1.973066	-3.309520
1	-1.318260	-1.396901	-3.511792
1	-0.668100	-3.032118	-3.206215
1	0.276876	-1.859718	-4.165451
1	-1.601896	0.738181	1.489201
8	-0.283934	1.276459	-2.305484
6	0.411318	1.530711	-3.552298
1	0.006468	2.461101	-3.968025
1	0.245250	0.719650	-4.276041
1	1.492687	1.652088	-3.404049
1	1.713906	-0.489440	1.517020

TS1-Sn=Sn=Sn-1MeOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

8	-0.435519	-2.481040	-1.114049
50	0.053892	-1.062475	0.396227
50	-2.527382	-0.375479	-0.502968
1	-1.579785	-1.928274	-1.341429
6	-0.138087	-3.871557	-1.447362
1	0.016277	-4.463674	-0.535816
1	0.754363	-3.926103	-2.078029
1	-0.998036	-4.274506	-1.996176
50	2.331897	0.209933	-0.217731
14	4.351628	-1.225922	-1.051690
6	5.956156	-0.234816	-0.743203
1	6.106722	-0.079969	0.333149
1	5.899190	0.757012	-1.208162
1	6.845277	-0.742276	-1.140462
6	4.505936	-2.923422	-0.066053
6	5.842812	-3.626207	-0.440415
1	6.712504	-2.991457	-0.228548

1	5.876689	-3.909903	-1.498895
1	5.952179	-4.546466	0.154255
6	4.528986	-2.632219	1.462455
1	3.587200	-2.183307	1.804434
1	5.351470	-1.963490	1.747110
1	4.663447	-3.575514	2.014729
6	3.337543	-3.908011	-0.332023
1	2.367434	-3.467543	-0.069002
1	3.467824	-4.808602	0.288830
1	3.295307	-4.232441	-1.378493
6	4.034928	-1.329329	-2.988882
6	5.200295	-2.062922	-3.708241
1	6.175135	-1.614731	-3.473661
1	5.060686	-2.004428	-4.799030
1	5.238127	-3.125773	-3.438372
6	2.699169	-2.039008	-3.347416
1	2.716798	-3.103115	-3.084387
1	2.526106	-1.971624	-4.433100
1	1.834844	-1.581099	-2.848207
6	3.953358	0.122846	-3.547778
1	4.868349	0.699414	-3.358839
1	3.104518	0.674828	-3.118170
1	3.798795	0.091689	-4.637271
14	2.507822	2.145460	1.570425
6	3.517272	3.605437	0.724575
6	3.020319	4.981386	1.254714
1	1.963376	5.148880	1.012576
1	3.599567	5.791124	0.783901
1	3.136547	5.076348	2.341455
6	3.275372	3.579266	-0.813714
1	2.207456	3.583431	-1.072977
1	3.731126	2.695201	-1.282669
1	3.733217	4.465013	-1.281096
6	5.044489	3.491326	0.972369
1	5.575478	4.269716	0.402376
1	5.441147	2.518084	0.653611
1	5.295225	3.628397	2.031406
6	0.703282	2.764049	1.739484
1	0.627984	3.566870	2.485709
1	0.018962	1.962408	2.041882
1	0.335203	3.158841	0.784573
6	3.090599	1.592621	3.357632
6	2.057739	0.583942	3.938328
1	1.053418	1.018405	4.024217
1	2.372145	0.273526	4.946885
1	1.980508	-0.323295	3.323837

6	3.149109	2.825472	4.304550
1	2.181398	3.341541	4.364217
1	3.905764	3.553400	3.985195
1	3.411546	2.499482	5.323065
6	4.477772	0.896911	3.343587
1	5.274269	1.562575	2.992855
1	4.471210	0.007841	2.701893
1	4.740462	0.568204	4.361504
14	-2.709771	1.870563	-1.868507
6	-0.940986	2.442452	-2.322653
1	-0.480666	2.991486	-1.490403
1	-0.954035	3.107378	-3.198615
1	-0.290023	1.588886	-2.547052
6	-3.598620	3.393467	-1.010947
6	-3.263444	4.708904	-1.774084
1	-3.769253	5.558446	-1.288112
1	-3.591225	4.680560	-2.819679
1	-2.185931	4.917706	-1.763144
6	-5.139946	3.221365	-0.955476
1	-5.427644	2.288665	-0.452466
1	-5.588812	3.218507	-1.956454
1	-5.589118	4.055768	-0.393860
6	-3.076655	3.544887	0.445143
1	-3.339726	2.677393	1.061317
1	-3.522803	4.438300	0.910924
1	-1.985722	3.662165	0.484597
6	-3.560012	1.221355	-3.520911
6	-3.927770	2.386519	-4.480409
1	-4.697797	3.041997	-4.055286
1	-4.324724	1.977015	-5.422922
1	-3.053398	3.002499	-4.731760
6	-4.845377	0.401100	-3.216497
1	-4.620530	-0.488339	-2.611071
1	-5.298523	0.047461	-4.155726
1	-5.599478	0.990897	-2.681658
6	-2.557226	0.287622	-4.261021
1	-2.242979	-0.555460	-3.632870
1	-1.655186	0.826191	-4.578921
1	-3.034389	-0.127911	-5.162713
14	-4.031153	-1.112599	1.523323
6	-5.715051	-0.210540	1.383416
1	-6.457326	-0.602070	2.091471
1	-6.127914	-0.316140	0.371708
1	-5.599520	0.863500	1.578130
6	-4.349314	-3.024844	1.160338
6	-5.508245	-3.579510	2.033656

1	-5.289521	-3.519503	3.106081
1	-5.682070	-4.639089	1.787608
1	-6.445500	-3.039425	1.845389
6	-4.769711	-3.197668	-0.330611
1	-5.628054	-2.565483	-0.597455
1	-5.057049	-4.245013	-0.513806
1	-3.948182	-2.953187	-1.014551
6	-3.080117	-3.890632	1.396555
1	-2.820024	-3.958536	2.459492
1	-2.208700	-3.494566	0.858254
1	-3.253453	-4.916399	1.033415
6	-3.305931	-0.680556	3.312553
6	-3.054059	0.854068	3.383097
1	-2.668977	1.119789	4.380568
1	-3.970271	1.436107	3.218169
1	-2.309510	1.174507	2.642165
6	-4.338240	-1.055623	4.415427
1	-3.980365	-0.693889	5.392484
1	-4.465543	-2.142403	4.495636
1	-5.323368	-0.606913	4.235727
6	-1.967778	-1.383258	3.665439
1	-1.608355	-1.023600	4.643469
1	-1.181261	-1.164040	2.932129
1	-2.067461	-2.472773	3.731490

Int-Sn=Sn=Sn-1MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-2.569387	0.303791	-0.134585
50	0.079506	-0.903945	-0.284507
50	2.526537	0.258390	0.287152
14	-4.031741	-0.804618	-2.071004
14	-3.544569	1.181569	2.203607
14	4.493238	-1.583646	0.538249
14	2.881181	2.360625	-1.352691
6	-2.920448	-0.587263	-3.615790
1	-2.801242	0.474518	-3.868224
1	-3.352024	-1.093180	-4.491083
1	-1.917722	-0.999616	-3.451799

6	-5.667785	0.232690	-2.397002
6	-6.167311	0.008320	-3.855775
1	-7.083284	0.596675	-4.023672
1	-6.406253	-1.041159	-4.060348
1	-5.425123	0.337921	-4.593430
6	-6.813976	-0.139355	-1.417016
1	-6.509473	-0.031176	-0.368268
1	-7.164061	-1.168928	-1.564922
1	-7.675718	0.526732	-1.581350
6	-4.313147	-2.724074	-1.795581
6	-5.281164	-3.307430	-2.866256
1	-6.294815	-2.899755	-2.771164
1	-5.351252	-4.399313	-2.741730
1	-4.929740	-3.115580	-3.888947
6	-4.891517	-3.032441	-0.387154
1	-4.219672	-2.692515	0.411682
1	-5.026403	-4.118899	-0.267157
1	-5.867204	-2.558408	-0.227412
6	-5.360270	1.749500	-2.236296
1	-5.092679	2.006328	-1.202700
1	-6.250235	2.339850	-2.505711
1	-4.536529	2.076192	-2.885103
6	-2.953323	-3.465964	-1.941305
1	-2.202293	-3.117811	-1.221126
1	-2.532171	-3.351088	-2.948009
1	-3.099086	-4.542903	-1.764234
6	-5.447122	1.347333	2.062551
1	-5.848747	1.892577	2.928830
1	-5.929364	0.362150	2.037628
1	-5.750870	1.888272	1.159099
6	-3.206968	-0.090131	3.655921
6	-4.068018	0.258618	4.906014
1	-3.825154	1.243360	5.319508
1	-3.883187	-0.486768	5.695611
1	-5.141943	0.238528	4.681326
6	-3.623170	-1.514926	3.191007
1	-4.678511	-1.560615	2.889338
1	-3.483135	-2.231031	4.015773
1	-3.013557	-1.861830	2.348333
6	-1.710700	-0.123932	4.071458
1	-1.387425	0.826606	4.514986
1	-1.049756	-0.338821	3.220155
1	-1.549290	-0.909597	4.826159
6	-2.815344	2.983495	2.467098
6	-3.466622	3.942122	1.427326
1	-3.031427	4.947953	1.532774

1	-4.549989	4.034734	1.576538
1	-3.287924	3.612178	0.395353
6	-3.147578	3.519335	3.890353
1	-2.844128	4.575563	3.962529
1	-2.606780	2.969875	4.670730
1	-4.221425	3.469663	4.117157
6	-1.275721	3.032128	2.272212
1	-0.912577	4.058212	2.441648
1	-0.989413	2.745719	1.252627
1	-0.743855	2.373395	2.968237
6	3.636087	1.988529	-3.129677
6	1.126931	3.071205	-1.649540
1	1.180980	4.075296	-2.094534
1	0.556924	3.150502	-0.716588
1	0.549271	2.435383	-2.332419
6	3.866056	3.696160	-0.295230
6	5.166262	1.737003	-3.081822
1	5.527572	1.441153	-4.079607
1	5.423549	0.932674	-2.381198
1	5.722760	2.635155	-2.784398
6	3.352940	3.172788	-4.101172
1	2.276878	3.344904	-4.230818
1	3.771330	2.939669	-5.093470
1	3.808446	4.109919	-3.763519
6	2.949204	0.725357	-3.721066
1	1.856680	0.833384	-3.768204
1	3.170860	-0.170923	-3.130456
1	3.309984	0.551819	-4.747464
6	2.963769	4.169386	0.882183
1	2.055811	4.671797	0.525750
1	3.517731	4.887291	1.507631
1	2.655487	3.334582	1.527574
6	4.225247	4.946881	-1.148445
1	3.341804	5.382409	-1.634164
1	4.964847	4.717931	-1.925399
1	4.660717	5.723198	-0.499105
6	5.177109	3.121093	0.308308
1	5.860569	2.746981	-0.462818
1	4.973985	2.298890	1.009399
1	5.705625	3.906553	0.871465
6	4.287032	-3.229295	-0.519062
6	6.149286	-0.791965	-0.017903
1	6.249219	0.243768	0.324803
1	6.236886	-0.789060	-1.111646
1	7.001866	-1.361344	0.379101
6	4.625216	-1.858539	2.479731

6	5.656765	-3.969102	-0.608230
1	6.423008	-3.357832	-1.101506
1	5.532825	-4.887033	-1.204329
1	6.038035	-4.264193	0.375906
6	3.232917	-4.205131	0.074341
1	3.547026	-4.596390	1.051164
1	3.115938	-5.069208	-0.599664
1	2.246513	-3.739453	0.191841
6	3.859096	-2.873480	-1.970669
1	4.557938	-2.172519	-2.448660
1	2.856863	-2.429468	-1.999804
1	3.836749	-3.788120	-2.583745
6	5.672002	-2.956979	2.823870
1	6.657578	-2.743661	2.387695
1	5.353397	-3.947637	2.477745
1	5.801665	-3.016524	3.916333
6	5.093578	-0.528119	3.138072
1	4.397933	0.298579	2.931648
1	6.091582	-0.226762	2.795056
1	5.139895	-0.650946	4.231660
6	3.262640	-2.257881	3.113688
1	2.505315	-1.475779	2.966447
1	3.387253	-2.403815	4.198923
1	2.862478	-3.186986	2.693394
8	0.113613	-2.652797	0.591139
6	-0.717057	-3.413034	1.485244
1	-0.376711	-4.456219	1.478096
1	-1.776628	-3.395589	1.181277
1	-0.644786	-3.028564	2.513992
1	-2.112852	1.776365	-0.935670

TS2-Sn=Sn=Sn-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-2.332088	0.029021	0.247418
50	0.080049	-0.568925	-0.997552
50	2.567189	0.561896	-0.534447
14	-3.777339	1.820947	-0.965800
14	-3.138421	-2.042507	1.610562

14	4.261296	-1.394789	-0.250232
14	2.392412	2.694578	0.969069
6	-2.497217	2.982787	-1.785321
1	-1.948635	3.554546	-1.026398
1	-2.982381	3.701847	-2.459993
1	-1.751691	2.420534	-2.358072
6	-4.741989	2.863980	0.388428
6	-4.995402	4.302666	-0.146969
1	-5.562718	4.880216	0.599081
1	-5.568945	4.308381	-1.082046
1	-4.051506	4.832826	-0.326595
6	-6.095186	2.212660	0.776375
1	-5.965609	1.174740	1.111184
1	-6.807210	2.214596	-0.058247
1	-6.553703	2.773151	1.605589
6	-4.850624	1.003444	-2.378817
6	-5.721930	2.073750	-3.093877
1	-6.463518	2.517721	-2.418042
1	-6.269164	1.612098	-3.930348
1	-5.109306	2.885946	-3.508021
6	-5.769618	-0.128055	-1.844376
1	-5.186364	-0.915191	-1.351037
1	-6.313036	-0.595556	-2.680283
1	-6.511698	0.239592	-1.128106
6	-3.886854	2.989098	1.683784
1	-3.783997	2.026647	2.200513
1	-4.376080	3.687325	2.380444
1	-2.874485	3.367018	1.488823
6	-3.896604	0.376177	-3.437230
1	-3.254482	-0.401172	-3.000711
1	-3.251625	1.130852	-3.904430
1	-4.489103	-0.096872	-4.235560
6	-4.964015	-1.682551	2.052670
1	-5.374067	-2.423627	2.751254
1	-5.588971	-1.687213	1.150153
1	-5.061312	-0.692311	2.515046
6	-3.069965	-3.691050	0.544317
6	-4.066148	-4.726788	1.141540
1	-3.807483	-5.003092	2.170988
1	-4.048866	-5.645561	0.535293
1	-5.095751	-4.346868	1.139488
6	-3.504853	-3.400944	-0.920408
1	-4.515866	-2.977095	-0.981808
1	-3.505170	-4.339241	-1.497051
1	-2.807528	-2.716322	-1.418297
6	-1.653170	-4.325364	0.491023

1	-1.288328	-4.609058	1.485333
1	-0.919265	-3.661955	0.017633
1	-1.690139	-5.243196	-0.117247
6	-2.088839	-2.048078	3.269257
6	-2.392227	-0.749470	4.073033
1	-1.831146	-0.766765	5.020322
1	-3.457070	-0.650805	4.320510
1	-2.080719	0.148578	3.525456
6	-2.494557	-3.268254	4.143744
1	-1.970133	-3.220949	5.110662
1	-2.225917	-4.219938	3.668526
1	-3.572886	-3.280874	4.352882
6	-0.556081	-2.098361	3.020287
1	-0.025473	-2.072903	3.985177
1	-0.207799	-1.233927	2.440140
1	-0.242858	-3.006041	2.495197
6	3.810138	3.854490	0.230206
6	0.714328	3.466780	0.462147
1	0.567117	4.448470	0.933175
1	-0.118798	2.819135	0.760975
1	0.657482	3.600552	-0.625534
6	2.373473	2.530388	2.922945
6	5.159859	3.654154	0.969203
1	5.951108	4.232245	0.466452
1	5.469287	2.599604	0.966945
1	5.112504	3.991293	2.011494
6	3.384876	5.347633	0.317532
1	2.488706	5.539101	-0.286934
1	4.191381	5.986259	-0.076397
1	3.174037	5.666354	1.345148
6	4.054380	3.539160	-1.275196
1	3.131229	3.568085	-1.868311
1	4.499621	2.545029	-1.418877
1	4.754903	4.276650	-1.697926
6	1.074893	1.790292	3.355000
1	0.167515	2.330058	3.057660
1	1.056893	1.686818	4.451719
1	1.019229	0.780650	2.926934
6	2.365998	3.939900	3.582102
1	1.516968	4.546709	3.238687
1	3.288924	4.496026	3.374377
1	2.279141	3.839964	4.675710
6	3.576721	1.719826	3.475334
1	4.539779	2.190851	3.250631
1	3.592001	0.702676	3.066332
1	3.495266	1.634238	4.570953

6	4.611722	-2.044678	-2.077203
6	5.841715	-0.534056	0.410157
1	5.639048	-0.054527	1.376592
1	6.169129	0.254092	-0.281771
1	6.678915	-1.230813	0.545872
6	3.768527	-2.791637	1.046354
6	6.083491	-2.533657	-2.183974
1	6.788228	-1.709167	-2.013067
1	6.271208	-2.926434	-3.195519
1	6.313786	-3.330107	-1.465988
6	3.650230	-3.194783	-2.488253
1	3.852639	-4.116953	-1.929038
1	3.787955	-3.423018	-3.557581
1	2.595663	-2.930084	-2.333383
6	4.429065	-0.897531	-3.113926
1	4.990212	0.009016	-2.846194
1	3.376704	-0.608113	-3.215106
1	4.783423	-1.233776	-4.101119
6	4.910573	-3.846939	1.116401
1	5.874940	-3.391841	1.378579
1	5.030943	-4.381125	0.165595
1	4.677403	-4.597104	1.888562
6	3.607146	-2.152233	2.455154
1	2.784428	-1.425094	2.473362
1	4.519503	-1.646064	2.795428
1	3.369600	-2.938179	3.189901
6	2.438822	-3.526299	0.724347
1	1.593199	-2.831776	0.657620
1	2.214999	-4.242340	1.532178
1	2.475636	-4.084727	-0.214370
8	0.092190	-2.307030	-1.897234
6	-0.372445	-2.643745	-3.221466
1	-1.377918	-2.236418	-3.427362
1	-0.419101	-3.735727	-3.305147
1	0.318551	-2.261106	-3.988693
1	-1.542540	0.997394	1.440590
8	0.410307	0.699414	-2.664790
6	-0.002032	0.916891	-4.050675
1	0.044690	1.990161	-4.269731
1	-1.026650	0.562468	-4.194663
1	0.670413	0.373072	-4.726054
1	1.576748	0.985908	-2.257099

TS3-Sn=Sn=Sn-3MeOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

50	2.511243	-0.431015	-0.178700
50	0.016205	0.491454	-1.252793
50	-2.296854	-0.014703	0.107099
14	2.260812	-1.880683	2.028533
14	4.188409	1.610395	-0.397319
14	-4.223033	-1.644786	-0.694978
14	-2.815168	2.363597	1.197523
6	0.761561	-3.007450	1.642480
1	-0.180802	-2.452558	1.720098
1	0.710557	-3.858221	2.336453
1	0.821864	-3.403318	0.621404
6	1.881092	-0.983568	3.734068
6	1.145309	-1.955216	4.704543
1	0.936909	-1.441085	5.656598
1	1.740205	-2.847807	4.932256
1	0.184003	-2.287226	4.292161
6	3.158426	-0.450399	4.435609
1	3.733168	0.220226	3.782328
1	3.822486	-1.262911	4.756174
1	2.878308	0.120264	5.335494
6	3.836106	-3.065750	2.056031
6	3.778224	-4.036825	3.269059
1	3.850492	-3.507696	4.227461
1	4.620930	-4.745204	3.218294
1	2.852481	-4.627970	3.274026
6	5.169940	-2.272096	2.108085
1	5.281622	-1.624699	1.227977
1	6.022404	-2.970135	2.114108
1	5.247647	-1.642107	3.001147
6	0.940517	0.224599	3.472407
1	1.438572	0.994510	2.868784
1	0.640882	0.681989	4.429491
1	0.027287	-0.076146	2.941381
6	3.848173	-3.926387	0.758386
1	3.895228	-3.301054	-0.142745
1	2.957569	-4.561885	0.677347
1	4.731848	-4.584380	0.759099
6	5.320981	1.686733	1.146066
1	6.002289	2.548367	1.104019

1	5.931138	0.779803	1.240497
1	4.724361	1.775400	2.062362
6	5.320500	1.103141	-1.929511
6	6.600610	1.981111	-2.016642
1	6.373940	3.037157	-2.192901
1	7.232379	1.632103	-2.849066
1	7.197635	1.909781	-1.097960
6	5.791883	-0.371207	-1.760419
1	6.334167	-0.526599	-0.817649
1	6.474344	-0.638650	-2.582659
1	4.949921	-1.074065	-1.784502
6	4.538182	1.202914	-3.268184
1	4.261317	2.237713	-3.506702
1	3.618186	0.601184	-3.241192
1	5.157938	0.826488	-4.097734
6	3.357696	3.398965	-0.536634
6	2.785057	3.775170	0.861931
1	2.243582	4.732402	0.796420
1	3.579043	3.893420	1.609676
1	2.077233	3.022181	1.233884
6	4.411033	4.475367	-0.931180
1	3.964631	5.476669	-0.822186
1	4.719936	4.369673	-1.978582
1	5.309570	4.442046	-0.301936
6	2.198817	3.500102	-1.562926
1	1.857765	4.545268	-1.638358
1	1.333153	2.900652	-1.256200
1	2.488917	3.170371	-2.568033
6	-3.751108	2.140244	2.911358
6	-1.089868	3.089362	1.600700
1	-1.175232	4.100819	2.021285
1	-0.464540	3.155466	0.703194
1	-0.555926	2.469189	2.329856
6	-3.657275	3.601140	-0.080990
6	-5.293089	2.093924	2.747026
1	-5.764705	1.871534	3.717082
1	-5.607436	1.317078	2.037563
1	-5.693132	3.054325	2.398827
6	-3.386229	3.302329	3.881374
1	-2.313772	3.315070	4.112059
1	-3.927448	3.173701	4.832031
1	-3.656025	4.285177	3.475678
6	-3.295115	0.810485	3.578428
1	-2.205405	0.760656	3.705974
1	-3.605969	-0.064558	2.991278
1	-3.750256	0.716212	4.577023

6	-2.716109	3.812592	-1.301419
1	-1.736636	4.213633	-1.009900
1	-3.175614	4.530395	-1.998921
1	-2.541324	2.879363	-1.850597
6	-3.878476	4.987128	0.591714
1	-2.936314	5.419812	0.954522
1	-4.577833	4.931959	1.435355
1	-4.300742	5.690099	-0.143646
6	-5.015894	3.078519	-0.622510
1	-5.770100	2.978784	0.165413
1	-4.905372	2.102012	-1.111497
1	-5.410098	3.780610	-1.374298
6	-3.743534	-3.349450	0.162644
6	-5.897889	-1.085233	0.041475
1	-6.120148	-0.045937	-0.228662
1	-5.883124	-1.143099	1.137774
1	-6.727711	-1.711914	-0.313905
6	-4.393779	-1.675742	-2.648811
6	-4.933181	-4.349849	0.120119
1	-5.821753	-3.946880	0.623516
1	-4.650555	-5.278468	0.641072
1	-5.214375	-4.618369	-0.904452
6	-2.501915	-4.012529	-0.494454
1	-2.709952	-4.345844	-1.518430
1	-2.201083	-4.897736	0.087529
1	-1.639342	-3.335129	-0.527066
6	-3.411592	-3.085519	1.661184
1	-4.247334	-2.614272	2.196736
1	-2.526281	-2.444862	1.777939
1	-3.187684	-4.038001	2.165999
6	-5.410709	-2.765404	-3.093938
1	-6.378736	-2.669332	-2.584373
1	-5.025414	-3.775807	-2.909084
1	-5.594802	-2.677316	-4.176315
6	-4.925510	-0.289163	-3.114737
1	-4.228209	0.518981	-2.853638
1	-5.904082	-0.049263	-2.679011
1	-5.040039	-0.286046	-4.210049
6	-3.047578	-1.936820	-3.375062
1	-2.277911	-1.205816	-3.105277
1	-3.202043	-1.874438	-4.464889
1	-2.640526	-2.930587	-3.155965
8	0.168594	-0.666746	-3.001568
6	-0.041278	-0.037420	-4.301995
1	0.895625	0.405801	-4.672571
1	-0.793512	0.758714	-4.220336

1	-0.399660	-0.787914	-5.016636
8	1.806824	-2.405870	-2.620628
6	2.635932	-3.089603	-3.602940
1	3.132287	-2.378644	-4.278776
1	2.018034	-3.784428	-4.183331
1	3.395571	-3.658886	-3.057067
1	1.019808	-1.693781	-2.940822
1	2.354937	-1.750372	-1.668048

TS4-Sn=Sn=Sn-3MeOH			

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

50	-2.257302	-0.006163	-0.260525
50	0.054858	0.402240	1.171529
50	2.212121	-0.183777	-0.250567
14	-3.705041	-1.891952	0.735442
14	-3.130853	2.122970	-1.441133
14	4.170223	1.414395	0.112474
14	2.227901	-2.555756	-1.247784
6	-2.467091	-3.030058	1.648972
1	-1.784245	-3.521348	0.946293
1	-2.987490	-3.814326	2.215366
1	-1.849098	-2.452022	2.346375
6	-4.492913	-2.898447	-0.751902
6	-4.653994	-4.384594	-0.328464
1	-5.132736	-4.954542	-1.139146
1	-5.268619	-4.495518	0.573578
1	-3.677653	-4.845192	-0.131172
6	-5.869130	-2.324154	-1.178109
1	-5.799785	-1.261878	-1.447570
1	-6.620954	-2.424509	-0.386025
1	-6.239432	-2.865883	-2.061783
6	-4.928477	-1.182411	2.082660
6	-5.769465	-2.332003	2.698917
1	-6.408701	-2.812732	1.947615
1	-6.423633	-1.940999	3.493419
1	-5.129551	-3.104911	3.145888
6	-5.877535	-0.090095	1.523721
1	-5.308644	0.739841	1.088472

1	-6.493250	0.322963	2.338095
1	-6.554241	-0.473980	0.753852
6	-3.565026	-2.865558	-2.002211
1	-3.504410	-1.863781	-2.444924
1	-3.964866	-3.542771	-2.772702
1	-2.539195	-3.183893	-1.775995
6	-4.084254	-0.527987	3.214988
1	-3.470520	0.299879	2.832536
1	-3.415006	-1.248924	3.698993
1	-4.752141	-0.115827	3.987957
6	-4.898181	1.635721	-1.988045
1	-5.347412	2.382295	-2.655117
1	-5.559075	1.511598	-1.120994
1	-4.877864	0.676888	-2.521682
6	-3.231320	3.672375	-0.247956
6	-4.309229	4.655136	-0.789121
1	-4.075452	5.007785	-1.800489
1	-4.372223	5.536873	-0.133112
1	-5.302489	4.188157	-0.814791
6	-3.662305	3.244372	1.183716
1	-4.656757	2.780369	1.200919
1	-3.703246	4.132443	1.834569
1	-2.945938	2.544082	1.631656
6	-1.871767	4.414793	-0.120944
1	-1.546118	4.847021	-1.074753
1	-1.077254	3.757081	0.254243
1	-1.979113	5.247262	0.593522
6	-2.044097	2.357094	-3.052923
6	-2.224657	1.119488	-3.980316
1	-1.623770	1.258594	-4.891957
1	-3.268792	0.978183	-4.287772
1	-1.877519	0.196794	-3.501365
6	-2.526353	3.616621	-3.824851
1	-1.984117	3.695410	-4.779503
1	-2.335330	4.536639	-3.259061
1	-3.599575	3.570147	-4.055237
6	-0.528649	2.500639	-2.748269
1	0.031954	2.568331	-3.693901
1	-0.130641	1.639852	-2.196556
1	-0.298145	3.397570	-2.164390
6	3.756051	-3.666463	-0.701799
6	0.643268	-3.426562	-0.628617
1	0.478391	-4.380033	-1.148308
1	-0.231325	-2.789694	-0.799410
1	0.706501	-3.630535	0.447867
6	2.058831	-2.268967	-3.185700

6	5.023460	-3.390199	-1.553047
1	5.869002	-3.978204	-1.162876
1	5.313930	-2.332434	-1.522727
1	4.881650	-3.671947	-2.603199
6	3.368016	-5.167095	-0.837589
1	2.545932	-5.427932	-0.159011
1	4.229528	-5.800522	-0.574976
1	3.059408	-5.426777	-1.857511
6	4.118309	-3.413513	0.787822
1	3.264530	-3.603044	1.452017
1	4.451336	-2.380282	0.951804
1	4.937675	-4.085744	1.089548
6	0.717670	-1.537337	-3.473968
1	-0.154629	-2.120288	-3.153384
1	0.621847	-1.354644	-4.556032
1	0.676339	-0.566531	-2.965276
6	2.043073	-3.621515	-3.947624
1	1.228853	-4.270233	-3.595615
1	2.988194	-4.168170	-3.841137
1	1.880155	-3.441806	-5.021812
6	3.195384	-1.367553	-3.742614
1	4.185522	-1.824643	-3.644294
1	3.214219	-0.396699	-3.229993
1	3.021576	-1.167581	-4.811697
6	4.587142	1.750620	1.999240
6	5.670420	0.549513	-0.699989
1	5.453496	0.331496	-1.754119
1	5.873523	-0.407500	-0.204266
1	6.585860	1.154198	-0.660861
6	3.713329	2.988683	-0.980091
6	5.537850	2.969216	2.144197
1	6.420069	2.884227	1.495763
1	5.891338	3.048385	3.184222
1	5.021391	3.905134	1.897644
6	3.327286	2.010180	2.868606
1	2.720386	2.843018	2.499099
1	3.633988	2.235900	3.903897
1	2.673988	1.127795	2.895685
6	5.299577	0.489703	2.564839
1	6.274821	0.319807	2.092368
1	4.688600	-0.410540	2.408788
1	5.466433	0.606333	3.647825
6	4.961098	3.888121	-1.194965
1	5.792024	3.321371	-1.636154
1	5.311235	4.341499	-0.261822
1	4.711785	4.704115	-1.891149

6	3.233212	2.527010	-2.387762
1	2.343185	1.890730	-2.324906
1	4.011021	1.970303	-2.929245
1	2.973735	3.409827	-2.993416
6	2.572097	3.823318	-0.336854
1	1.669625	3.226021	-0.158422
1	2.296843	4.654674	-1.006597
1	2.870999	4.259067	0.625627
8	0.143095	2.255595	1.780555
6	-0.253013	2.820421	3.039315
1	0.410318	2.485503	3.852099
1	-1.292398	2.553491	3.301097
1	-0.189506	3.912091	2.961136
1	-1.458212	-0.852068	-1.524596
8	-0.174340	-0.568758	3.227742
6	-0.715122	-0.274149	4.559884
1	-1.131316	-1.189171	4.997291
1	-1.507196	0.466367	4.446735
1	0.076453	0.127439	5.205402
1	0.586016	-1.271939	3.248329
8	1.856064	-2.037680	3.039248
1	2.225441	-1.647030	2.188145
6	2.834675	-2.073941	4.131265
1	3.763176	-2.541249	3.789006
1	2.390562	-2.679736	4.924324
1	3.044069	-1.060829	4.499108

Pro-Sn=Sn=Sn-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

50	2.510038	-0.055711	0.382556
50	0.014642	-0.057105	-1.066284
50	-2.498508	-0.066327	0.318865
14	4.194352	-1.752231	-0.793967
14	3.213732	2.251934	1.508726
14	-4.480487	1.394295	-0.704301
14	-2.733798	-2.536459	1.274789
6	3.078063	-3.257509	-1.162647
1	2.815363	-3.785218	-0.235723

1	3.586146	-3.975035	-1.823034
1	2.142581	-2.936415	-1.637581
6	5.584717	-2.344392	0.466007
6	6.123109	-3.739293	0.027270
1	6.905894	-4.067923	0.729354
1	6.564478	-3.720354	-0.975494
1	5.332501	-4.499808	0.034362
6	6.780480	-1.359353	0.561453
1	6.457922	-0.342863	0.821875
1	7.343795	-1.305878	-0.378673
1	7.478390	-1.696941	1.343941
6	4.869555	-1.051986	-2.495368
6	5.890867	-2.036950	-3.134870
1	6.811173	-2.117567	-2.543321
1	6.173912	-1.674823	-4.135912
1	5.472943	-3.045348	-3.256715
6	5.547936	0.336802	-2.345449
1	4.848486	1.084037	-1.951007
1	5.889479	0.692243	-3.330696
1	6.420791	0.307093	-1.683478
6	4.973748	-2.504752	1.887667
1	4.679828	-1.538911	2.318784
1	5.719134	-2.955602	2.561552
1	4.088230	-3.153988	1.889309
6	3.674049	-0.897657	-3.478899
1	2.916646	-0.202563	-3.095461
1	3.173833	-1.853474	-3.673002
1	4.036821	-0.501040	-4.440622
6	5.108347	2.217770	1.781843
1	5.428179	3.074943	2.391261
1	5.649419	2.265368	0.828207
1	5.428636	1.306171	2.299562
6	2.842318	3.784513	0.341920
6	3.560121	5.063587	0.867769
1	3.192455	5.375897	1.850730
1	3.381377	5.895274	0.168253
1	4.646365	4.923216	0.939906
6	3.406662	3.494052	-1.077955
1	4.489588	3.312206	-1.061676
1	3.227259	4.361202	-1.732563
1	2.921250	2.626513	-1.542851
6	1.323892	4.081914	0.209369
1	0.871894	4.358788	1.170136
1	0.767620	3.228000	-0.199425
1	1.170781	4.926413	-0.480899
6	2.365954	2.305607	3.279415

6	3.032082	1.227253	4.184453
1	2.537477	1.218044	5.168156
1	4.096854	1.433794	4.352434
1	2.939453	0.218565	3.761193
6	2.567852	3.689856	3.961831
1	2.205451	3.640961	5.000604
1	2.002698	4.482239	3.455963
1	3.624170	3.989511	3.996093
6	0.842422	2.008187	3.217215
1	0.410195	2.070908	4.228399
1	0.637679	0.998776	2.839421
1	0.302428	2.721440	2.583568
6	-3.864210	-3.687961	0.161070
6	-0.962555	-3.256249	1.208090
1	-0.924646	-4.252796	1.670474
1	-0.245081	-2.617726	1.737846
1	-0.611132	-3.348317	0.172159
6	-3.272074	-2.412189	3.159592
6	-5.378516	-3.425810	0.378965
1	-5.967777	-4.039721	-0.320509
1	-5.643143	-2.375655	0.201649
1	-5.698563	-3.688221	1.395045
6	-3.571067	-5.189746	0.452329
1	-2.526118	-5.448696	0.240268
1	-4.204036	-5.818145	-0.194046
1	-3.784792	-5.464827	1.491152
6	-3.533463	-3.431239	-1.336115
1	-2.471146	-3.599896	-1.555677
1	-3.785671	-2.406842	-1.638949
1	-4.117034	-4.117559	-1.969857
6	-2.093625	-1.817585	3.985020
1	-1.213508	-2.472565	3.968598
1	-2.402302	-1.702493	5.035882
1	-1.789241	-0.828583	3.619288
6	-3.595606	-3.818874	3.742482
1	-2.762679	-4.522642	3.609106
1	-4.491492	-4.259116	3.287495
1	-3.784345	-3.733020	4.824278
6	-4.511604	-1.496247	3.358357
1	-5.383776	-1.845046	2.792304
1	-4.301198	-0.461507	3.056893
1	-4.792951	-1.475734	4.423185
6	-4.374062	1.565381	-2.653548
6	-6.127022	0.497258	-0.311711
1	-6.164846	0.147775	0.726561
1	-6.270987	-0.374993	-0.962425

1	-6.980047	1.171952	-0.469881
6	-4.482027	3.088417	0.289324
6	-5.760326	1.988572	-3.226326
1	-6.541327	1.250199	-3.003491
1	-5.688571	2.073075	-4.321974
1	-6.091832	2.960002	-2.842346
6	-3.304246	2.596232	-3.107395
1	-3.552130	3.613630	-2.777855
1	-3.262530	2.612941	-4.208989
1	-2.302584	2.337022	-2.740661
6	-4.010399	0.187532	-3.276481
1	-4.716086	-0.602533	-2.983085
1	-2.998194	-0.126684	-2.993948
1	-4.036832	0.260063	-4.375075
6	-5.505973	4.086395	-0.327000
1	-6.518412	3.663766	-0.384087
1	-5.210789	4.405697	-1.333764
1	-5.561543	4.988624	0.302251
6	-4.909265	2.812116	1.760614
1	-4.223814	2.117912	2.264418
1	-5.924178	2.398746	1.822707
1	-4.899061	3.754759	2.329670
6	-3.084178	3.767750	0.308543
1	-2.340224	3.147989	0.824277
1	-3.146940	4.725394	0.849557
1	-2.708009	3.977387	-0.698831
8	-0.210724	1.374387	-2.391131
6	0.574582	1.766522	-3.538473
1	1.557588	2.167356	-3.244453
1	0.027999	2.555546	-4.070943
1	0.737457	0.926039	-4.231617
1	1.950230	-0.993915	1.731114
8	0.252276	-1.674577	-2.164138
6	-0.408888	-2.102646	-3.376386
1	-0.045183	-3.107714	-3.627413
1	-0.183715	-1.430483	-4.219020
1	-1.503234	-2.151708	-3.259446
1	-2.031241	0.814866	1.737206

TS1-Pb=Pb=Pb-1MeOH			

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

8	-0.524688	-2.427584	-1.182575
82	0.015553	-1.144251	0.504106
82	-2.577692	-0.235154	-0.534974
1	-1.756955	-1.718564	-1.434761
6	-0.192423	-3.751843	-1.685620
1	-0.009529	-4.457840	-0.861606
1	0.695759	-3.713874	-2.329164
1	-1.042914	-4.118901	-2.277285
82	2.368158	0.226816	-0.205483
14	4.459021	-1.146464	-1.179010
6	6.103113	-0.231883	-0.842536
1	6.301280	-0.186231	0.236164
1	6.062099	0.801069	-1.209026
1	6.959026	-0.726799	-1.322004
6	4.579475	-2.916286	-0.322548
6	5.897678	-3.627243	-0.746282
1	6.784539	-3.037265	-0.482491
1	5.929398	-3.828716	-1.823773
1	5.976047	-4.594620	-0.225404
6	4.610879	-2.732783	1.223020
1	3.670944	-2.309194	1.601644
1	5.433773	-2.083395	1.548949
1	4.748601	-3.711854	1.708350
6	3.385835	-3.847633	-0.661134
1	2.421546	-3.387065	-0.410830
1	3.468429	-4.779054	-0.078505
1	3.365222	-4.124727	-1.721885
6	4.104545	-1.113966	-3.113529
6	5.236584	-1.820273	-3.911012
1	6.225330	-1.398289	-3.686373
1	5.061892	-1.700115	-4.991948
1	5.268781	-2.896956	-3.701984
6	2.747350	-1.772986	-3.489866
1	2.754439	-2.854669	-3.313407
1	2.544409	-1.615796	-4.561043
1	1.903386	-1.349054	-2.929253
6	4.045595	0.374952	-3.568725
1	4.975934	0.916945	-3.354696
1	3.216262	0.915406	-3.088590
1	3.874045	0.424212	-4.655039
14	2.646908	2.087042	1.750620
6	3.670598	3.598484	1.020005

6	3.211155	4.939664	1.662673
1	2.152766	5.145006	1.458294
1	3.796259	5.772410	1.241023
1	3.352804	4.950564	2.750124
6	3.402752	3.694537	-0.511027
1	2.330475	3.753563	-0.745298
1	3.820491	2.832487	-1.050663
1	3.880405	4.597615	-0.922183
6	5.199089	3.437422	1.234020
1	5.737498	4.247344	0.717093
1	5.573052	2.483973	0.837450
1	5.467484	3.489594	2.296576
6	0.845224	2.717458	1.951643
1	0.766437	3.446766	2.770152
1	0.141405	1.902176	2.161948
1	0.499915	3.209614	1.033407
6	3.208448	1.421455	3.509600
6	2.146085	0.410913	4.030247
1	1.156133	0.871180	4.145836
1	2.450784	0.027905	5.016658
1	2.041855	-0.454050	3.360283
6	3.300814	2.592572	4.529995
1	2.350851	3.137399	4.616590
1	4.084093	3.311828	4.259509
1	3.545306	2.197266	5.528684
6	4.576159	0.689296	3.455551
1	5.389144	1.351685	3.137325
1	4.545518	-0.164359	2.767397
1	4.832264	0.301277	4.454313
14	-2.660270	2.153074	-1.770920
6	-0.861710	2.692314	-2.142130
1	-0.358531	3.033998	-1.227608
1	-0.839189	3.515419	-2.872255
1	-0.269795	1.862841	-2.547741
6	-3.506420	3.622428	-0.788222
6	-3.146879	4.988751	-1.444723
1	-3.631246	5.805488	-0.886214
1	-3.482952	5.054152	-2.485996
1	-2.065389	5.174615	-1.425608
6	-5.050745	3.479638	-0.735260
1	-5.354983	2.515121	-0.307174
1	-5.505356	3.568179	-1.729824
1	-5.478239	4.275032	-0.104515
6	-2.971299	3.642494	0.671307
1	-3.254468	2.735831	1.218697
1	-3.390834	4.507176	1.209979

1	-1.877367	3.727966	0.711403
6	-3.506163	1.680321	-3.483310
6	-3.817753	2.938054	-4.342017
1	-4.579736	3.576087	-3.877238
1	-4.204222	2.625436	-5.325181
1	-2.921301	3.547833	-4.518845
6	-4.825160	0.885001	-3.271302
1	-4.642008	-0.067174	-2.753830
1	-5.279471	0.643468	-4.245023
1	-5.563252	1.448540	-2.688177
6	-2.524130	0.778651	-4.287993
1	-2.243036	-0.124027	-3.729751
1	-1.602884	1.313020	-4.552954
1	-3.002803	0.454567	-5.225517
14	-4.181146	-1.073341	1.450784
6	-5.844721	-0.128024	1.354621
1	-6.600272	-0.562332	2.023370
1	-6.250054	-0.145260	0.334993
1	-5.713164	0.924429	1.637420
6	-4.533766	-2.950883	0.964357
6	-5.661526	-3.560431	1.843114
1	-5.384920	-3.601931	2.903544
1	-5.867594	-4.591593	1.514490
1	-6.597594	-2.993140	1.755343
6	-5.012581	-3.000436	-0.517897
1	-5.881837	-2.353247	-0.697354
1	-5.304596	-4.030373	-0.776725
1	-4.216142	-2.700329	-1.210469
6	-3.270187	-3.849010	1.080449
1	-2.947666	-3.975956	2.120787
1	-2.425867	-3.446693	0.505374
1	-3.490445	-4.851887	0.680031
6	-3.476972	-0.764270	3.274059
6	-3.098162	0.739525	3.410465
1	-2.735125	0.938872	4.431368
1	-3.955710	1.402194	3.231325
1	-2.299904	1.023564	2.711735
6	-4.571525	-1.081381	4.336345
1	-4.196990	-0.815016	5.337636
1	-4.825312	-2.148692	4.355278
1	-5.494585	-0.513110	4.166087
6	-2.221072	-1.600886	3.638679
1	-1.848591	-1.296221	4.630142
1	-1.398702	-1.450490	2.926220
1	-2.432834	-2.675949	3.682763

Int-Pb=Pb=Pb-1MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-2.699843	0.301395	-0.098390
82	0.055719	-0.906583	-0.361660
82	2.638083	0.312523	0.362185
14	-4.245087	-0.843803	-2.000606
14	-3.601012	1.307359	2.262477
14	4.661071	-1.569613	0.577734
14	3.009845	2.328888	-1.492522
6	-3.160255	-0.673333	-3.570772
1	-3.043347	0.380806	-3.853278
1	-3.606813	-1.202768	-4.424377
1	-2.155039	-1.084011	-3.415005
6	-5.887543	0.183261	-2.331624
6	-6.420772	-0.107064	-3.766329
1	-7.344289	0.468500	-3.937400
1	-6.657254	-1.165936	-3.918703
1	-5.699374	0.194425	-4.536249
6	-7.006522	-0.143496	-1.306476
1	-6.673955	0.017727	-0.272630
1	-7.354337	-1.180550	-1.394201
1	-7.874995	0.510921	-1.481347
6	-4.511476	-2.755238	-1.652970
6	-5.500117	-3.384776	-2.677678
1	-6.514802	-2.981046	-2.575493
1	-5.560015	-4.471698	-2.509719
1	-5.172673	-3.230826	-3.714883
6	-5.054112	-3.013335	-0.220431
1	-4.361253	-2.645814	0.547734
1	-5.184204	-4.095009	-0.058127
1	-6.026170	-2.533831	-0.052680
6	-5.576921	1.705692	-2.246879
1	-5.296794	2.010835	-1.230351
1	-6.470475	2.282245	-2.533389
1	-4.760958	2.001065	-2.919797
6	-3.150161	-3.494378	-1.800249
1	-2.388090	-3.110054	-1.109242

1	-2.751933	-3.418870	-2.820248
1	-3.282811	-4.564142	-1.575595
6	-5.506989	1.468352	2.178792
1	-5.885819	2.036425	3.041166
1	-5.989115	0.482339	2.192613
1	-5.833980	1.986107	1.269800
6	-3.201931	0.073226	3.732707
6	-4.005952	0.463975	5.008924
1	-3.734726	1.455723	5.386447
1	-3.797339	-0.263572	5.809064
1	-5.088359	0.452138	4.827852
6	-3.642550	-1.361545	3.326156
1	-4.710483	-1.409916	3.073237
1	-3.469772	-2.054628	4.164264
1	-3.071784	-1.733516	2.467071
6	-1.689801	0.041505	4.084485
1	-1.343939	1.001179	4.488842
1	-1.066127	-0.202207	3.213257
1	-1.500916	-0.725653	4.851720
6	-2.849590	3.113921	2.429708
6	-3.535010	4.038599	1.381445
1	-3.093636	5.045880	1.436482
1	-4.612370	4.139638	1.565501
1	-3.393082	3.670854	0.356945
6	-3.123051	3.702772	3.844442
1	-2.808105	4.758027	3.867387
1	-2.558406	3.176563	4.624044
1	-4.188170	3.671929	4.111996
6	-1.318802	3.141952	2.168831
1	-0.940364	4.168572	2.295117
1	-1.084716	2.827115	1.144422
1	-0.764118	2.495840	2.859399
6	3.690807	1.876476	-3.281030
6	1.242578	3.031103	-1.755365
1	1.274563	4.017530	-2.240378
1	0.706760	3.145544	-0.805230
1	0.640959	2.369316	-2.391956
6	4.031069	3.718998	-0.540841
6	5.223621	1.631763	-3.286952
1	5.544197	1.290303	-4.284147
1	5.518951	0.863285	-2.561252
1	5.785583	2.546304	-3.057771
6	3.364307	3.011243	-4.298035
1	2.283474	3.177398	-4.388845
1	3.739622	2.728843	-5.294982
1	3.832059	3.964322	-4.027274

6	2.986848	0.583956	-3.783993
1	1.892521	0.687576	-3.790881
1	3.239337	-0.285068	-3.165220
1	3.303372	0.364422	-4.816183
6	3.171697	4.241605	0.648303
1	2.250648	4.727809	0.303593
1	3.745590	4.984492	1.224678
1	2.885071	3.437042	1.340921
6	4.355960	4.932628	-1.458084
1	3.452201	5.357419	-1.915096
1	5.051951	4.664719	-2.262611
1	4.831560	5.729819	-0.864075
6	5.364529	3.166991	0.033744
1	6.022438	2.773320	-0.749934
1	5.188830	2.359968	0.758797
1	5.909101	3.967838	0.558738
6	4.383445	-3.240975	-0.422320
6	6.319342	-0.830284	-0.041709
1	6.472314	0.194992	0.314579
1	6.350542	-0.805647	-1.138550
1	7.171628	-1.434954	0.300875
6	4.827412	-1.791775	2.525987
6	5.729191	-4.020697	-0.535544
1	6.491280	-3.448763	-1.079934
1	5.559190	-4.956440	-1.091617
1	6.140664	-4.289587	0.443938
6	3.324849	-4.168276	0.234967
1	3.666566	-4.543871	1.208547
1	3.157756	-5.045260	-0.411479
1	2.356948	-3.671036	0.377851
6	3.915001	-2.914943	-1.868616
1	4.607239	-2.235498	-2.385370
1	2.917309	-2.458254	-1.877234
1	3.859276	-3.843060	-2.459181
6	5.873370	-2.886438	2.885646
1	6.851594	-2.693988	2.424164
1	5.540131	-3.884869	2.576972
1	6.023032	-2.912646	3.977003
6	5.316293	-0.445274	3.135801
1	4.619862	0.380282	2.924356
1	6.306594	-0.157363	2.760434
1	5.387913	-0.535947	4.230995
6	3.476265	-2.162216	3.200226
1	2.712916	-1.389235	3.039513
1	3.620773	-2.265195	4.287899
1	3.068795	-3.106806	2.824679

8	0.132294	-2.654647	0.681572
6	-0.750694	-3.376356	1.562861
1	-0.460225	-4.436210	1.564894
1	-1.805831	-3.311907	1.245519
1	-0.678151	-2.992604	2.593060
1	-2.258466	1.781255	-0.994104

TS2-Pb=Pb=Pb-2MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

82	-2.492116	0.026363	0.248543
82	0.088805	-0.599529	-0.939331
82	2.735788	0.565070	-0.477341
14	-3.858721	1.942932	-0.990863
14	-3.349657	-2.050274	1.692473
14	4.375852	-1.518980	-0.119661
14	2.477031	2.732471	1.103025
6	-2.501450	3.053862	-1.751634
1	-1.981660	3.622528	-0.970050
1	-2.932048	3.775216	-2.461241
1	-1.739998	2.466187	-2.277245
6	-4.842698	3.021826	0.320449
6	-5.093898	4.447278	-0.254064
1	-5.658485	5.044788	0.478858
1	-5.671659	4.430241	-1.186309
1	-4.150299	4.972600	-0.449619
6	-6.200195	2.379622	0.709038
1	-6.074051	1.348707	1.067605
1	-6.903306	2.363641	-0.133331
1	-6.668232	2.958960	1.519974
6	-4.901545	1.151129	-2.441271
6	-5.743690	2.233810	-3.174776
1	-6.511088	2.669707	-2.522640
1	-6.259497	1.783006	-4.037083
1	-5.116198	3.050872	-3.556371
6	-5.849177	0.027661	-1.939403
1	-5.290635	-0.774281	-1.439614
1	-6.380791	-0.422259	-2.792369
1	-6.602265	0.401180	-1.236930

6	-3.995913	3.180818	1.616859
1	-3.877245	2.228186	2.147587
1	-4.498028	3.883563	2.300043
1	-2.989981	3.572587	1.415405
6	-3.917923	0.523543	-3.471547
1	-3.284763	-0.249387	-3.013934
1	-3.259959	1.278256	-3.920527
1	-4.486782	0.048302	-4.285542
6	-5.182380	-1.706663	2.122538
1	-5.580609	-2.455454	2.821291
1	-5.805056	-1.726485	1.218392
1	-5.301797	-0.719153	2.584728
6	-3.273684	-3.699732	0.627597
6	-4.261979	-4.747329	1.220144
1	-4.001539	-5.029348	2.247708
1	-4.234977	-5.662011	0.607703
1	-5.295694	-4.378791	1.219528
6	-3.715436	-3.400636	-0.833362
1	-4.715771	-2.949303	-0.884235
1	-3.745990	-4.338205	-1.409967
1	-3.006562	-2.732428	-1.337885
6	-1.853823	-4.327412	0.570948
1	-1.493543	-4.624971	1.563548
1	-1.117583	-3.655438	0.112397
1	-1.882994	-5.236259	-0.050879
6	-2.310691	-2.059921	3.357967
6	-2.640989	-0.776212	4.174353
1	-2.064041	-0.779688	5.112483
1	-3.704442	-0.715612	4.440311
1	-2.369966	0.133772	3.624209
6	-2.696144	-3.296701	4.220453
1	-2.173056	-3.247711	5.188480
1	-2.409575	-4.240095	3.739172
1	-3.773993	-3.331942	4.430247
6	-0.776854	-2.081991	3.110088
1	-0.247328	-2.081597	4.076046
1	-0.444717	-1.193105	2.557988
1	-0.452604	-2.968561	2.555373
6	3.909529	3.920935	0.448044
6	0.811102	3.488356	0.539858
1	0.631577	4.456806	1.028369
1	-0.025779	2.824750	0.789900
1	0.792042	3.648451	-0.545527
6	2.390249	2.524302	3.050795
6	5.247841	3.680724	1.196339
1	6.050076	4.273957	0.730105

1	5.552139	2.624998	1.159357
1	5.186602	3.977887	2.250240
6	3.492678	5.412434	0.605504
1	2.605392	5.644593	0.002514
1	4.309751	6.062573	0.254046
1	3.275026	5.682305	1.645419
6	4.161753	3.674579	-1.068578
1	3.240388	3.729498	-1.663108
1	4.618990	2.692319	-1.254438
1	4.858539	4.434042	-1.456484
6	1.071034	1.788901	3.422737
1	0.179888	2.342992	3.104251
1	1.014027	1.665778	4.515845
1	1.020138	0.788025	2.973889
6	2.371561	3.920874	3.740023
1	1.549694	4.550753	3.373245
1	3.312156	4.466244	3.592435
1	2.230792	3.795390	4.825371
6	3.571236	1.698186	3.628081
1	4.542629	2.171358	3.446597
1	3.599842	0.688467	3.201386
1	3.451219	1.593262	4.718376
6	4.750043	-2.206592	-1.924231
6	5.974491	-0.720147	0.573773
1	5.773687	-0.213569	1.526458
1	6.372768	0.031598	-0.120994
1	6.763783	-1.464086	0.746847
6	3.771791	-2.856037	1.188257
6	6.187567	-2.801381	-1.973113
1	6.947917	-2.033326	-1.779131
1	6.380006	-3.212178	-2.976667
1	6.332079	-3.612542	-1.248759
6	3.729540	-3.293764	-2.364636
1	3.854377	-4.223195	-1.794151
1	3.893316	-3.538934	-3.426251
1	2.687657	-2.964309	-2.252764
6	4.686517	-1.052163	-2.967203
1	5.309316	-0.190795	-2.684266
1	3.661261	-0.690479	-3.110139
1	5.048306	-1.417352	-3.941007
6	4.861022	-3.962165	1.324122
1	5.836539	-3.549133	1.613405
1	4.988632	-4.526735	0.392062
1	4.560931	-4.678841	2.104666
6	3.593327	-2.178061	2.576619
1	2.799538	-1.419410	2.555642

1	4.514811	-1.701823	2.935237
1	3.301790	-2.937120	3.319634
6	2.424310	-3.539082	0.830211
1	1.610963	-2.812453	0.720813
1	2.143535	-4.231580	1.640277
1	2.470201	-4.113273	-0.098410
8	0.116389	-2.416347	-1.895927
6	-0.434381	-2.748490	-3.191245
1	-1.476757	-2.399563	-3.314721
1	-0.429884	-3.841916	-3.302044
1	0.167226	-2.315846	-4.008165
1	-1.632057	0.994813	1.471972
8	0.482354	0.725481	-2.621325
6	0.086352	0.885846	-4.009890
1	0.166738	1.945888	-4.290320
1	-0.952299	0.563016	-4.164431
1	0.737217	0.293441	-4.670708
1	1.861485	0.968476	-2.123242

TS3-Pb=Pb=Pb-3MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-2.576051	0.448736	-0.121797
82	-0.039391	-0.717416	-1.238928
82	2.355018	0.066833	0.143899
14	-2.266700	2.043097	2.038706
14	-4.299439	-1.634648	-0.173419
14	4.346468	1.678066	-0.763261
14	2.966849	-2.272293	1.434890
6	-0.757534	3.119771	1.556875
1	0.175078	2.547959	1.637319
1	-0.669524	4.002108	2.207071
1	-0.835860	3.468533	0.519936
6	-1.855946	1.226903	3.777828
6	-1.116662	2.251190	4.690479
1	-0.888497	1.784168	5.661988
1	-1.719537	3.146046	4.885720
1	-0.165987	2.575196	4.248443
6	-3.120761	0.722297	4.522023

1	-3.698831	0.013796	3.913325
1	-3.786877	1.546617	4.806243
1	-2.826199	0.203620	5.448322
6	-3.828677	3.242738	2.040129
6	-3.752430	4.265770	3.209895
1	-3.820842	3.779275	4.190960
1	-4.591544	4.976149	3.134155
1	-2.823688	4.851806	3.182380
6	-5.168200	2.463599	2.146219
1	-5.299132	1.773368	1.302175
1	-6.014376	3.169006	2.130475
1	-5.237832	1.879257	3.070701
6	-0.909290	0.014206	3.560516
1	-1.404681	-0.784200	2.992313
1	-0.600177	-0.400370	4.533823
1	-0.000905	0.297960	3.011391
6	-3.845469	4.048542	0.707534
1	-3.888100	3.390582	-0.169967
1	-2.958259	4.685335	0.601995
1	-4.731928	4.701993	0.681517
6	-5.369154	-1.617275	1.416618
1	-6.052658	-2.477598	1.453680
1	-5.975184	-0.704970	1.481938
1	-4.736896	-1.653660	2.312311
6	-5.489635	-1.216163	-1.687248
6	-6.760253	-2.112559	-1.684612
1	-6.524361	-3.172601	-1.823748
1	-7.427185	-1.810077	-2.507836
1	-7.324385	-2.009114	-0.748424
6	-5.969080	0.260374	-1.563294
1	-6.472831	0.451955	-0.605977
1	-6.689083	0.484491	-2.366143
1	-5.137841	0.970757	-1.657128
6	-4.762581	-1.370759	-3.051763
1	-4.510023	-2.417099	-3.266056
1	-3.835015	-0.782029	-3.088003
1	-5.413161	-1.016264	-3.867135
6	-3.465590	-3.425687	-0.232191
6	-2.757208	-3.673363	1.132527
1	-2.223955	-4.637024	1.106142
1	-3.473670	-3.714596	1.962534
1	-2.018402	-2.892971	1.361612
6	-4.541448	-4.536059	-0.424267
1	-4.079351	-5.522605	-0.260057
1	-4.946287	-4.532416	-1.443795
1	-5.378768	-4.441685	0.278464

6	-2.413301	-3.616635	-1.356593
1	-2.059731	-4.660264	-1.362090
1	-1.530992	-2.982827	-1.200213
1	-2.810925	-3.393747	-2.353793
6	3.917997	-1.942322	3.123310
6	1.241918	-2.964430	1.914965
1	1.330155	-3.944971	2.403733
1	0.599502	-3.091923	1.035491
1	0.720307	-2.293764	2.608327
6	3.787159	-3.606232	0.240065
6	5.456296	-1.870594	2.934497
1	5.936335	-1.580651	3.882429
1	5.743333	-1.131258	2.174817
1	5.873200	-2.841327	2.637905
6	3.593503	-3.055211	4.162947
1	2.524406	-3.082945	4.407784
1	4.141639	-2.859325	5.098257
1	3.884965	-4.052091	3.810494
6	3.434828	-0.586921	3.716237
1	2.345155	-0.559842	3.854492
1	3.717243	0.259312	3.074259
1	3.896503	-0.420567	4.702385
6	2.813358	-3.921921	-0.931198
1	1.852983	-4.319713	-0.577753
1	3.263748	-4.680035	-1.591049
1	2.601835	-3.034933	-1.542327
6	4.045978	-4.934003	1.009943
1	3.122343	-5.342789	1.441879
1	4.775767	-4.807374	1.819347
1	4.447412	-5.690394	0.316810
6	5.123408	-3.110323	-0.376516
1	5.893743	-2.937372	0.382970
1	4.985810	-2.175793	-0.936098
1	5.511809	-3.863900	-1.080069
6	3.858650	3.431827	-0.016823
6	6.055947	1.205557	-0.044154
1	6.297971	0.156767	-0.253964
1	6.071254	1.334026	1.046067
1	6.858662	1.827793	-0.464935
6	4.456271	1.573123	-2.720894
6	5.033117	4.443472	-0.146581
1	5.933617	4.093091	0.374430
1	4.742662	5.405871	0.304425
1	5.299315	4.636650	-1.192304
6	2.598129	4.037856	-0.693441
1	2.789317	4.320045	-1.735734

1	2.288939	4.948436	-0.156581
1	1.746385	3.345410	-0.682446
6	3.551413	3.259453	1.500557
1	4.389715	2.808374	2.048952
1	2.658134	2.639820	1.668976
1	3.347571	4.241848	1.954067
6	5.468022	2.616491	-3.276354
1	6.455085	2.536946	-2.801744
1	5.105059	3.643068	-3.141858
1	5.606052	2.456861	-4.357615
6	4.962202	0.151226	-3.102300
1	4.268249	-0.630224	-2.761589
1	5.951960	-0.065350	-2.680303
1	5.041734	0.067128	-4.197468
6	3.089266	1.797259	-3.422053
1	2.316422	1.103764	-3.071662
1	3.205789	1.644467	-4.507448
1	2.705992	2.812526	-3.272054
8	-0.244205	0.444969	-3.077889
6	0.114860	-0.143523	-4.359259
1	-0.747209	-0.663199	-4.807568
1	0.930269	-0.873348	-4.240069
1	0.457236	0.641446	-5.047623
8	-1.883559	2.248295	-2.767719
6	-2.732906	2.757401	-3.831332
1	-3.175155	1.944672	-4.427459
1	-2.157550	3.422121	-4.489173
1	-3.538359	3.335711	-3.365116
1	-1.133594	1.520939	-3.035446
1	-2.476115	1.597855	-1.653364

TS4-Pb=Pb=Pb-3MeOH

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-2.359289	0.032923	0.303416
82	0.047180	-0.452840	-1.032563
82	2.352958	0.280699	0.159949
14	-3.710285	1.957834	-0.792208
14	-3.206651	-2.104564	1.518224

14	4.193660	-1.491120	-0.033643
14	2.240573	2.603280	1.281478
6	-2.419428	3.037910	-1.696681
1	-1.750946	3.541907	-0.988281
1	-2.904959	3.811277	-2.307335
1	-1.790951	2.426865	-2.354338
6	-4.503948	2.994642	0.667841
6	-4.659044	4.470606	0.208441
1	-5.139099	5.061623	1.003068
1	-5.268799	4.561954	-0.698848
1	-3.679636	4.922260	0.004382
6	-5.881523	2.425620	1.096259
1	-5.810242	1.368446	1.386121
1	-6.628408	2.507586	0.297425
1	-6.259045	2.982437	1.967180
6	-4.909444	1.212883	-2.139120
6	-5.736307	2.351749	-2.793180
1	-6.388396	2.848260	-2.063514
1	-6.375065	1.947229	-3.593114
1	-5.084662	3.113727	-3.241779
6	-5.868032	0.134581	-1.568646
1	-5.306326	-0.691450	-1.115630
1	-6.477131	-0.289694	-2.381781
1	-6.550563	0.533257	-0.811452
6	-3.583412	2.988707	1.924599
1	-3.526210	1.996935	2.389325
1	-3.988554	3.682547	2.676933
1	-2.555768	3.301399	1.699069
6	-4.047710	0.529467	-3.241575
1	-3.445905	-0.293409	-2.833043
1	-3.364248	1.234261	-3.729742
1	-4.705262	0.104333	-4.016246
6	-4.974918	-1.589295	2.032599
1	-5.455586	-2.322637	2.692256
1	-5.611046	-1.457677	1.148406
1	-4.949649	-0.627063	2.560177
6	-3.290990	-3.653886	0.326818
6	-4.389751	-4.618005	0.859453
1	-4.178640	-4.957808	1.880589
1	-4.446834	-5.507861	0.214655
1	-5.378559	-4.141012	0.857635
6	-3.690860	-3.232357	-1.116511
1	-4.676776	-2.751103	-1.156292
1	-3.737239	-4.127337	-1.757013
1	-2.954550	-2.552232	-1.562086
6	-1.937732	-4.412388	0.231914

1	-1.628571	-4.830832	1.197587
1	-1.133045	-3.772690	-0.150829
1	-2.047689	-5.256331	-0.468301
6	-2.112952	-2.299358	3.126800
6	-2.288454	-1.041522	4.027724
1	-1.694302	-1.167476	4.945550
1	-3.333021	-0.884047	4.325762
1	-1.930362	-0.132450	3.531241
6	-2.601592	-3.542226	3.922446
1	-2.060061	-3.606418	4.878211
1	-2.416671	-4.473199	3.372651
1	-3.674688	-3.483714	4.151174
6	-0.597604	-2.455118	2.824068
1	-0.038982	-2.510572	3.771448
1	-0.193715	-1.603762	2.261896
1	-0.370526	-3.360853	2.253243
6	3.785504	3.689799	0.739849
6	0.659912	3.452081	0.632595
1	0.491937	4.417654	1.128682
1	-0.216647	2.819289	0.814010
1	0.732200	3.630037	-0.447568
6	2.047454	2.298423	3.211814
6	5.041051	3.392681	1.601823
1	5.899601	3.964321	1.216800
1	5.313899	2.329478	1.572456
1	4.897445	3.675706	2.651457
6	3.409779	5.193465	0.869474
1	2.596505	5.455982	0.180866
1	4.278751	5.817728	0.610789
1	3.093961	5.460045	1.885310
6	4.159224	3.433139	-0.746810
1	3.309339	3.605966	-1.419743
1	4.497839	2.401697	-0.905668
1	4.975977	4.111116	-1.043727
6	0.698103	1.575162	3.479985
1	-0.167123	2.165944	3.155672
1	0.590331	1.385435	4.559776
1	0.656005	0.608718	2.963337
6	2.033608	3.652510	3.972586
1	1.229377	4.307935	3.610364
1	2.984906	4.190659	3.876493
1	1.856555	3.475499	5.044869
6	3.169064	1.386935	3.780912
1	4.165433	1.832226	3.690941
1	3.179432	0.415197	3.269981
1	2.982427	1.192870	4.848935

6	4.607292	-1.844254	-1.913259
6	5.677306	-0.613263	0.792848
1	5.440821	-0.380453	1.839591
1	5.883018	0.336492	0.284522
1	6.595191	-1.214979	0.777082
6	3.672586	-3.018079	1.084592
6	5.551044	-3.069389	-2.037578
1	6.432897	-2.976772	-1.389100
1	5.904941	-3.165457	-3.075506
1	5.028718	-3.998694	-1.776960
6	3.342627	-2.104740	-2.775248
1	2.738847	-2.939168	-2.403548
1	3.644452	-2.328696	-3.811941
1	2.691752	-1.221429	-2.798536
6	5.323008	-0.590925	-2.492748
1	6.292298	-0.406321	-2.012801
1	4.703374	0.306906	-2.360786
1	5.501511	-0.727899	-3.571083
6	4.908316	-3.923763	1.343235
1	5.734558	-3.356638	1.793444
1	5.274370	-4.394022	0.424231
1	4.636527	-4.726453	2.045918
6	3.169757	-2.507364	2.465803
1	2.299431	-1.849833	2.358774
1	3.946658	-1.955090	3.012223
1	2.874287	-3.366446	3.087970
6	2.535888	-3.855041	0.438066
1	1.644366	-3.255849	0.219408
1	2.237875	-4.665158	1.123838
1	2.851325	-4.320264	-0.505039
8	0.121350	-2.401336	-1.620504
6	-0.187883	-2.932725	-2.919289
1	0.510221	-2.561175	-3.688033
1	-1.216961	-2.686721	-3.234830
1	-0.101149	-4.025814	-2.869150
1	-1.478973	0.906180	1.551992
8	-0.146483	0.509584	-3.243187
6	-0.682786	0.182260	-4.559541
1	-1.133517	1.072889	-5.012456
1	-1.450816	-0.582609	-4.426278
1	0.108261	-0.207307	-5.213261
1	0.628785	1.188041	-3.271063
8	1.909609	1.977152	-3.054194
1	2.280027	1.589252	-2.191885
6	2.901985	2.008150	-4.131379
1	3.810344	2.517465	-3.793175

1	2.453896	2.570800	-4.953782
1	3.152787	0.991199	-4.462682

Pro-Pb=Pb=Pb-2MeOH			

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

82	-2.649234	0.032845	0.399325
82	-0.012135	0.039154	-0.975770
82	2.629820	0.064061	0.351471
14	-4.286117	1.806148	-0.819190
14	-3.302739	-2.324731	1.544357
14	4.591723	-1.454335	-0.725411
14	2.809384	2.576498	1.317025
6	-3.134050	3.288598	-1.149589
1	-2.888733	3.809862	-0.214472
1	-3.612188	4.016327	-1.821608
1	-2.190279	2.955476	-1.600911
6	-5.686901	2.385327	0.432014
6	-6.242142	3.768908	-0.022317
1	-7.028674	4.095633	0.676472
1	-6.683475	3.734068	-1.024638
1	-5.460277	4.538618	-0.022776
6	-6.865149	1.379923	0.528801
1	-6.524150	0.371949	0.801467
1	-7.420443	1.306332	-0.414694
1	-7.574317	1.711809	1.303383
6	-4.926830	1.092440	-2.526078
6	-5.950465	2.065083	-3.182275
1	-6.881092	2.136655	-2.605392
1	-6.213505	1.696778	-4.186431
1	-5.542122	3.077834	-3.301402
6	-5.592239	-0.303162	-2.379351
1	-4.889582	-1.041760	-1.973111
1	-5.916336	-0.665044	-3.368126
1	-6.474489	-0.281001	-1.728890
6	-5.084355	2.566614	1.854783
1	-4.777800	1.609261	2.295618
1	-5.839962	3.011897	2.520864
1	-4.208768	3.228874	1.855035

6	-3.713902	0.948917	-3.489944
1	-2.953491	0.265095	-3.093217
1	-3.221928	1.909874	-3.679961
1	-4.057753	0.545252	-4.455580
6	-5.197059	-2.302403	1.818920
1	-5.512103	-3.159230	2.431794
1	-5.736921	-2.357878	0.864957
1	-5.523027	-1.390387	2.332670
6	-2.911593	-3.830676	0.351899
6	-3.637620	-5.117194	0.848655
1	-3.292650	-5.437947	1.837703
1	-3.438842	-5.941295	0.145576
1	-4.725781	-4.980680	0.895511
6	-3.453865	-3.512162	-1.070607
1	-4.533234	-3.308594	-1.065629
1	-3.283433	-4.374512	-1.733653
1	-2.943599	-2.649582	-1.517903
6	-1.391395	-4.126624	0.236052
1	-0.953847	-4.426059	1.196768
1	-0.828461	-3.264443	-0.144917
1	-1.229131	-4.954816	-0.471356
6	-2.434223	-2.370887	3.301485
6	-3.107410	-1.309916	4.221368
1	-2.605660	-1.303692	5.201424
1	-4.168475	-1.530694	4.395076
1	-3.029189	-0.296926	3.805621
6	-2.605360	-3.764639	3.973842
1	-2.218513	-3.722118	5.004057
1	-2.045053	-4.546433	3.446451
1	-3.657765	-4.075053	4.030827
6	-0.916847	-2.045772	3.219869
1	-0.471167	-2.100728	4.225601
1	-0.737050	-1.032551	2.839297
1	-0.371656	-2.748850	2.579484
6	3.933959	3.714617	0.186092
6	1.023957	3.251759	1.229139
1	0.965496	4.261590	1.660178
1	0.322811	2.615273	1.783030
1	0.667177	3.301239	0.192112
6	3.346796	2.461293	3.201829
6	5.448790	3.457772	0.407407
1	6.036526	4.063545	-0.300146
1	5.714461	2.405227	0.242326
1	5.769262	3.732731	1.420072
6	3.634353	5.218489	0.462166
1	2.588794	5.470651	0.244774

1	4.266035	5.842589	-0.189461
1	3.844966	5.505497	1.498646
6	3.604142	3.438366	-1.308061
1	2.539785	3.588893	-1.529853
1	3.871439	2.415035	-1.601703
1	4.177960	4.126878	-1.948148
6	2.173852	1.854721	4.026264
1	1.286136	2.499344	4.007551
1	2.482353	1.744806	5.077674
1	1.882451	0.861800	3.660412
6	3.654337	3.874484	3.778524
1	2.813688	4.568488	3.642224
1	4.545684	4.322348	3.321875
1	3.843652	3.794670	4.860687
6	4.596785	1.560388	3.404266
1	5.466142	1.919212	2.840276
1	4.399138	0.522916	3.103232
1	4.875060	1.544504	4.469907
6	4.454339	-1.589445	-2.673520
6	6.238122	-0.560914	-0.326536
1	6.288534	-0.242628	0.721349
1	6.369594	0.330522	-0.953396
1	7.092038	-1.227184	-0.514726
6	4.569710	-3.152230	0.256385
6	5.831169	-2.022205	-3.263762
1	6.623838	-1.297168	-3.037380
1	5.747637	-2.088707	-4.359688
1	6.153167	-3.004285	-2.898359
6	3.365914	-2.598864	-3.131646
1	3.598921	-3.623675	-2.813699
1	3.320833	-2.603489	-4.233099
1	2.368214	-2.327126	-2.762025
6	4.102418	-0.196857	-3.270330
1	4.814726	0.582537	-2.963971
1	3.092435	0.119391	-2.983546
1	4.128189	-0.251218	-4.369846
6	5.572080	-4.160222	-0.379968
1	6.591164	-3.753864	-0.440192
1	5.263597	-4.463437	-1.387666
1	5.617048	-5.069860	0.239302
6	5.013759	-2.897620	1.726683
1	4.345437	-2.195204	2.241976
1	6.037293	-2.505331	1.785076
1	4.989084	-3.845548	2.286305
6	3.159133	-3.805015	0.279768
1	2.432138	-3.175886	0.808450

1	3.208957	-4.769302	0.810199
1	2.770136	-3.996290	-0.726383
8	0.272945	-1.397273	-2.420376
6	-0.569183	-1.724891	-3.549610
1	-1.547135	-2.129588	-3.237001
1	-0.060279	-2.496915	-4.144451
1	-0.752304	-0.854214	-4.200929
1	-2.046610	0.982500	1.779759
8	-0.278050	1.744154	-2.110282
6	0.403195	2.098097	-3.337597
1	0.080120	3.107398	-3.631679
1	0.160039	1.405476	-4.159543
1	1.500469	2.114067	-3.222540
1	2.137599	-0.846247	1.799098

TS-C=C=C-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

6	-0.055512	0.255097	-0.268231
6	-0.638306	-0.521705	0.584595
14	-2.090057	1.553592	-1.758532
14	-1.651895	-1.630274	1.765915
6	1.473952	0.166288	-0.099531
6	-1.154448	2.488177	-3.145543
1	-0.629949	1.789987	-3.808460
1	-0.419749	3.201760	-2.755181
1	-1.874631	3.053207	-3.756257
6	-3.265978	0.270352	-2.737421
6	-2.399853	-0.754311	-3.513562
1	-1.729097	-0.270732	-4.235559
1	-3.056132	-1.440428	-4.074834
1	-1.790080	-1.358225	-2.841710
6	-4.126595	1.004946	-3.812282
1	-3.500188	1.454791	-4.592230
1	-4.768662	1.787801	-3.397707
1	-4.785188	0.268303	-4.302505
6	-4.220212	-0.518802	-1.795398
1	-4.575545	-1.434738	-2.293905

1	-5.103950	0.064982	-1.522138
1	-3.723729	-0.820182	-0.867141
6	-3.219438	2.923786	-0.780696
6	-3.087279	4.305164	-1.487031
1	-3.487509	4.294862	-2.509227
1	-2.046669	4.648870	-1.529673
1	-3.660658	5.052048	-0.913751
6	-2.744622	3.113706	0.680614
1	-2.819966	2.185728	1.251710
1	-3.377651	3.862765	1.184420
1	-1.709481	3.463060	0.729197
6	-4.741972	2.597496	-0.709625
1	-5.207311	2.509428	-1.695527
1	-5.251952	3.420117	-0.182691
1	-4.953807	1.680164	-0.152354
6	-0.364320	-2.173779	3.049081
1	0.513442	-2.608377	2.571011
1	-0.788035	-2.920770	3.726859
1	-0.029463	-1.320822	3.643870
6	-3.004464	-0.646080	2.812142
6	-2.372895	0.616344	3.465357
1	-1.878970	1.268518	2.741442
1	-1.635602	0.351274	4.231525
1	-3.163143	1.203871	3.957983
6	-4.275269	-0.216613	2.030643
1	-4.041791	0.403421	1.160778
1	-4.922756	0.379664	2.693104
1	-4.863673	-1.072370	1.687190
6	-3.447430	-1.584842	3.976473
1	-3.901241	-2.518156	3.622954
1	-4.198137	-1.065229	4.590665
1	-2.606753	-1.839350	4.632116
6	-2.325956	-3.239472	0.822514
6	-1.748562	-4.491732	1.549201
1	-0.663143	-4.434500	1.690980
1	-1.956562	-5.388388	0.945595
1	-2.211189	-4.635749	2.535509
6	-3.874230	-3.391297	0.806642
1	-4.125545	-4.350457	0.328233
1	-4.365285	-2.603229	0.227393
1	-4.310496	-3.404051	1.811077
6	-1.859955	-3.278707	-0.656240
1	-0.779171	-3.173742	-0.761923
1	-2.327879	-2.488048	-1.246310
1	-2.150085	-4.242514	-1.103353
14	2.505873	1.452729	1.008727

6	3.977466	0.506065	1.814492
1	4.470433	-0.231551	1.185733
1	3.617837	-0.027421	2.699899
1	4.742099	1.216393	2.149078
6	1.726844	2.215868	2.677261
6	2.827152	3.025433	3.435481
1	3.224976	3.864447	2.855745
1	3.671418	2.392895	3.733791
1	2.391531	3.442645	4.357256
6	1.282765	1.077993	3.634296
1	0.464531	0.507502	3.194012
1	0.922685	1.518507	4.578456
1	2.093210	0.385594	3.887412
6	0.489097	3.128652	2.482592
1	0.738403	4.091157	2.030627
1	0.028975	3.338764	3.461722
1	-0.265349	2.643812	1.858478
6	3.239522	2.965997	-0.095257
6	3.195398	2.688306	-1.624552
1	3.390584	3.626502	-2.167940
1	2.220705	2.304682	-1.946324
1	3.959944	1.973258	-1.932197
6	4.725205	3.235170	0.297282
1	5.115664	4.075917	-0.298104
1	5.368813	2.368628	0.101013
1	4.841144	3.501619	1.355351
6	2.456428	4.296586	0.109987
1	2.908281	5.073070	-0.526916
1	2.496644	4.663083	1.139074
1	1.402639	4.201763	-0.180901
14	2.634239	-1.197274	-1.008309
6	4.387945	-0.461881	-1.336139
1	5.110299	-1.284049	-1.360811
1	4.751662	0.269661	-0.618365
1	4.412668	0.010404	-2.320930
6	2.997516	-2.896945	0.028854
6	2.144641	-1.630295	-2.882347
6	2.987887	-2.673264	1.569107
1	3.942777	-2.270159	1.920712
1	2.834546	-3.636751	2.082349
1	2.203742	-1.982210	1.887118
6	4.401443	-3.492722	-0.307215
1	4.539094	-3.710245	-1.371660
1	4.519781	-4.441368	0.241016
1	5.216186	-2.834111	0.014538
6	1.961006	-4.010300	-0.290592

1	1.972332	-4.296630	-1.347156
1	0.941009	-3.714989	-0.027604
1	2.203571	-4.912992	0.292864
6	3.256462	-2.515240	-3.528942
1	3.038328	-2.641103	-4.601139
1	3.290137	-3.517986	-3.086696
1	4.256711	-2.074946	-3.447813
6	2.061076	-0.306092	-3.698305
1	1.797752	-0.538863	-4.742202
1	3.013307	0.235808	-3.721393
1	1.297981	0.371526	-3.297305
6	0.799533	-2.370081	-3.078406
1	0.561522	-2.419581	-4.153521
1	-0.014389	-1.845567	-2.578272
1	0.824713	-3.398078	-2.705195

Pro-C=C=C-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

6	1.034680	0.001555	0.000857
6	-0.475724	-0.480746	0.470308
6	-0.475723	0.478746	-0.471803
14	2.212687	1.303735	1.104235
14	2.219917	-1.296058	-1.101471
14	-1.513915	1.742071	-1.604444
14	-1.511594	-1.745859	1.602532
6	3.780202	-0.376799	-1.728600
1	4.438486	-1.104522	-2.213467
1	4.364601	0.124108	-0.955692
1	3.515160	0.367922	-2.479843
6	2.976490	-2.906744	-0.132546
6	1.499211	-1.897362	-2.863051
6	3.129877	-2.735318	1.407923
1	4.052032	-2.204794	1.655163
1	3.191713	-3.726962	1.883278
1	2.297247	-2.196605	1.864841
6	4.410813	-3.213115	-0.671881
1	4.425780	-3.443391	-1.742942
1	4.804428	-4.094229	-0.140316

1	5.106673	-2.385910	-0.492799
6	2.145550	-4.203079	-0.348023
1	2.009776	-4.454891	-1.403125
1	1.161660	-4.141250	0.117771
1	2.676574	-5.046390	0.121539
6	2.537953	-2.744831	-3.661984
1	2.106716	-2.987982	-4.646917
1	2.778010	-3.694969	-3.173232
1	3.474422	-2.205002	-3.843210
6	1.219488	-0.634887	-3.725334
1	0.761455	-0.933494	-4.681515
1	2.140198	-0.089907	-3.962896
1	0.535850	0.051629	-3.224143
6	0.202068	-2.742089	-2.792842
1	-0.254665	-2.814792	-3.792371
1	-0.536867	-2.304327	-2.120216
1	0.403030	-3.762736	-2.455830
6	3.775612	0.394050	1.738554
1	4.376259	-0.093441	0.969634
1	3.508773	-0.359818	2.479747
1	4.418254	1.125729	2.238013
6	2.961477	2.917521	0.133316
6	3.104363	2.746288	-1.408475
1	3.149629	3.737750	-1.886268
1	2.275222	2.195805	-1.857773
1	4.031344	2.227593	-1.662835
6	4.397475	3.226375	0.665837
1	4.788831	4.106482	0.130871
1	5.092872	2.398958	0.486025
1	4.415498	3.459524	1.736409
6	2.128240	4.211626	0.355218
1	2.650236	5.054812	-0.124755
1	2.004979	4.468648	1.410942
1	1.138040	4.145425	-0.096634
6	1.489060	1.902248	2.865313
6	2.524764	2.752192	3.665440
1	2.769702	3.698330	3.171502
1	3.459801	2.212872	3.855769
1	2.088446	3.002057	4.646395
6	1.209675	0.639050	3.726184
1	0.528818	-0.047973	3.221948
1	0.748633	0.936298	4.681382
1	2.129818	0.094409	3.966188
6	0.190234	2.744674	2.796779
1	0.388392	3.767990	2.466240
1	-0.268068	2.810857	3.796055

1	-0.548180	2.309869	2.121529
6	-0.281967	-2.690477	2.701639
1	0.475514	-3.206790	2.107430
1	-0.825953	-3.453022	3.274228
1	0.240529	-2.050508	3.420268
6	-2.825442	-0.897872	2.828984
6	-2.446874	-3.190556	0.593398
6	-1.415814	-4.210560	0.045540
1	-0.680711	-3.746120	-0.607384
1	-1.941367	-4.978412	-0.544223
1	-0.886042	-4.726739	0.854984
6	-3.387954	-4.019492	1.520196
1	-3.752988	-4.887851	0.949552
1	-4.266671	-3.457137	1.848803
1	-2.870792	-4.408886	2.406106
6	-3.301480	-2.682871	-0.593002
1	-2.705364	-2.125391	-1.318029
1	-4.124328	-2.040603	-0.264444
1	-3.744682	-3.541523	-1.122272
6	-2.274614	0.391194	3.487729
1	-1.915061	1.114754	2.759126
1	-1.451148	0.171257	4.174393
1	-3.073704	0.872224	4.074392
6	-4.152360	-0.545892	2.099334
1	-3.982997	0.063677	1.206905
1	-4.803359	0.031400	2.774181
1	-4.706672	-1.440047	1.796144
6	-3.158574	-1.845699	4.025060
1	-3.641633	-2.777687	3.727149
1	-3.850050	-1.319243	4.701878
1	-2.262700	-2.095323	4.606676
6	-0.288833	2.700525	-2.697584
1	0.256753	2.064979	-3.402368
1	0.448661	3.238685	-2.097663
1	-0.841084	3.446088	-3.284753
6	-2.820127	0.887915	-2.834900
6	-2.266525	-0.400399	-3.491980
1	-1.437471	-0.181901	-4.173180
1	-3.063210	-0.878509	-4.084958
1	-1.914863	-1.126414	-2.761279
6	-3.156217	1.833716	-4.031737
1	-2.261997	2.078588	-4.617955
1	-3.635251	2.768271	-3.734680
1	-3.852477	1.307385	-4.703850
6	-4.146871	0.530759	-2.106108
1	-4.794634	-0.050242	-2.781118

1	-4.706588	1.422405	-1.805463
1	-3.976856	-0.077387	-1.212578
6	-2.459245	3.179357	-0.595013
6	-1.437428	4.205930	-0.042127
1	-0.905321	4.724390	-0.848498
1	-0.704634	3.745514	0.616206
1	-1.971321	4.971347	0.543275
6	-3.312774	2.663590	0.588305
1	-4.135438	2.022773	0.256332
1	-3.756940	3.518070	1.123396
1	-2.715536	2.101435	1.308671
6	-3.403255	4.003075	-1.523299
1	-2.883181	4.402605	-2.402968
1	-3.781619	4.864143	-0.950429
1	-4.272288	3.432037	-1.862140

TS-Si=Si=Si-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

14	0.158804	0.782212	-1.886164
14	-2.976710	1.343905	-1.181447
14	-1.158434	-0.114725	-0.101431
14	-1.965541	-1.545593	1.798105
14	1.593528	0.147466	-0.157650
6	-2.764372	3.287009	-1.500510
6	-1.760388	3.722932	-2.600499
1	-0.732015	3.435950	-2.353927
1	-1.792524	4.820449	-2.697166
1	-1.992395	3.297210	-3.580731
6	-2.329966	3.974204	-0.175499
1	-1.350599	3.613099	0.161396
1	-3.052042	3.813558	0.634760
1	-2.250650	5.060501	-0.337352
6	-4.166111	3.853179	-1.902389
1	-4.096027	4.947689	-1.997773
1	-4.940971	3.642141	-1.155706
1	-4.508620	3.464833	-2.869074
6	-3.700788	0.384323	-2.775149

6	-3.279027	-1.107346	-2.851382
1	-2.196235	-1.218854	-2.970160
1	-3.768097	-1.573855	-3.721716
1	-3.578679	-1.673359	-1.966219
6	-3.281632	1.028542	-4.127044
1	-2.193197	1.029444	-4.256485
1	-3.644344	2.056218	-4.234718
1	-3.718128	0.439737	-4.949995
6	-5.259044	0.427086	-2.683071
1	-5.651533	1.450992	-2.661446
1	-5.634848	-0.096664	-1.795528
1	-5.686019	-0.073210	-3.566542
6	-4.294555	1.280236	0.202079
1	-3.888461	1.739072	1.111276
1	-4.580788	0.252985	0.438610
1	-5.206229	1.825218	-0.074928
6	-3.075658	-3.004835	1.064588
6	-2.308868	-3.664268	-0.117743
1	-1.388367	-4.154950	0.222027
1	-2.036478	-2.936637	-0.890642
1	-2.940459	-4.435806	-0.584884
6	-3.302188	-4.103103	2.147362
1	-2.360342	-4.490296	2.555485
1	-3.834648	-4.951469	1.689266
1	-3.918333	-3.743368	2.980637
6	-4.474922	-2.557164	0.562992
1	-4.989572	-3.413582	0.099882
1	-4.413756	-1.767681	-0.190854
1	-5.109639	-2.195482	1.379038
6	-2.750743	-0.657086	3.399520
6	-2.522339	-1.589279	4.634760
1	-1.462181	-1.787277	4.827437
1	-3.039064	-2.551674	4.534174
1	-2.931561	-1.090319	5.527029
6	-2.010123	0.677690	3.683255
1	-0.933768	0.526177	3.827765
1	-2.407366	1.129114	4.606800
1	-2.140802	1.403538	2.870738
6	-4.275881	-0.364919	3.353818
1	-4.871998	-1.273270	3.198840
1	-4.545689	0.358445	2.580625
1	-4.581317	0.063183	4.322577
6	-0.377506	-2.370055	2.445481
1	0.175824	-2.846357	1.635063
1	-0.611147	-3.137806	3.194122
1	0.286483	-1.633009	2.910672

14	2.944235	1.737460	1.135574
6	2.017179	2.348791	2.752881
6	1.905784	1.141240	3.729389
1	2.892146	0.801530	4.070275
1	1.396463	0.286196	3.266925
1	1.330957	1.436240	4.621209
6	0.592794	2.885878	2.455966
1	0.618838	3.790236	1.837369
1	0.087671	3.145273	3.399937
1	-0.022204	2.141082	1.939124
6	2.813692	3.467780	3.485657
1	2.828829	4.402584	2.912594
1	3.851664	3.178009	3.697722
1	2.329496	3.684147	4.451194
6	3.555463	3.198605	-0.033756
6	4.515809	0.851248	1.776025
1	4.980967	1.451516	2.570283
1	5.262478	0.715452	0.986780
1	4.284979	-0.134685	2.195272
6	4.777872	3.928632	0.601007
1	5.123427	4.720475	-0.082444
1	5.621360	3.245016	0.762529
1	4.538474	4.401159	1.558997
6	4.029028	2.637252	-1.403505
1	4.355932	3.468048	-2.048082
1	3.231364	2.099332	-1.930304
1	4.884663	1.960069	-1.287109
6	2.434139	4.238853	-0.302415
1	2.794607	4.994942	-1.017417
1	2.136851	4.766841	0.611795
1	1.537844	3.774305	-0.735034
14	2.912215	-1.779571	-1.065786
6	2.457389	-2.086257	-2.965230
6	3.332506	-3.230862	-3.561990
1	4.407469	-3.066172	-3.413464
1	3.156214	-3.282170	-4.647938
1	3.070841	-4.209670	-3.143961
6	0.972966	-2.469305	-3.202364
1	0.701479	-3.401637	-2.693405
1	0.792076	-2.608645	-4.280145
1	0.285557	-1.690269	-2.851278
6	2.781371	-0.803247	-3.786266
1	3.846758	-0.544955	-3.739961
1	2.210405	0.071541	-3.448408
1	2.523481	-0.968693	-4.843603
6	3.020892	-3.417497	0.011161

6	3.179765	-3.034573	1.510333
1	4.098212	-2.455986	1.678627
1	3.250797	-3.948392	2.121082
1	2.337570	-2.445289	1.884259
6	4.277659	-4.261292	-0.367240
1	5.210543	-3.710763	-0.194652
1	4.267265	-4.593828	-1.409775
1	4.306446	-5.162174	0.266116
6	1.768790	-4.315087	-0.173949
1	1.775339	-5.133740	0.562687
1	1.747836	-4.770597	-1.172336
1	0.834936	-3.756841	-0.048942
6	4.710118	-1.122351	-1.120863
1	5.186411	-1.163218	-0.136753
1	4.777866	-0.096748	-1.492204
1	5.294299	-1.760021	-1.799194

Pro-Si=Si=Si-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	0.417648	1.203044	-0.176498
14	1.022411	-0.867158	-0.257288
14	-1.311724	-0.462408	0.160316
14	1.451686	3.357363	-0.347805
14	2.828659	-2.413478	-0.455945
14	-2.935833	-0.834861	-1.623650
14	-2.159225	-0.929484	2.401119
6	2.141956	-4.150373	-0.065671
1	1.859132	-4.235949	0.990857
1	2.890596	-4.926497	-0.278392
1	1.250796	-4.370427	-0.665054
6	4.175605	-1.976692	0.901172
6	3.482258	-1.757479	2.276248
1	2.928045	-2.646573	2.605583
1	2.783494	-0.911682	2.250958
1	4.244530	-1.542100	3.041164
6	5.182917	-3.153531	1.066466
1	4.678257	-4.084164	1.357524
1	5.902131	-2.907048	1.863091

1	5.756419	-3.348179	0.153639
6	4.960628	-0.684705	0.546346
1	5.652852	-0.434087	1.365306
1	4.287557	0.171737	0.406724
1	5.558752	-0.801724	-0.365975
6	3.462968	-2.395473	-2.310679
6	4.805944	-3.169591	-2.450678
1	4.745798	-4.189204	-2.045617
1	5.634137	-2.651204	-1.951864
1	5.067232	-3.254749	-3.517046
6	2.405041	-3.108222	-3.201946
1	2.293251	-4.167539	-2.936873
1	2.721519	-3.061588	-4.255676
1	1.419290	-2.634371	-3.131412
6	3.664244	-0.954005	-2.853463
1	4.414202	-0.394631	-2.280966
1	2.729214	-0.379831	-2.832131
1	4.008527	-0.998532	-3.898762
6	2.960272	3.069761	-1.483155
1	2.668856	2.578391	-2.418311
1	3.705679	2.430763	-0.993378
1	3.447412	4.021895	-1.737664
6	2.136373	3.939836	1.394329
6	2.925217	2.776323	2.060492
1	2.295132	1.897827	2.238981
1	3.321996	3.110823	3.031760
1	3.780157	2.457977	1.448836
6	0.996130	4.380087	2.350685
1	0.259374	3.582516	2.505906
1	0.466962	5.264560	1.974003
1	1.415911	4.640890	3.334748
6	3.129489	5.127258	1.214351
1	2.648932	6.019954	0.800850
1	3.972616	4.860373	0.563549
1	3.546950	5.401137	2.195814
6	0.227677	4.594015	-1.238434
6	-1.192240	4.559183	-0.608371
1	-1.642316	3.561846	-0.674500
1	-1.853115	5.258058	-1.144657
1	-1.183392	4.855517	0.447506
6	0.119489	4.176331	-2.734875
1	-0.169085	3.124038	-2.853554
1	1.068024	4.326005	-3.266556
1	-0.644209	4.790409	-3.236183
6	0.748958	6.059696	-1.192873
1	0.105814	6.693254	-1.823214

1	1.774951	6.151423	-1.574202
1	0.722584	6.474590	-0.177689
6	-4.071842	-0.865525	2.389817
1	-4.499413	-1.728770	1.868116
1	-4.451015	0.041296	1.906925
1	-4.455357	-0.880577	3.419011
6	-1.689521	-2.771697	2.916288
6	-1.604895	0.444318	3.691979
6	-1.904838	-3.721732	1.703598
1	-2.943059	-3.698625	1.346957
1	-1.682307	-4.758607	2.001551
1	-1.247911	-3.467482	0.862197
6	-2.607564	-3.275514	4.068864
1	-3.665455	-3.278583	3.777553
1	-2.509504	-2.670360	4.976936
1	-2.334087	-4.310904	4.328367
6	-0.211207	-2.899477	3.372505
1	0.036225	-3.960582	3.538779
1	-0.026499	-2.368532	4.314749
1	0.483464	-2.505053	2.620417
6	-2.121789	0.116443	5.122821
1	-3.205967	-0.053385	5.151534
1	-1.903068	0.963303	5.792748
1	-1.625208	-0.767650	5.541591
6	-0.067347	0.634409	3.772786
1	0.440377	-0.257182	4.158471
1	0.167774	1.469220	4.452585
1	0.362372	0.865867	2.792534
6	-2.238881	1.796875	3.252085
1	-3.335391	1.755014	3.251675
1	-1.909567	2.094511	2.247872
1	-1.938701	2.592110	3.952746
6	-4.273954	-2.062709	-1.014885
1	-4.884741	-2.399005	-1.863695
1	-4.948912	-1.595376	-0.289356
1	-3.841807	-2.953385	-0.545850
6	-3.899441	0.832304	-2.030971
6	-2.113003	-1.700817	-3.184985
6	-5.249087	0.537003	-2.749111
1	-5.771479	1.486591	-2.948790
1	-5.914431	-0.080778	-2.133377
1	-5.110246	0.029637	-3.709933
6	-4.236150	1.572823	-0.704936
1	-4.782278	2.503105	-0.928347
1	-3.334406	1.841578	-0.140956
1	-4.876956	0.965465	-0.052662

6	-3.066574	1.787470	-2.926019
1	-3.585295	2.754092	-3.026370
1	-2.930305	1.381772	-3.936074
1	-2.074517	1.983249	-2.502885
6	-1.598750	-3.100843	-2.738201
1	-2.417705	-3.746666	-2.395874
1	-0.863905	-3.025204	-1.925845
1	-1.110727	-3.605873	-3.586522
6	-3.155153	-1.917452	-4.320876
1	-3.482445	-0.967503	-4.761435
1	-4.045424	-2.461325	-3.979010
1	-2.697162	-2.511715	-5.127521
6	-0.918572	-0.906940	-3.780671
1	-1.227888	0.066758	-4.176659
1	-0.476254	-1.476431	-4.614180
1	-0.132652	-0.728323	-3.038777

TS-Ge=Ge=Ge-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	0.157156	-2.017021	-0.690859
32	-1.143596	0.218588	-0.686179
14	-3.158906	-1.792941	-0.373424
14	-1.865269	2.687669	-0.073311
32	1.591488	-0.152928	0.164893
6	-4.352359	-0.599248	-1.291095
1	-3.990029	-0.440827	-2.313488
1	-4.411294	0.381416	-0.816424
1	-5.370758	-1.007101	-1.350295
6	-3.854509	-2.133454	1.445558
6	-3.173031	-1.187920	2.462936
1	-3.264586	-0.142636	2.163590
1	-2.105128	-1.414578	2.564951
1	-3.643245	-1.297398	3.453808
6	-3.625475	-3.583708	1.950081
1	-2.564681	-3.863591	1.926839
1	-4.190870	-4.325512	1.375257
1	-3.963940	-3.653697	2.996078

6	-5.386593	-1.841481	1.463523
1	-5.943987	-2.490396	0.777142
1	-5.609364	-0.801089	1.196576
1	-5.778803	-2.014053	2.478211
6	-3.238770	-3.419084	-1.524252
6	-2.398306	-4.643563	-1.071781
1	-1.325158	-4.427258	-1.086413
1	-2.582387	-5.478628	-1.767557
1	-2.661716	-4.989982	-0.068579
6	-2.826720	-3.077603	-2.984747
1	-1.781961	-2.750491	-3.045897
1	-3.458888	-2.296981	-3.425289
1	-2.934768	-3.978273	-3.610286
6	-4.737916	-3.867872	-1.547805
1	-4.839842	-4.723699	-2.233582
1	-5.410891	-3.081067	-1.908330
1	-5.090010	-4.196926	-0.563128
6	-0.295481	3.634888	0.436556
1	-0.033030	3.412598	1.474780
1	-0.460352	4.719084	0.354414
1	0.565129	3.372765	-0.183958
6	-3.099082	2.929433	1.453261
6	-2.478564	2.292626	2.734633
1	-1.739867	2.967289	3.185609
1	-1.979763	1.336454	2.550055
1	-3.267882	2.119744	3.483976
6	-3.269237	4.448276	1.779374
1	-2.305786	4.956604	1.908663
1	-3.815168	4.537817	2.731945
1	-3.844622	4.986046	1.021070
6	-4.514608	2.347206	1.204745
1	-5.159647	2.560064	2.071612
1	-4.498153	1.261746	1.070348
1	-4.991684	2.793451	0.322253
6	-2.468050	3.483333	-1.772131
6	-3.023839	4.920070	-1.540837
1	-2.349991	5.545753	-0.941583
1	-4.005827	4.907228	-1.053423
1	-3.150005	5.414102	-2.516627
6	-1.237456	3.602815	-2.714007
1	-0.465759	4.264111	-2.302044
1	-1.556749	4.025009	-3.679467
1	-0.778288	2.629300	-2.914398
6	-3.555551	2.661390	-2.508910
1	-4.457379	2.518167	-1.901363
1	-3.181752	1.673030	-2.800313

1	-3.855517	3.190945	-3.427159
14	3.266756	0.241484	-1.734364
6	4.748744	1.202703	-0.993468
1	5.402855	1.556770	-1.803401
1	5.352175	0.570373	-0.334001
1	4.425797	2.077712	-0.417683
6	3.998227	-1.502400	-2.319866
6	5.369017	-1.300530	-3.038534
1	5.766198	-2.283980	-3.337503
1	6.111679	-0.834978	-2.378665
1	5.288659	-0.690639	-3.943274
6	4.267838	-2.423999	-1.098280
1	4.699471	-3.376553	-1.444234
1	3.350025	-2.651268	-0.543676
1	4.985075	-1.974275	-0.399056
6	3.046484	-2.252115	-3.290254
1	3.454356	-3.250406	-3.514892
1	2.927591	-1.722925	-4.243779
1	2.044923	-2.397647	-2.860214
6	2.614118	1.340657	-3.224409
6	2.453034	2.796841	-2.703333
1	3.419614	3.232577	-2.419582
1	1.790653	2.843779	-1.830665
1	2.018210	3.430796	-3.491417
6	3.628456	1.374592	-4.405722
1	3.693045	0.406805	-4.917265
1	4.639145	1.665536	-4.089870
1	3.289734	2.114040	-5.148684
6	1.254321	0.849378	-3.784271
1	1.323555	-0.161526	-4.202625
1	0.915324	1.521928	-4.588513
1	0.478063	0.826102	-3.011973
14	2.686350	-0.117410	2.450861
6	4.589400	-0.249286	2.274555
1	5.024026	0.692551	1.921989
1	4.901154	-1.043662	1.589003
1	5.028347	-0.467378	3.258639
6	2.394109	1.597794	3.363490
6	2.122638	-1.711109	3.449114
6	2.728921	2.750060	2.373333
1	3.791653	2.750049	2.096105
1	2.511101	3.722031	2.844610
1	2.140025	2.682898	1.453350
6	3.324010	1.773247	4.599423
1	4.385478	1.730973	4.324119
1	3.141705	1.021381	5.374865

1	3.140712	2.762616	5.049694
6	0.924546	1.746742	3.829902
1	0.745879	2.765860	4.209987
1	0.684119	1.048025	4.641506
1	0.221566	1.565529	3.010616
6	2.689807	-1.711052	4.898175
1	3.778424	-1.568330	4.921137
1	2.474788	-2.680301	5.375261
1	2.230035	-0.932523	5.519263
6	0.579863	-1.850577	3.526033
1	0.112618	-1.008753	4.050819
1	0.313079	-2.771998	4.068079
1	0.133838	-1.913334	2.525551
6	2.683996	-2.964491	2.716834
1	3.781261	-2.967508	2.688384
1	2.318591	-3.027074	1.683209
1	2.361379	-3.876810	3.242251

Pro-Ge=Ge=Ge-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

32	0.432269	1.273705	-0.254275
32	1.087138	-0.920230	-0.182436
32	-1.394948	-0.480503	0.155659
14	1.522150	3.476659	-0.282414
14	2.931466	-2.508212	-0.428160
14	-3.007787	-0.818460	-1.723636
14	-2.287179	-0.958822	2.439198
6	2.240148	-4.254214	-0.091359
1	1.960494	-4.371373	0.963082
1	2.980383	-5.030180	-0.332655
1	1.343834	-4.445675	-0.693135
6	4.247864	-2.080496	0.957222
6	3.528453	-1.912801	2.327366
1	2.965070	-2.810794	2.615237
1	2.831941	-1.064091	2.319459
1	4.277193	-1.725177	3.112489
6	5.277945	-3.239133	1.102138
1	4.790226	-4.184350	1.373362

1	5.992484	-2.994558	1.902775
1	5.853107	-3.404859	0.184063
6	5.003552	-0.759753	0.647874
1	5.681969	-0.516638	1.480233
1	4.309875	0.082797	0.526691
1	5.612240	-0.836240	-0.262636
6	3.558387	-2.413795	-2.281674
6	4.909720	-3.166736	-2.451616
1	4.861202	-4.200989	-2.083650
1	5.730344	-2.656622	-1.931845
1	5.172357	-3.208237	-3.520186
6	2.500773	-3.102935	-3.192528
1	2.399744	-4.172471	-2.966836
1	2.808204	-3.012254	-4.245508
1	1.511175	-2.639238	-3.096067
6	3.739370	-0.950870	-2.772465
1	4.479069	-0.399520	-2.180047
1	2.795386	-0.392703	-2.733112
1	4.084589	-0.954264	-3.818477
6	3.057551	3.218876	-1.389207
1	2.786814	2.750118	-2.342490
1	3.788033	2.565552	-0.896303
1	3.553678	4.174870	-1.609958
6	2.153018	3.977972	1.502082
6	2.914235	2.780175	2.139815
1	2.269040	1.902390	2.263115
1	3.287479	3.069726	3.134398
1	3.781527	2.476127	1.538167
6	0.986638	4.378363	2.444294
1	0.248808	3.572349	2.545920
1	0.464826	5.276991	2.091081
1	1.379661	4.598074	3.449294
6	3.153161	5.168040	1.398252
1	2.685098	6.075399	1.000568
1	4.015731	4.922214	0.764912
1	3.539610	5.407213	2.401309
6	0.297379	4.717651	-1.163208
6	-1.128914	4.657842	-0.549254
1	-1.565775	3.654757	-0.634224
1	-1.792709	5.355195	-1.083995
1	-1.136888	4.937869	0.511243
6	0.203772	4.320061	-2.665762
1	-0.092532	3.270642	-2.797575
1	1.158993	4.467446	-3.186033
1	-0.550486	4.945256	-3.167931
6	0.809605	6.184111	-1.084465

1	0.168036	6.829253	-1.704796
1	1.837986	6.286840	-1.456985
1	0.775704	6.575581	-0.059898
6	-4.198736	-0.888094	2.385838
1	-4.614058	-1.739940	1.835616
1	-4.557066	0.028187	1.903075
1	-4.614463	-0.915072	3.402255
6	-1.811090	-2.807376	2.917540
6	-1.727174	0.409586	3.730911
6	-2.030358	-3.729647	1.683395
1	-3.064453	-3.684022	1.316545
1	-1.824137	-4.775660	1.960159
1	-1.362300	-3.466812	0.853251
6	-2.726753	-3.331165	4.062254
1	-3.785195	-3.328122	3.772480
1	-2.625830	-2.740975	4.980077
1	-2.453863	-4.370880	4.304097
6	-0.330516	-2.943628	3.365211
1	-0.083993	-4.007688	3.511267
1	-0.142103	-2.429981	4.316215
1	0.362245	-2.536875	2.618116
6	-2.254247	0.075102	5.156404
1	-3.340766	-0.082576	5.177026
1	-2.029621	0.912657	5.835780
1	-1.770273	-0.818943	5.568669
6	-0.188112	0.590962	3.816707
1	0.315755	-0.306261	4.193295
1	0.047629	1.416899	4.507220
1	0.246379	0.833894	2.840841
6	-2.348075	1.769068	3.293430
1	-3.445030	1.734852	3.274446
1	-1.998896	2.073754	2.297640
1	-2.053848	2.556380	4.005556
6	-4.360510	-2.043135	-1.141506
1	-4.981133	-2.359462	-1.991213
1	-5.024069	-1.582292	-0.400544
1	-3.931115	-2.945249	-0.690609
6	-3.930759	0.875266	-2.114546
6	-2.135799	-1.665456	-3.266497
6	-5.273320	0.611530	-2.857878
1	-5.781365	1.570997	-3.046415
1	-5.954509	-0.010224	-2.263735
1	-5.124881	0.121133	-3.826667
6	-4.271707	1.595556	-0.777996
1	-4.815171	2.530461	-0.987990
1	-3.369478	1.854346	-0.208455

1	-4.914326	0.979821	-0.134644
6	-3.072063	1.836505	-2.979163
1	-3.584447	2.807099	-3.076525
1	-2.916495	1.444102	-3.991711
1	-2.087728	2.023311	-2.532897
6	-1.643474	-3.075620	-2.825898
1	-2.474694	-3.722239	-2.516267
1	-0.930409	-3.014772	-1.992911
1	-1.133675	-3.570066	-3.667663
6	-3.144677	-1.850701	-4.436645
1	-3.452569	-0.888638	-4.864829
1	-4.047866	-2.394938	-4.130689
1	-2.667712	-2.430814	-5.242498
6	-0.915051	-0.871384	-3.805276
1	-1.199038	0.116953	-4.183693
1	-0.454769	-1.425525	-4.639427
1	-0.149379	-0.723040	-3.036195

TS-Sn=Sn=Sn-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

50	0.267921	-2.424514	-0.522841
50	-1.231188	0.088973	-0.683674
14	-3.354920	-1.712764	0.097151
14	-1.942583	2.746414	-0.641038
50	1.580037	-0.014577	0.262599
6	-4.536897	-0.702795	-1.040710
1	-4.190057	-0.771700	-2.078743
1	-4.558808	0.358393	-0.783271
1	-5.566951	-1.081070	-1.001696
6	-4.014299	-1.615798	1.961047
6	-3.299791	-0.481003	2.736899
1	-3.407015	0.484277	2.238244
1	-2.227375	-0.684458	2.853044
1	-3.737733	-0.383301	3.743893
6	-3.785807	-2.922012	2.768608
1	-2.725659	-3.206360	2.793810
1	-4.359738	-3.767980	2.375240

1	-4.109161	-2.761109	3.809194
6	-5.540825	-1.299805	1.947224
1	-6.123883	-2.074114	1.433631
1	-5.754456	-0.340684	1.458922
1	-5.911755	-1.233704	2.982275
6	-3.495760	-3.541689	-0.670732
6	-2.656219	-4.651079	0.018467
1	-1.580618	-4.473824	-0.090805
1	-2.877081	-5.619594	-0.457794
1	-2.875124	-4.747970	1.085224
6	-3.116948	-3.523718	-2.180079
1	-2.075397	-3.219020	-2.337255
1	-3.760055	-2.852641	-2.762411
1	-3.233955	-4.536666	-2.596660
6	-4.995782	-3.964905	-0.566568
1	-5.123624	-4.941429	-1.059082
1	-5.667647	-3.256599	-1.065288
1	-5.323168	-4.077493	0.473652
6	-0.314111	3.686281	-0.331175
1	-0.051771	3.651228	0.730685
1	-0.416358	4.741972	-0.621141
1	0.524727	3.260562	-0.888441
6	-3.126750	3.342825	0.819811
6	-2.487464	2.965364	2.192785
1	-1.729739	3.702436	2.487793
1	-2.005121	1.982330	2.195165
1	-3.262336	2.958540	2.976145
6	-3.248925	4.898910	0.819465
1	-2.267735	5.389569	0.819827
1	-3.769895	5.208535	1.739209
1	-3.824758	5.279076	-0.028756
6	-4.559622	2.756421	0.729101
1	-5.184928	3.178672	1.531374
1	-4.568878	1.668668	0.850375
1	-5.042899	2.996112	-0.227417
6	-2.517685	3.185270	-2.467521
6	-3.045172	4.646738	-2.545878
1	-2.352594	5.368099	-2.092790
1	-4.021209	4.754325	-2.058169
1	-3.172198	4.929444	-3.602211
6	-1.278699	3.077058	-3.400300
1	-0.495351	3.794566	-3.127980
1	-1.580752	3.289623	-4.437290
1	-0.838013	2.073674	-3.385289
6	-3.615827	2.237851	-3.014260
1	-4.520173	2.240856	-2.392798

1	-3.255563	1.203674	-3.080056
1	-3.906903	2.555307	-4.027894
14	3.367278	0.042015	-1.765538
6	4.811893	1.166707	-1.203649
1	5.503764	1.354557	-2.037230
1	5.383654	0.700519	-0.392913
1	4.448161	2.135134	-0.841076
6	4.141143	-1.768660	-1.976600
6	5.517453	-1.687345	-2.704449
1	5.941928	-2.700279	-2.792028
1	6.235361	-1.077525	-2.142527
1	5.435895	-1.274843	-3.714737
6	4.406612	-2.420229	-0.590100
1	4.858149	-3.415582	-0.728637
1	3.485513	-2.548149	-0.008120
1	5.103565	-1.823442	0.013783
6	3.222442	-2.714892	-2.792358
1	3.636856	-3.735030	-2.798748
1	3.112632	-2.390771	-3.833997
1	2.207434	-2.785413	-2.367000
6	2.682918	0.795942	-3.446368
6	2.503662	2.327856	-3.244784
1	3.465053	2.832145	-3.085003
1	1.857818	2.552494	-2.387123
1	2.038241	2.770740	-4.139027
6	3.677538	0.585888	-4.623988
1	3.751758	-0.470093	-4.910554
1	4.686413	0.952472	-4.393361
1	3.317119	1.139075	-5.505747
6	1.317397	0.191497	-3.864881
1	1.375657	-0.887647	-4.052704
1	0.961676	0.671050	-4.791033
1	0.552135	0.341854	-3.096353
14	2.733075	0.476699	2.608086
6	4.634367	0.306879	2.461095
1	5.060947	1.146273	1.899255
1	4.927125	-0.618590	1.953453
1	5.095715	0.304848	3.458670
6	2.406816	2.349390	3.114212
6	2.125399	-0.882108	3.885202
6	2.732568	3.264779	1.897970
1	3.788686	3.196189	1.603989
1	2.529836	4.316052	2.158958
1	2.122230	3.016499	1.022877
6	3.323346	2.799271	4.287676
1	4.386636	2.716413	4.028548

1	3.148327	2.220545	5.201637
1	3.122893	3.857601	4.521374
6	0.928624	2.578837	3.519967
1	0.734952	3.654893	3.658341
1	0.683334	2.077456	4.464707
1	0.238089	2.209875	2.753367
6	2.686587	-0.617107	5.310020
1	3.780318	-0.517165	5.311506
1	2.430309	-1.459040	5.972299
1	2.259627	0.291405	5.752648
6	0.577340	-0.967399	3.968711
1	0.129140	-0.038310	4.339540
1	0.283018	-1.777560	4.654796
1	0.132358	-1.186209	2.989583
6	2.655579	-2.263317	3.400492
1	3.752361	-2.296691	3.370602
1	2.283125	-2.507522	2.396175
1	2.314942	-3.055059	4.085777

Pro-Sn=Sn=Sn-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	0.157645	1.597421	-0.601301
50	1.553526	-0.628504	-0.040323
50	-1.331025	-0.842335	0.121669
14	0.680499	4.188325	-0.156451
14	3.808364	-2.013374	-0.389667
14	-2.972272	-1.562085	-1.883096
14	-2.260426	-1.600419	2.527987
6	3.449423	-3.871046	-0.124016
1	3.205577	-4.080179	0.925180
1	4.321841	-4.483860	-0.394071
1	2.601312	-4.206363	-0.732285
6	5.063294	-1.446315	1.010037
6	4.336906	-1.467735	2.386292
1	3.908405	-2.453532	2.614799
1	3.527662	-0.725761	2.429932
1	5.052676	-1.224965	3.187217
6	6.263192	-2.436386	1.091616

1	5.933646	-3.458716	1.319027
1	6.943752	-2.122105	1.898912
1	6.844286	-2.465293	0.163076
6	5.606524	-0.011277	0.771777
1	6.233656	0.295170	1.623799
1	4.794913	0.723729	0.677198
1	6.227356	0.049040	-0.131087
6	4.392777	-1.743536	-2.241827
6	5.826358	-2.309354	-2.462462
1	5.912877	-3.361296	-2.157159
1	6.583044	-1.730620	-1.917798
1	6.079424	-2.255021	-3.533013
6	3.418662	-2.510888	-3.183218
1	3.444022	-3.593741	-3.005162
1	3.708681	-2.338863	-4.231339
1	2.380038	-2.171378	-3.067723
6	4.384568	-0.245050	-2.651234
1	5.070112	0.355851	-2.041951
1	3.382738	0.195310	-2.560819
1	4.698320	-0.146361	-3.702192
6	2.262050	4.521176	-1.184079
1	2.176828	4.104941	-2.194675
1	3.141079	4.062358	-0.712859
1	2.454772	5.600014	-1.276631
6	1.099193	4.615018	1.712018
6	2.102471	3.567367	2.274201
1	1.657005	2.567369	2.337664
1	2.412571	3.862402	3.289035
1	3.010754	3.490537	1.660648
6	-0.162569	4.612066	2.615479
1	-0.696662	3.653864	2.563102
1	-0.864857	5.411124	2.344980
1	0.130917	4.772863	3.664821
6	1.782713	6.013273	1.797785
1	1.133157	6.821525	1.443631
1	2.714927	6.046902	1.219418
1	2.038141	6.229115	2.847311
6	-0.798158	5.191546	-0.964476
6	-2.181065	4.745916	-0.413258
1	-2.369415	3.679877	-0.600130
1	-2.981097	5.315759	-0.911505
1	-2.273276	4.917627	0.665520
6	-0.785637	4.939896	-2.500684
1	-0.888047	3.872754	-2.743003
1	0.136122	5.305798	-2.970916
1	-1.631049	5.467693	-2.968738

6	-0.640143	6.721910	-0.727786
1	-1.414172	7.263598	-1.294002
1	0.336209	7.096596	-1.064742
1	-0.761964	6.987437	0.329624
6	-4.150921	-1.892341	2.406989
1	-4.379105	-2.786856	1.815133
1	-4.664352	-1.043592	1.940569
1	-4.582471	-2.036195	3.407556
6	-1.465947	-3.334414	3.016707
6	-2.001954	-0.163753	3.841217
6	-1.483929	-4.270058	1.773389
1	-2.496989	-4.392318	1.366413
1	-1.117405	-5.270389	2.053348
1	-0.838025	-3.892378	0.969459
6	-2.298492	-4.026261	4.136486
1	-3.330326	-4.219890	3.816887
1	-2.335760	-3.432045	5.056401
1	-1.842937	-4.997901	4.386711
6	0.003122	-3.200422	3.502881
1	0.435886	-4.201402	3.660489
1	0.071276	-2.659741	4.455353
1	0.632172	-2.676525	2.770500
6	-2.430327	-0.619837	5.265928
1	-3.457437	-1.008261	5.288973
1	-2.386448	0.237687	5.956121
1	-1.762442	-1.394069	5.663518
6	-0.533456	0.335223	3.907571
1	0.154361	-0.446361	4.251115
1	-0.458439	1.177057	4.614553
1	-0.178606	0.686527	2.931120
6	-2.902878	1.037369	3.429043
1	-3.968710	0.775615	3.445199
1	-2.657866	1.404985	2.423273
1	-2.755262	1.870664	4.134059
6	-4.021857	-3.050064	-1.283227
1	-4.584105	-3.489735	-2.119419
1	-4.747368	-2.745379	-0.519187
1	-3.395829	-3.840175	-0.851995
6	-4.241563	-0.099023	-2.243181
6	-1.955712	-2.191390	-3.441723
6	-5.491435	-0.626820	-3.008540
1	-6.201715	0.201153	-3.164520
1	-6.016743	-1.408426	-2.445314
1	-5.237204	-1.032073	-3.994305
6	-4.737013	0.486284	-0.889040
1	-5.485498	1.272870	-1.074202

1	-3.916169	0.935234	-0.313820
1	-5.212774	-0.279516	-0.261486
6	-3.608489	1.053981	-3.068845
1	-4.327527	1.883834	-3.160190
1	-3.347176	0.732767	-4.084967
1	-2.701011	1.450572	-2.594889
6	-1.206936	-3.496074	-3.040830
1	-1.900727	-4.298353	-2.758273
1	-0.519402	-3.326811	-2.201170
1	-0.610115	-3.857376	-3.893131
6	-2.906648	-2.524912	-4.627626
1	-3.384304	-1.624421	-5.033258
1	-3.696224	-3.233964	-4.344636
1	-2.327913	-2.985286	-5.444111
6	-0.902193	-1.163875	-3.935608
1	-1.361848	-0.227260	-4.271255
1	-0.344618	-1.584943	-4.787962
1	-0.176342	-0.913049	-3.153383

TS-Pb=Pb=Pb-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.175379	-2.320153	-0.106987
82	-1.404759	0.189001	-0.914188
14	-3.437653	-1.646649	0.330504
14	-1.942189	2.950965	-0.546702
82	1.568824	0.212931	0.209680
6	-4.702041	-0.627301	-0.722314
1	-4.465747	-0.712355	-1.790956
1	-4.689328	0.437280	-0.471706
1	-5.728253	-0.991119	-0.577727
6	-3.982726	-1.479954	2.226598
6	-3.184288	-0.338317	2.905149
1	-3.306416	0.608496	2.373266
1	-2.110742	-0.562679	2.944562
1	-3.539432	-0.189231	3.938052
6	-3.738971	-2.770426	3.052757
1	-2.690166	-3.093388	3.010002

1	-4.368527	-3.603365	2.719003
1	-3.982512	-2.575852	4.109409
6	-5.496359	-1.119531	2.311861
1	-6.134272	-1.884472	1.851225
1	-5.714934	-0.161785	1.823228
1	-5.794364	-1.026925	3.368499
6	-3.664191	-3.475694	-0.409134
6	-2.830669	-4.592030	0.274971
1	-1.753766	-4.413527	0.172062
1	-3.049254	-5.557744	-0.208158
1	-3.057421	-4.695334	1.339912
6	-3.292070	-3.468717	-1.920427
1	-2.236578	-3.210671	-2.075319
1	-3.903090	-2.763306	-2.497315
1	-3.454253	-4.471615	-2.346420
6	-5.167774	-3.870322	-0.282718
1	-5.321921	-4.861902	-0.736750
1	-5.827838	-3.166060	-0.802389
1	-5.489618	-3.934394	0.764374
6	-0.294207	3.899037	-0.354866
1	0.047721	3.866437	0.684646
1	-0.415585	4.954152	-0.642316
1	0.497653	3.464890	-0.971674
6	-3.053191	3.557142	0.960557
6	-2.347429	3.156250	2.291404
1	-1.526463	3.845999	2.524226
1	-1.930492	2.143375	2.266848
1	-3.065259	3.204555	3.125706
6	-3.167810	5.112438	0.972866
1	-2.184286	5.597083	0.929630
1	-3.647204	5.425875	1.913895
1	-3.777101	5.495834	0.148857
6	-4.487277	2.968454	0.933956
1	-5.071171	3.369112	1.777523
1	-4.484160	1.877314	1.028377
1	-5.021474	3.227232	0.010035
6	-2.610827	3.369057	-2.353666
6	-3.103930	4.842072	-2.437062
1	-2.368033	5.553056	-2.038819
1	-4.047041	4.985442	-1.896295
1	-3.284949	5.107320	-3.490557
6	-1.432181	3.205767	-3.356187
1	-0.612362	3.902486	-3.142950
1	-1.786766	3.408798	-4.378630
1	-1.018767	2.188902	-3.350349
6	-3.767677	2.442407	-2.812864

1	-4.626261	2.474213	-2.130353
1	-3.444018	1.396018	-2.894419
1	-4.120361	2.753626	-3.808878
14	3.344894	-0.012088	-1.887726
6	4.848383	1.079334	-1.416378
1	5.506516	1.233357	-2.283911
1	5.442718	0.612666	-0.622389
1	4.530558	2.065568	-1.057841
6	4.038693	-1.847732	-2.105088
6	5.356062	-1.832271	-2.939004
1	5.740835	-2.860245	-3.033311
1	6.134467	-1.233440	-2.450078
1	5.210243	-1.440171	-3.950310
6	4.388000	-2.464008	-0.721214
1	4.807071	-3.473235	-0.859733
1	3.506887	-2.549023	-0.073770
1	5.137897	-1.865995	-0.185606
6	3.018972	-2.776820	-2.813823
1	3.394298	-3.811852	-2.831089
1	2.834505	-2.471999	-3.851341
1	2.046189	-2.792547	-2.296467
6	2.595781	0.759520	-3.537567
6	2.441988	2.293323	-3.324032
1	3.414121	2.789314	-3.208966
1	1.838158	2.521667	-2.436059
1	1.939713	2.742771	-4.195196
6	3.530503	0.539182	-4.761708
1	3.569434	-0.516336	-5.057590
1	4.556257	0.883817	-4.576153
1	3.140948	1.105867	-5.622564
6	1.203458	0.178398	-3.895369
1	1.231193	-0.903124	-4.075615
1	0.817136	0.658706	-4.808836
1	0.475984	0.357369	-3.095344
14	2.879031	0.670467	2.552434
6	4.758375	0.422536	2.289828
1	5.185567	1.236659	1.692822
1	4.975585	-0.519991	1.775240
1	5.281086	0.407197	3.257318
6	2.629771	2.555739	3.046559
6	2.307791	-0.649256	3.892915
6	2.922644	3.444105	1.802436
1	3.956847	3.327920	1.450242
1	2.778079	4.505471	2.060778
1	2.253498	3.211301	0.966178
6	3.612738	2.995259	4.170064

1	4.660099	2.873243	3.865006
1	3.461741	2.438302	5.101187
1	3.456859	4.063183	4.393371
6	1.176462	2.825407	3.514144
1	1.012428	3.907357	3.642669
1	0.962540	2.343923	4.476864
1	0.444575	2.459654	2.784430
6	2.909364	-0.328085	5.291825
1	4.002463	-0.225787	5.260779
1	2.674248	-1.146438	5.990671
1	2.490645	0.593967	5.712854
6	0.763263	-0.724735	4.027453
1	0.330623	0.217928	4.382137
1	0.485866	-1.511351	4.747097
1	0.288779	-0.968468	3.067794
6	2.825355	-2.051257	3.459235
1	3.921289	-2.091432	3.418884
1	2.442301	-2.333689	2.469165
1	2.489174	-2.811308	4.181820

Pro-Pb=Pb=Pb-TR

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	0.454436	1.700101	-0.632500
82	1.456785	-0.890458	-0.182357
82	-1.538021	-0.641520	0.104266
14	2.282882	3.575780	0.207769
14	2.669663	-3.317021	-0.462798
14	-3.364890	-0.151465	-1.898328
14	-2.805162	-0.864155	2.524227
6	1.507721	-4.821912	-0.290702
1	1.143493	-4.927386	0.738704
1	2.034479	-5.750901	-0.556905
1	0.633109	-4.732783	-0.944673
6	3.992764	-3.410421	0.982136
6	3.266150	-3.198849	2.342685
1	2.472589	-3.940373	2.507816
1	2.816120	-2.198942	2.415953
1	3.987605	-3.297088	3.168538

6	4.673447	-4.811025	1.022366
1	3.942060	-5.616450	1.170095
1	5.381577	-4.849742	1.865132
1	5.237147	-5.026535	0.107765
6	5.090987	-2.321773	0.839705
1	5.764379	-2.353880	1.710225
1	4.662129	-1.310501	0.793058
1	5.704328	-2.472201	-0.058008
6	3.374753	-3.270731	-2.297022
6	4.442297	-4.381079	-2.520264
1	4.071900	-5.378760	-2.247869
1	5.358540	-4.187016	-1.948624
1	4.720749	-4.410763	-3.585660
6	2.195090	-3.523356	-3.280742
1	1.764421	-4.525031	-3.155873
1	2.555667	-3.442512	-4.317954
1	1.388191	-2.788543	-3.152680
6	4.014410	-1.899611	-2.653018
1	4.845360	-1.639470	-1.986419
1	3.279881	-1.083307	-2.610546
1	4.407840	-1.929111	-3.681253
6	3.885641	3.246733	-0.792028
1	3.661844	3.023176	-1.842086
1	4.425957	2.383040	-0.382202
1	4.565856	4.111144	-0.768251
6	2.796572	3.623973	2.102911
6	3.211504	2.198275	2.565447
1	2.373660	1.491524	2.510781
1	3.557310	2.233928	3.611071
1	4.034357	1.792892	1.960275
6	1.638374	4.110460	3.014569
1	0.737468	3.494092	2.890622
1	1.366911	5.155070	2.813598
1	1.943031	4.047123	4.071400
6	4.026996	4.559551	2.304035
1	3.815119	5.596539	2.020086
1	4.895005	4.219177	1.724376
1	4.319614	4.559261	3.366297
6	1.451962	5.215038	-0.499060
6	-0.008632	5.383983	0.007546
1	-0.648068	4.540891	-0.292801
1	-0.452093	6.296953	-0.420903
1	-0.062909	5.466356	1.099605
6	1.414180	5.112308	-2.052954
1	0.869892	4.220927	-2.398091
1	2.422099	5.074571	-2.485098

1	0.901153	5.991513	-2.473052
6	2.252821	6.494163	-0.125949
1	1.818938	7.366536	-0.640926
1	3.306713	6.423293	-0.427208
1	2.217678	6.697699	0.951633
6	-4.637730	-0.320499	2.385669
1	-5.211707	-1.007517	1.751867
1	-4.727872	0.683403	1.955305
1	-5.113716	-0.303728	3.376957
6	-2.825789	-2.791284	2.927390
6	-1.988062	0.276608	3.902742
6	-3.226001	-3.569408	1.639543
1	-4.189597	-3.230159	1.235283
1	-3.319357	-4.643718	1.864229
1	-2.470778	-3.464079	0.847745
6	-3.879822	-3.127021	4.022308
1	-4.893142	-2.843799	3.710304
1	-3.666538	-2.626703	4.973432
1	-3.883761	-4.212801	4.211114
6	-1.437181	-3.306496	3.393020
1	-1.457355	-4.403558	3.492412
1	-1.155813	-2.892005	4.368944
1	-0.644979	-3.051243	2.675638
6	-2.597719	-0.017450	5.304448
1	-3.693253	0.060746	5.308663
1	-2.212615	0.713165	6.033739
1	-2.324493	-1.016326	5.667250
6	-0.446925	0.109216	3.994298
1	-0.154162	-0.909990	4.273159
1	-0.044702	0.791553	4.760416
1	0.044059	0.354543	3.044081
6	-2.285516	1.763802	3.549578
1	-3.361700	1.979265	3.542163
1	-1.874484	2.037872	2.568448
1	-1.821090	2.421514	4.301403
6	-4.938439	-1.122784	-1.386815
1	-5.628825	-1.221061	-2.236909
1	-5.473289	-0.609596	-0.578991
1	-4.696384	-2.133571	-1.036802
6	-3.918503	1.724279	-2.111929
6	-2.682736	-1.018260	-3.526988
6	-5.252905	1.816303	-2.913032
1	-5.556607	2.872641	-2.991525
1	-6.068296	1.276220	-2.415589
1	-5.157081	1.424807	-3.932005
6	-4.175871	2.347206	-0.709816

1	-4.526278	3.385311	-0.823255	
1	-3.267213	2.364437	-0.094754	
1	-4.949425	1.797587	-0.156539	
6	-2.851643	2.582540	-2.843326	
1	-3.160493	3.639994	-2.847989	
1	-2.719966	2.272601	-3.887817	
1	-1.872890	2.522285	-2.349199	
6	-2.557166	-2.545144	-3.248660	
1	-3.530284	-3.006581	-3.037132	
1	-1.890665	-2.749894	-2.399398	
1	-2.134538	-3.049232	-4.132039	
6	-3.659973	-0.825917	-4.722420	
1	-3.698679	0.219282	-5.053240	
1	-4.682287	-1.148518	-4.483879	
1	-3.314742	-1.427634	-5.578339	
6	-1.284912	-0.493778	-3.952468	
1	-1.293315	0.577568	-4.185282	
1	-0.946858	-1.028429	-4.854885	
1	-0.534072	-0.654947	-3.169839	-----

