

Supporting Information

A Mechanistic Study of the Activation of Small Molecules (H_2 and C_2H_2) by Group 14 Analogues of Selenophene

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Figure S1. The curve of intrinsic reaction coordinate (IRC) of transition state for $\text{H}_2 + \text{Rea-E}$ ($\text{E} = \text{C}, \text{Si}, \text{Ge}, \text{Sn}, \text{and Pb}$) at B3PW91/def2-SVP level of theory.

Figure S2. The curve of intrinsic reaction coordinate (IRC) of transition state for $\text{C}_2\text{H}_2 + \text{Rea-E}$ ($\text{E} = \text{C}, \text{Si}, \text{Ge}, \text{Sn}, \text{and Pb}$) at B3PW91/def2-SVP level of theory.

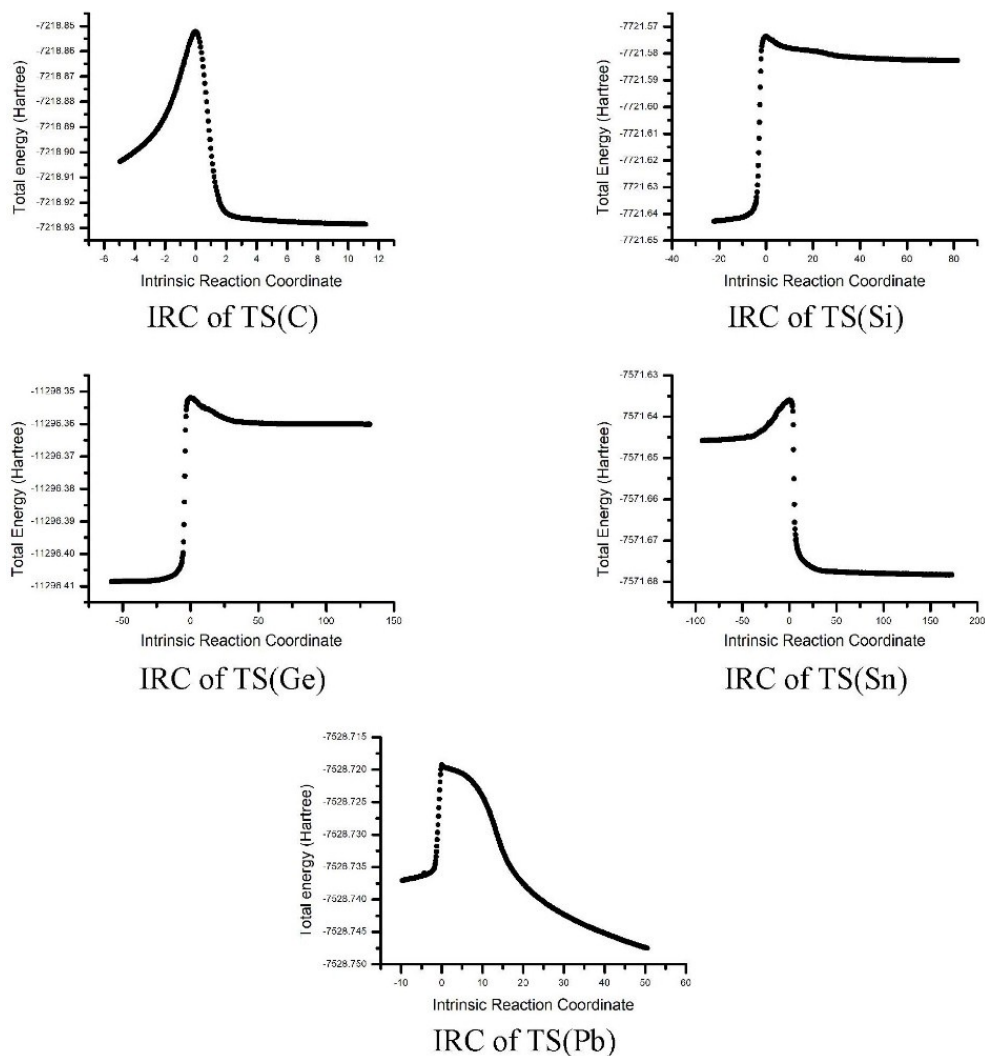


Figure S1. The curve of intrinsic reaction coordinate (IRC) of transition state for H₂ + **Rea-E** (E = C, Si, Ge, Sn, and Pb) at B3PW91/def2-SVP level of theory.

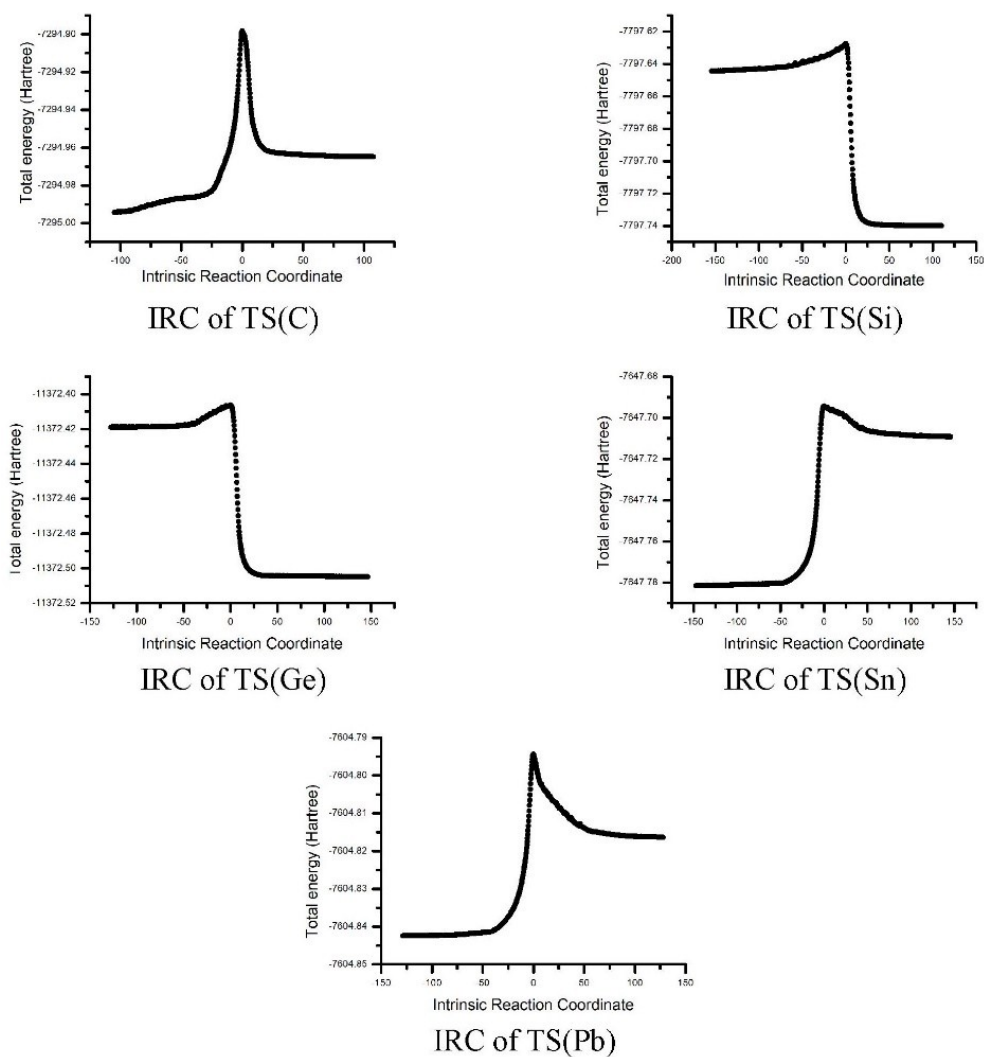


Figure S2. The curve of intrinsic reaction coordinate (IRC) of transition state for $\text{C}_2\text{H}_2 + \text{Rea-E}$ (E = C, Si, Ge, Sn, and Pb) at B3PW91/def2-SVP level of theory.

Table S1-S26. Geometrical coordinates of the reactants, transition states, and products at B3PW91/def2-SVP level of theory.

Table S1

B3PW91/def2-SVP

Rea-E₁₄ (E₁₄ = C)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
34	-0.000008	-0.000086	-1.165757
6	-1.327696	-0.063627	0.162629
6	1.327603	0.063567	0.162654
6	-0.732242	-0.017675	1.412259
6	0.732051	0.017714	1.412285
6	-1.509632	0.047530	2.682474
6	-2.551904	-0.849991	2.962307
1	-2.843617	-1.577929	2.207557
6	-3.207184	-0.835683	4.194363
1	-4.004426	-1.557725	4.388897
6	-2.847494	0.091792	5.172316
1	-3.356934	0.100998	6.139266
6	-1.841405	1.019501	4.895881
1	-1.561463	1.765619	5.643863
6	-1.183556	0.997893	3.667388
1	-0.388338	1.719674	3.473253
6	1.509364	-0.047587	2.682551
6	2.551672	0.849812	2.962575
1	2.843579	1.577769	2.207909
6	3.206753	0.835358	4.194740
1	4.004045	1.557299	4.389441
6	2.846822	-0.092138	5.172584
1	3.356130	-0.101446	6.139603
6	1.840694	-1.019742	4.895946
1	1.560566	-1.765877	5.643841
6	1.183038	-0.997989	3.667351
1	0.387762	-1.719663	3.473060
6	-2.779878	-0.147177	-0.185919
6	-3.367398	-1.402072	-0.528190
6	-4.763847	-1.478124	-0.681513
1	-5.190150	-2.456712	-0.894806
6	-5.606529	-0.372692	-0.577087
6	-4.993787	0.861552	-0.347858
1	-5.611592	1.761185	-0.304053
6	-3.613389	1.013766	-0.150986
6	-2.577950	-2.669350	-0.809009
1	-1.499456	-2.446996	-0.719222
14	-2.767666	-3.128912	-2.676779
14	-2.817391	-4.124995	0.442579
6	-2.553141	-1.571778	-3.722332
1	-2.689581	-1.815489	-4.789066
1	-1.550476	-1.131138	-3.608514
1	-3.297793	-0.807375	-3.452893
6	-1.444935	-4.367985	-3.215959
1	-1.661369	-5.392303	-2.881777
1	-0.441883	-4.095250	-2.856754
1	-1.405848	-4.381824	-4.317978
6	-4.456299	-3.860318	-3.131745
1	-4.384532	-4.312982	-4.134895
1	-5.235282	-3.084874	-3.178623
1	-4.797881	-4.645604	-2.440339
6	-2.782081	-5.847625	-0.344925
1	-1.800766	-6.084386	-0.782554
1	-3.549094	-5.998280	-1.119201

1	-2.970477	-6.585838	0.452602
6	-4.446675	-4.018250	1.397820
1	-4.425018	-4.757543	2.215715
1	-5.308377	-4.262392	0.756861
1	-4.630663	-3.027048	1.837684
6	-1.366407	-4.113781	1.653782
1	-1.284361	-3.174933	2.219259
1	-0.418783	-4.258668	1.111591
1	-1.461845	-4.938838	2.378606
6	-3.094012	2.421288	0.045244
1	-2.028916	2.375562	0.336214
14	-3.073715	3.377301	-1.630031
14	-3.929723	3.421360	1.478262
6	-2.073195	2.440519	-2.924816
1	-2.108495	2.983832	-3.883608
1	-2.488398	1.435538	-3.094952
1	-1.018579	2.322578	-2.639197
6	-4.780394	3.615949	-2.409758
1	-5.500618	4.141184	-1.768063
1	-5.218374	2.650071	-2.704304
1	-4.655901	4.212449	-3.329358
6	-2.269143	5.073244	-1.381368
1	-2.145967	5.569083	-2.358121
1	-1.269743	4.982278	-0.927421
1	-2.867986	5.741731	-0.744642
6	-4.718551	2.291624	2.759369
1	-5.103231	2.902932	3.592636
1	-3.996992	1.573733	3.170649
1	-5.560513	1.718958	2.343314
6	-5.303603	4.607896	0.925059
1	-5.677614	5.129840	1.822019
1	-6.161813	4.082950	0.476995
1	-4.968787	5.379227	0.215330
6	-2.601520	4.469997	2.318843
1	-2.131740	5.183856	1.625351
1	-1.807490	3.838297	2.744946
1	-3.045985	5.050666	3.143922
6	-7.134071	-0.464567	-0.721245
6	-7.801886	0.096832	0.548414
1	-7.493160	-0.469289	1.441062
1	-7.544674	1.153163	0.716698
1	-8.899173	0.032490	0.466971
6	-7.583707	0.359891	-1.942399
1	-8.678005	0.306274	-2.063358
1	-7.312681	1.421532	-1.843228
1	-7.121249	-0.019079	-2.867374
6	-7.614590	-1.908800	-0.911461
1	-7.331335	-2.549500	-0.062271
1	-8.712912	-1.929447	-0.989052
1	-7.213924	-2.361237	-1.831233
6	2.779810	0.147178	-0.185804
6	3.367232	1.402137	-0.527977
6	4.763690	1.478271	-0.681344
1	5.189929	2.456886	-0.894623
6	5.606435	0.372897	-0.577018
6	4.993781	-0.861407	-0.347824
1	5.611665	-1.760993	-0.304091
6	3.613416	-1.013717	-0.150940
6	2.577717	2.669371	-0.808821
1	1.499243	2.446865	-0.719183
14	2.817146	4.125104	0.442668
14	2.767643	3.128729	-2.676676
6	4.446762	4.018804	1.397402

1	5.308155	4.263232	0.756130
1	4.631205	3.027588	1.837064
1	4.425242	4.757981	2.215397
6	1.366593	4.113596	1.654377
1	1.462573	4.938383	2.379445
1	1.284577	3.174562	2.219543
1	0.418748	4.258925	1.112698
6	2.781208	5.847661	-0.344893
1	2.969433	6.586078	0.452482
1	1.799833	6.084141	-0.782574
1	3.548149	5.998418	-1.119217
6	2.554187	1.571252	-3.721935
1	2.690036	1.814768	-4.788780
1	1.552008	1.129631	-3.607629
1	3.299683	0.807656	-3.452484
6	1.444468	4.367042	-3.216407
1	1.659167	5.391184	-2.880591
1	0.441155	4.092650	-2.859206
1	1.407202	4.382170	-4.318474
6	4.456098	3.860857	-3.131386
1	5.235284	3.085642	-3.178469
1	4.797400	4.646146	-2.439874
1	4.384065	4.313661	-4.134456
6	3.094191	-2.421294	0.045302
1	2.029083	-2.375750	0.336269
14	3.930039	-3.421061	1.478440
14	3.074096	-3.377478	-1.629841
6	2.602063	-4.470022	2.319000
1	3.046683	-5.050324	3.144262
1	2.132681	-5.184241	1.625616
1	1.807694	-3.838602	2.744888
6	4.718470	-2.291090	2.759579
1	3.996590	-1.573608	3.171012
1	5.560081	-1.717929	2.343492
1	5.103566	-2.902287	3.592731
6	5.304269	-4.607278	0.925410
1	6.162604	-4.082041	0.477910
1	4.969856	-5.378379	0.215250
1	5.677977	-5.129506	1.822329
6	2.270549	-5.073860	-1.380942
1	1.271029	-4.983648	-0.927116
1	2.869829	-5.741899	-0.744164
1	2.147856	-5.569790	-2.357717
6	2.072877	-2.441350	-2.924534
1	2.107774	-2.984929	-3.883188
1	2.487783	-1.436320	-3.095141
1	1.018365	-2.323525	-2.638454
6	4.780818	-3.615418	-2.409691
1	4.656526	-4.211966	-3.329292
1	5.501282	-4.140370	-1.768027
1	5.218410	-2.649380	-2.704292
6	7.133963	0.464861	-0.721309
6	7.614389	1.909134	-0.911483
1	8.712704	1.929834	-0.989148
1	7.331157	2.549775	-0.062242
1	7.213644	2.361598	-1.831207
6	7.801935	-0.096573	0.548245
1	7.544800	-1.152925	0.716512
1	7.493275	0.469488	1.440955
1	8.899211	-0.032171	0.466695
6	7.583510	-0.359502	-1.942563
1	7.312553	-1.421165	-1.843417
1	8.677793	-0.305815	-2.063638

1 7.120924 0.019497 -2.867460

Table S2

B3PW91/def2-SVP

Rea-E₁₄ (E₁₄ = Si)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
34	-0.000013	-0.000070	-1.387770
14	-1.592024	-0.244480	0.199867
14	1.592016	0.244693	0.199817
6	-0.718271	-0.015440	1.756263
6	0.718238	0.015910	1.756271
6	-1.477452	0.139285	3.022994
6	-2.543617	-0.709826	3.363501
1	-2.800134	-1.528823	2.687839
6	-3.250180	-0.547177	4.556700
1	-4.069263	-1.230027	4.796258
6	-2.905573	0.469991	5.446399
1	-3.453203	0.593696	6.384074
6	-1.848619	1.325231	5.125050
1	-1.566768	2.129303	5.810214
6	-1.146408	1.163153	3.934042
1	-0.321275	1.838022	3.699804
6	1.477431	-0.138641	3.023010
6	2.543667	0.710455	3.363334
1	2.800239	1.529305	2.687518
6	3.250219	0.548029	4.556569
1	4.069343	1.230883	4.795963
6	2.905538	-0.468904	5.446505
1	3.453156	-0.592436	6.384210
6	1.848523	-1.324141	5.125341
1	1.566606	-2.128039	5.810681
6	1.146324	-1.162282	3.934297
1	0.321165	-1.837173	3.700219
6	-3.384067	0.095152	-0.289715
6	-4.270321	-1.004659	-0.476670
6	-5.614091	-0.749267	-0.802331
1	-6.273431	-1.607155	-0.934101
6	-6.125244	0.540788	-0.944338
6	-5.228670	1.604646	-0.788771
1	-5.589604	2.628903	-0.903665
6	-3.871280	1.422579	-0.487369
6	-3.846717	-2.449779	-0.357188
1	-2.800376	-2.478282	0.019677
14	-3.674266	-3.294822	-2.079902
14	-4.822612	-3.470131	0.963444
6	-2.467387	-2.312831	-3.143134
1	-2.386564	-2.770752	-4.142903
1	-1.459437	-2.289462	-2.701459
1	-2.800588	-1.271763	-3.276709
6	-2.971244	-5.035767	-1.851697
1	-3.651600	-5.708142	-1.307709
1	-2.012919	-5.011924	-1.309208
1	-2.779465	-5.487951	-2.838686
6	-5.297746	-3.398285	-3.042053
1	-5.106931	-3.919142	-3.995431
1	-5.681210	-2.395886	-3.286569
1	-6.087870	-3.951496	-2.514476
6	-6.150561	-4.626007	0.262781
1	-5.756368	-5.395610	-0.417379

1	-6.944130	-4.075963	-0.266847
1	-6.627884	-5.148885	1.108756
6	-5.729916	-2.333141	2.169493
1	-6.038517	-2.909032	3.057933
1	-6.639405	-1.917848	1.709288
1	-5.118359	-1.483262	2.503023
6	-3.571280	-4.533633	1.900559
1	-2.810493	-3.921193	2.409868
1	-3.042282	-5.226198	1.227224
1	-4.080200	-5.138878	2.668559
6	-2.992473	2.644640	-0.397755
1	-1.955091	2.315972	-0.183655
14	-2.798621	3.526991	-2.099388
14	-3.390748	3.783975	1.112353
6	-2.315295	2.273949	-3.424041
1	-2.248051	2.773151	-4.404938
1	-3.071331	1.476906	-3.504063
1	-1.344558	1.800558	-3.215865
6	-4.357699	4.380387	-2.750010
1	-4.803373	5.099588	-2.049012
1	-5.128495	3.648511	-3.035188
1	-4.083636	4.933135	-3.664587
6	-1.432079	4.824898	-1.950004
1	-1.207478	5.249340	-2.942179
1	-0.502870	4.382105	-1.558589
1	-1.715921	5.659513	-1.290123
6	-4.292248	2.803672	2.442824
1	-4.455692	3.439748	3.328205
1	-3.719681	1.921526	2.765347
1	-5.275372	2.457585	2.088169
6	-4.476639	5.280470	0.700546
1	-4.659395	5.842467	1.631871
1	-5.459823	4.989855	0.298156
1	-4.004667	5.973260	-0.012867
6	-1.751445	4.433225	1.790358
1	-1.224717	5.066481	1.060118
1	-1.083354	3.601860	2.063125
1	-1.924198	5.037575	2.695883
6	-7.604491	0.817078	-1.256515
6	-8.213269	1.656551	-0.116876
1	-8.152225	1.122414	0.844163
1	-7.698154	2.621254	0.003298
1	-9.275274	1.869510	-0.321004
6	-7.713815	1.594618	-2.581761
1	-8.770544	1.788199	-2.827835
1	-7.203368	2.567526	-2.531458
1	-7.270335	1.024937	-3.413397
6	-8.422913	-0.473441	-1.391804
1	-8.413410	-1.067242	-0.464827
1	-9.472864	-0.225529	-1.611907
1	-8.056611	-1.110694	-2.211341
6	3.384053	-0.095108	-0.289711
6	4.270453	1.004575	-0.476727
6	5.614247	0.748975	-0.802114
1	6.273717	1.606763	-0.933895
6	6.125271	-0.541163	-0.943856
6	5.228543	-1.604893	-0.788332
1	5.589361	-2.629210	-0.903045
6	3.871127	-1.422620	-0.487185
6	3.847034	2.449775	-0.357571
1	2.800660	2.478548	0.019178
14	4.822919	3.470246	0.963001
14	3.674883	3.294508	-2.080444

6	5.730054	2.333346	2.169276
1	6.639955	1.918560	1.709420
1	5.118694	1.483130	2.502305
1	6.037991	2.909175	3.057986
6	3.571570	4.533957	1.899864
1	4.080421	5.139240	2.667877
1	2.810715	3.921576	2.409148
1	3.042659	5.226475	1.226417
6	6.151010	4.625903	0.262286
1	6.628471	5.148663	1.108262
1	5.756909	5.395615	-0.417805
1	6.944461	4.075758	-0.267411
6	2.468233	2.312371	-3.143805
1	2.387565	2.770248	-4.143607
1	1.460199	2.288934	-2.702324
1	2.801553	1.271327	-3.277280
6	2.971801	5.035476	-1.852557
1	3.652032	5.707900	-1.308476
1	2.013354	5.011663	-1.310286
1	2.780242	5.487570	-2.839630
6	5.298530	3.397859	-3.042320
1	5.682040	2.395424	-3.286626
1	6.088552	3.951121	-2.514641
1	5.107954	3.918594	-3.995812
6	2.992134	-2.644553	-0.397681
1	1.954746	-2.315693	-0.183894
14	3.389839	-3.783893	1.112577
14	2.798609	-3.527081	-2.099253
6	1.750216	-4.432637	1.790293
1	1.922608	-5.036989	2.695886
1	1.223477	-5.065789	1.059971
1	1.082284	-3.601073	2.062866
6	4.291466	-2.803871	2.443150
1	3.719110	-1.921618	2.765740
1	5.274697	-2.458005	2.088568
1	4.454714	-3.440075	3.328476
6	4.475330	-5.280731	0.700901
1	5.458591	-4.990455	0.298459
1	4.003105	-5.973400	-0.012468
1	4.657946	-5.842738	1.632246
6	1.431897	-4.824835	-1.950077
1	0.502752	-4.381986	-1.558576
1	1.715635	-5.659629	-1.290380
1	1.207224	-5.249018	-2.942348
6	2.315683	-2.274102	-3.424115
1	2.248247	-2.773378	-4.404959
1	3.071936	-1.477277	-3.504238
1	1.345092	-1.800395	-3.215965
6	4.357791	-4.380672	-2.749346
1	4.083855	-4.933933	-3.663650
1	4.803500	-5.099446	-2.047933
1	5.128506	-3.648837	-3.034848
6	7.604530	-0.817661	-1.255793
6	8.423157	0.472741	-1.390979
1	9.473118	0.224661	-1.610851
1	8.413547	1.066599	-0.464039
1	8.057129	1.110003	-2.210633
6	8.213030	-1.657203	-0.116061
1	7.697778	-2.621841	0.004055
1	8.151925	-1.123045	0.844963
1	9.275035	-1.870305	-0.320039
6	7.713924	-1.595230	-2.581018
1	7.203342	-2.568071	-2.530763

1	8.770659	-1.788948	-2.826964
1	7.270614	-1.025504	-3.412713

Table S3
B3PW91/def2-SVP
Rea-E₁₄ (E₁₄ = Ge)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
34	-0.000007	0.000045	-1.456261
32	-1.623311	-0.457055	0.155455
32	1.623313	0.457110	0.155447
6	-0.689521	-0.106123	1.798786
6	0.689530	0.106171	1.798783
6	-1.472914	-0.233885	3.054596
6	-2.294262	-1.349857	3.288845
1	-2.341423	-2.137928	2.532228
6	-3.009513	-1.486088	4.480267
1	-3.629233	-2.372085	4.639555
6	-2.923133	-0.505588	5.467860
1	-3.478584	-0.612665	6.402967
6	-2.114927	0.612671	5.249673
1	-2.040207	1.391745	6.012865
6	-1.398286	0.746320	4.063636
1	-0.768744	1.624175	3.912582
6	1.472918	0.233947	3.054594
6	2.294244	1.349939	3.288840
1	2.341383	2.138011	2.532223
6	3.009494	1.486189	4.480260
1	3.629191	2.372202	4.639546
6	2.923141	0.505687	5.467854
1	3.478589	0.612780	6.402961
6	2.114964	-0.612593	5.249669
1	2.040268	-1.391671	6.012859
6	1.398321	-0.746259	4.063635
1	0.768808	-1.624136	3.912582
6	-3.447298	0.176269	-0.289709
6	-4.433732	-0.804677	-0.573271
6	-5.749115	-0.383337	-0.845672
1	-6.492875	-1.153580	-1.049574
6	-6.126269	0.959447	-0.853264
6	-5.121652	1.904905	-0.617128
1	-5.372213	2.968311	-0.636137
6	-3.788099	1.556689	-0.353100
6	-4.152649	-2.289505	-0.624696
1	-3.113370	-2.464402	-0.270928
14	-4.074854	-2.931669	-2.440653
14	-5.214511	-3.350941	0.587033
6	-2.744680	-1.988263	-3.387211
1	-2.729302	-2.317755	-4.439461
1	-1.740923	-2.161991	-2.969678
1	-2.931485	-0.903231	-3.379362
6	-3.604326	-4.764069	-2.453288
1	-4.364953	-5.409317	-1.988092
1	-2.647363	-4.936368	-1.935436
1	-3.479253	-5.100599	-3.495760
6	-5.696125	-2.699952	-3.383496
1	-5.580851	-3.123346	-4.395358
1	-5.939467	-1.632524	-3.498564
1	-6.553089	-3.199511	-2.908968
6	-6.724700	-4.170914	-0.209640
1	-6.464234	-4.856317	-1.030341
1	-7.443873	-3.433443	-0.599117
1	-7.249561	-4.762493	0.559202
6	-5.858064	-2.291507	2.008998

1	-6.353980	-2.930819	2.758286
1	-6.593784	-1.553875	1.654381
1	-5.053305	-1.734854	2.511314
6	-4.110919	-4.722489	1.278828
1	-3.246495	-4.312334	1.824862
1	-3.721059	-5.377756	0.484855
1	-4.679421	-5.352980	1.982058
6	-2.785470	2.670959	-0.182198
1	-1.792679	2.221109	0.012535
14	-2.484940	3.607955	-1.840997
14	-3.075352	3.745330	1.394394
6	-2.404703	2.379588	-3.270252
1	-2.204531	2.916258	-4.212378
1	-3.363900	1.849893	-3.381745
1	-1.614221	1.628286	-3.131010
6	-3.821652	4.855756	-2.334048
1	-3.928391	5.697153	-1.636081
1	-4.806988	4.380298	-2.455707
1	-3.542985	5.272438	-3.316826
6	-0.843780	4.535073	-1.700047
1	-0.569597	4.974482	-2.672969
1	-0.030454	3.857901	-1.394139
1	-0.896046	5.357397	-0.969055
6	-4.085135	2.767939	2.649032
1	-4.153111	3.325647	3.597505
1	-3.637592	1.787210	2.865526
1	-5.108695	2.596723	2.281751
6	-3.995897	5.374748	1.104047
1	-4.185335	5.843604	2.084303
1	-4.971721	5.233587	0.613668
1	-3.412284	6.090717	0.505107
6	-1.380125	4.185963	2.107313
1	-0.818340	4.849150	1.431110
1	-0.767235	3.286741	2.274625
1	-1.488956	4.708097	3.072024
6	-7.570869	1.417018	-1.108897
6	-8.073650	2.211224	0.111969
1	-8.052194	1.592364	1.022640
1	-7.461446	3.105735	0.300948
1	-9.111596	2.546019	-0.047487
6	-7.611301	2.316965	-2.358410
1	-8.642221	2.650938	-2.559112
1	-6.989540	3.216193	-2.236266
1	-7.249650	1.777180	-3.247541
6	-8.524397	0.236636	-1.337166
1	-8.564441	-0.434937	-0.465644
1	-9.545466	0.611156	-1.510001
1	-8.241105	-0.360608	-2.217536
6	3.447285	-0.176263	-0.289710
6	4.433748	0.804647	-0.573291
6	5.749117	0.383261	-0.845695
1	6.492903	1.153477	-1.049607
6	6.126223	-0.959535	-0.853292
6	5.121576	-1.904958	-0.617138
1	5.372097	-2.968372	-0.636157
6	3.788041	-1.556694	-0.353083
6	4.152716	2.289483	-0.624718
1	3.113423	2.464412	-0.271009
14	5.214549	3.350860	0.587081
14	4.075061	2.931673	-2.440678
6	5.857954	2.291387	2.009082
1	6.593651	1.553708	1.654515
1	5.053128	1.734785	2.511350

1	6.353860	2.930671	2.758400
6	4.110973	4.722453	1.278815
1	4.679456	5.352911	1.982090
1	3.246492	4.312336	1.824787
1	3.721200	5.377745	0.484822
6	6.724821	4.170773	-0.209495
1	7.249658	4.762332	0.559378
1	6.464428	4.856185	-1.030211
1	7.443989	3.433274	-0.598930
6	2.744884	1.988355	-3.387320
1	2.729582	2.317850	-4.439570
1	1.741116	2.162151	-2.969840
1	2.931617	0.903311	-3.379464
6	3.604627	4.764097	-2.453327
1	4.365257	5.409312	-1.988090
1	2.647644	4.936436	-1.935523
1	3.479622	5.100636	-3.495804
6	5.696376	2.699874	-3.383424
1	5.939663	1.632433	-3.498487
1	6.553341	3.199378	-2.908842
1	5.581186	3.123284	-4.395290
6	2.785393	-2.670939	-0.182142
1	1.792602	-2.221072	0.012560
14	3.075252	-3.745225	1.394511
14	2.484863	-3.607995	-1.840905
6	1.380018	-4.185862	2.107408
1	1.488837	-4.707974	3.072132
1	0.818254	-4.849071	1.431209
1	0.767114	-3.286644	2.274685
6	4.084971	-2.767736	2.649124
1	3.637390	-1.787009	2.865551
1	5.108535	-2.596507	2.281861
1	4.152937	-3.325385	3.597632
6	3.995869	-5.374623	1.104277
1	4.971697	-5.233428	0.613915
1	3.412312	-6.090655	0.505358
1	4.185307	-5.843416	2.084562
6	0.843629	-4.534982	-1.699954
1	0.030362	-3.857726	-1.394072
1	0.895811	-5.357295	-0.968944
1	0.569425	-4.974386	-2.672872
6	2.404755	-2.379697	-3.270228
1	2.204585	-2.916404	-4.212333
1	3.363988	-1.850065	-3.381714
1	1.614315	-1.628337	-3.131054
6	3.821502	-4.855907	-2.333874
1	3.542831	-5.272590	-3.316651
1	3.928163	-5.697297	-1.635887
1	4.806878	-4.380526	-2.455515
6	7.570803	-1.417159	-1.108945
6	8.524362	-0.236815	-1.337275
1	9.545414	-0.611373	-1.510132
1	8.564453	0.434776	-0.465769
1	8.241060	0.360418	-2.217649
6	8.073586	-2.211342	0.111934
1	7.461354	-3.105825	0.300957
1	8.052173	-1.592452	1.022586
1	9.111517	-2.546179	-0.047535
6	7.611178	-2.317148	-2.358431
1	6.989383	-3.216347	-2.236247
1	8.642080	-2.651168	-2.559140
1	7.249533	-1.777377	-3.247573

Table S4
B3PW91/def2-SVP
 Rea-E₁₄ (E₁₄ = Sn)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
34	-0.000913	-0.004821	-1.691254
50	-1.745108	-0.658973	0.035275
50	1.744974	0.662641	0.030892
6	-0.652267	-0.176900	1.889951
6	0.652925	0.184835	1.888150
6	-1.439729	-0.454555	3.117491
6	-2.073994	-1.694669	3.305931
1	-1.970633	-2.468120	2.538827
6	-2.794263	-1.967477	4.470197
1	-3.265023	-2.945803	4.596428
6	-2.907553	-1.000674	5.468808
1	-3.472679	-1.211349	6.380150
6	-2.290069	0.239866	5.291973
1	-2.375116	1.008692	6.064462
6	-1.561443	0.510155	4.136005
1	-1.079264	1.481588	4.014811
6	1.441531	0.467187	3.113845
6	2.074025	1.708848	3.298096
1	1.968326	2.480069	2.529077
6	2.795471	1.985883	4.460643
1	3.264831	2.965297	4.583617
6	2.911735	1.021915	5.461649
1	3.477800	1.235902	6.371635
6	2.296017	-0.220096	5.288951
1	2.383394	-0.986729	6.063362
6	1.566195	-0.494621	4.134741
1	1.085309	-1.467109	4.016835
6	-3.730640	0.237208	-0.359807
6	-4.810176	-0.665320	-0.518898
6	-6.102825	-0.145204	-0.726069
1	-6.921873	-0.855735	-0.835567
6	-6.363147	1.223998	-0.786411
6	-5.268697	2.087741	-0.663664
1	-5.430884	3.166789	-0.719040
6	-3.954384	1.634616	-0.463331
6	-4.660255	-2.171978	-0.504739
1	-3.623877	-2.425754	-0.190761
14	-4.716424	-2.886819	-2.291911
14	-5.723100	-3.069103	0.828515
6	-3.342043	-2.090820	-3.309686
1	-3.376079	-2.460839	-4.347781
1	-2.343149	-2.324315	-2.908034
1	-3.443516	-0.994924	-3.340818
6	-4.413285	-4.754010	-2.258871
1	-5.225504	-5.310687	-1.766435
1	-3.469517	-5.002453	-1.747444
1	-4.337041	-5.129468	-3.292767
6	-6.351618	-2.548625	-3.175801
1	-6.321330	-3.019386	-4.172760
1	-6.510581	-1.469657	-3.323700
1	-7.223244	-2.955392	-2.642040
6	-7.399076	-3.684270	0.197108
1	-7.300762	-4.412216	-0.622982
1	-8.044502	-2.863250	-0.152232
1	-7.929054	-4.187913	1.022790
6	-6.038411	-1.916428	2.286636

1	-6.574449	-2.456072	3.084883
1	-6.649966	-1.050491	1.991620
1	-5.097858	-1.532279	2.710747
6	-4.750534	-4.570353	1.445125
1	-3.783154	-4.270069	1.878399
1	-4.548539	-5.296128	0.643292
1	-5.319264	-5.092213	2.232264
6	-2.853093	2.664406	-0.377751
1	-1.886090	2.136433	-0.260365
14	-2.589125	3.578052	-2.054646
14	-2.943508	3.748738	1.213576
6	-2.574291	2.322597	-3.461666
1	-2.397029	2.834706	-4.421939
1	-3.543551	1.803825	-3.530689
1	-1.788917	1.563853	-3.328559
6	-3.921996	4.844061	-2.510762
1	-4.043687	5.651649	-1.775739
1	-4.901757	4.368337	-2.669157
1	-3.631013	5.307452	-3.468774
6	-0.930329	4.482589	-1.986939
1	-0.696763	4.913685	-2.974252
1	-0.110560	3.797470	-1.718605
1	-0.938445	5.309823	-1.259557
6	-3.956070	2.860180	2.532243
1	-3.938821	3.434744	3.473102
1	-3.566306	1.853426	2.744395
1	-5.006076	2.751322	2.219669
6	-3.720349	5.459327	0.977159
1	-3.755278	5.964137	1.957220
1	-4.752861	5.410524	0.597503
1	-3.135300	6.099493	0.298902
6	-1.179767	4.014953	1.839548
1	-0.569892	4.579871	1.117379
1	-0.676699	3.052295	2.022008
1	-1.186578	4.580321	2.785885
6	-7.776653	1.793248	-0.988387
6	-8.114612	2.751971	0.169213
1	-8.078621	2.230108	1.138327
1	-7.416588	3.600857	0.220594
1	-9.128704	3.164805	0.042812
6	-7.829556	2.561359	-2.322723
1	-8.836620	2.977169	-2.489810
1	-7.116586	3.399112	-2.341174
1	-7.589902	1.899560	-3.169679
6	-8.847068	0.694621	-1.023540
1	-8.869188	0.113330	-0.088629
1	-9.842172	1.147909	-1.153540
1	-8.694687	-0.005377	-1.859388
6	3.729867	-0.238529	-0.359713
6	4.810593	0.662444	-0.520241
6	6.102807	0.140688	-0.725882
1	6.922501	0.850267	-0.836610
6	6.361945	-1.228839	-0.783168
6	5.266621	-2.091207	-0.658782
1	5.427813	-3.170535	-0.711702
6	3.952633	-1.636394	-0.460010
6	4.662630	2.169407	-0.509186
1	3.626787	2.425219	-0.195253
14	5.727133	3.067924	0.821757
14	4.718809	2.880705	-2.297731
6	6.041833	1.917930	2.282147
1	6.651886	1.050448	1.988598
1	5.100966	1.536138	2.707702

1	6.579180	2.458526	3.078870
6	4.756591	4.571506	1.435902
1	5.326526	5.094654	2.221311
1	3.789374	4.273006	1.870731
1	4.554490	5.295618	0.632598
6	7.403479	3.680057	0.188333
1	7.934465	4.184732	1.012736
1	7.305523	4.406569	-0.633075
1	8.047871	2.857716	-0.159805
6	3.342674	2.084809	-3.313276
1	3.377267	2.452073	-4.352332
1	2.344360	2.321409	-2.911985
1	3.441955	0.988627	-3.341603
6	4.418218	4.748376	-2.268093
1	5.231462	5.304818	-1.777091
1	3.475057	4.999071	-1.756644
1	4.341993	5.122023	-3.302649
6	6.353025	2.538766	-3.182043
1	6.510815	1.459319	-3.327654
1	7.225471	2.945877	-2.649881
1	6.322460	3.007337	-4.180031
6	2.850593	-2.665280	-0.372834
1	1.883963	-2.136346	-0.257148
14	2.939165	-3.746496	1.220716
14	2.587148	-3.582210	-2.047963
6	1.174970	-4.008398	1.847264
1	1.180684	-4.572855	2.794152
1	0.563915	-4.572767	1.125657
1	0.673909	-3.044525	2.028829
6	3.953319	-2.857147	2.537624
1	3.565851	-1.848927	2.746997
1	5.003678	-2.751457	2.225155
1	3.934426	-3.429302	3.479918
6	3.712761	-5.459040	0.987761
1	4.745545	-5.412982	0.608485
1	3.126757	-6.099245	0.310355
1	3.746298	-5.962273	1.968687
6	0.927896	-4.485901	-1.979386
1	0.108334	-3.799814	-1.712927
1	0.935197	-5.311634	-1.250288
1	0.694652	-4.918951	-2.965919
6	2.573655	-2.329818	-3.457799
1	2.397098	-2.844020	-4.417086
1	3.543094	-1.811420	-3.527166
1	1.788344	-1.570604	-3.327133
6	3.919706	-4.849648	-2.500988
1	3.628579	-5.315502	-3.457757
1	4.041323	-5.655293	-1.763840
1	4.899487	-4.374414	-2.660674
6	7.774971	-1.799801	-0.983697
6	8.846450	-0.702251	-1.020545
1	9.841168	-1.156731	-1.149358
1	8.868788	-0.119226	-0.086721
1	8.695012	-0.003689	-1.857764
6	8.111748	-2.756762	0.175698
1	7.412912	-3.604897	0.228441
1	8.076027	-2.233119	1.143861
1	9.125477	-3.170792	0.050281
6	7.827480	-2.570347	-2.316640
1	7.113629	-3.407375	-2.333768
1	8.834160	-2.987491	-2.482723
1	7.588719	-1.909810	-3.164834

Table S7
B3PW91/def2-SVP
 TS-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.254219	0.067934	0.126766
1	-0.450042	1.375029	0.032792
34	-0.012980	-0.610546	-1.184634
6	1.274524	-0.011995	0.117575
1	0.526076	1.364273	0.018513
6	-0.695813	-0.222949	1.434363
6	0.710023	-0.202754	1.433547
6	-1.490322	-0.325445	2.684384
6	-2.607177	0.481208	2.962838
1	-2.974231	1.174501	2.207951
6	-3.250461	0.418124	4.200005
1	-4.105706	1.070983	4.392734
6	-2.812035	-0.469587	5.182388
1	-3.315569	-0.515533	6.151295
6	-1.738246	-1.317469	4.902362
1	-1.398892	-2.039865	5.649144
6	-1.092053	-1.249630	3.670558
1	-0.251329	-1.915250	3.467432
6	1.521845	0.000256	2.669062
6	1.120081	0.948214	3.629332
1	0.240697	1.564712	3.437216
6	1.813379	1.101861	4.827987
1	1.471339	1.840089	5.557829
6	2.935553	0.315629	5.097044
1	3.473999	0.426197	6.041773
6	3.378159	-0.592795	4.135716
1	4.271588	-1.195027	4.319192
6	2.687976	-0.736575	2.931126
1	3.054964	-1.439729	2.185954
6	-2.726037	0.147350	-0.174692
6	-3.358707	1.408164	-0.433757
6	-4.761984	1.460988	-0.459307
1	-5.221868	2.436744	-0.618132
6	-5.584253	0.340317	-0.315616
6	-4.939760	-0.888087	-0.205692
1	-5.531451	-1.801866	-0.160337
6	-3.541732	-1.026893	-0.148193
6	-2.636164	2.703959	-0.770448
1	-1.550755	2.514676	-0.838315
14	-2.743512	4.107107	0.549068
6	-4.457983	4.260454	1.329570
1	-4.427917	5.047333	2.101552
1	-4.780777	3.326697	1.814006
1	-5.228973	4.546263	0.596902
6	-2.298981	5.803681	-0.165623
1	-2.981636	6.145954	-0.957584
1	-1.273312	5.829346	-0.564262
1	-2.349307	6.541261	0.652730
6	-1.485094	3.808007	1.925775
1	-0.471995	3.690221	1.511708
1	-1.709475	2.915896	2.526816
1	-1.467673	4.674753	2.607207
14	-3.067729	3.251252	-2.574922
6	-4.687057	4.225022	-2.728594
1	-4.740430	5.086028	-2.044950
1	-5.572178	3.595542	-2.553813

1	-4.766300	4.616433	-3.756613
6	-1.689891	4.326035	-3.295194
1	-0.706702	3.840948	-3.204125
1	-1.625093	5.320577	-2.832441
1	-1.885523	4.473327	-4.370565
6	-3.202115	1.722729	-3.672020
1	-3.451354	2.018354	-4.704510
1	-3.980538	1.030643	-3.317407
1	-2.245389	1.178316	-3.701139
6	-3.017346	-2.446571	-0.137821
1	-1.930959	-2.449862	0.059722
14	-3.747907	-3.628034	1.215895
6	-2.335936	-4.718045	1.838388
1	-1.566557	-4.107279	2.335371
1	-1.852293	-5.284044	1.027769
1	-2.712393	-5.444952	2.576573
6	-5.137282	-4.777597	0.622272
1	-5.394544	-5.443250	1.463562
1	-4.870243	-5.417310	-0.231048
1	-6.053648	-4.225337	0.360539
6	-4.484222	-2.709074	2.683522
1	-4.817144	-3.448949	3.430633
1	-5.356682	-2.101766	2.400813
1	-3.755396	-2.046739	3.166821
14	-3.172565	-3.211307	-1.910487
6	-2.403886	-4.941547	-1.937975
1	-2.384167	-5.312508	-2.976021
1	-2.955772	-5.677414	-1.334841
1	-1.363410	-4.922294	-1.577423
6	-4.954460	-3.304036	-2.540776
1	-4.941101	-3.802903	-3.524593
1	-5.367218	-2.294582	-2.691648
1	-5.642152	-3.865178	-1.894116
6	-2.270723	-2.181730	-3.212488
1	-1.178228	-2.292338	-3.162071
1	-2.514880	-1.111792	-3.133087
1	-2.590132	-2.518283	-4.213012
6	-7.114345	0.483052	-0.314289
6	-7.821599	-0.865754	-0.129210
1	-7.594599	-1.566647	-0.947053
1	-8.912427	-0.715780	-0.118684
1	-7.545494	-1.346696	0.821706
6	-7.581446	1.089859	-1.650694
1	-7.152750	2.088443	-1.820523
1	-8.678592	1.194870	-1.663981
1	-7.291708	0.451281	-2.499839
6	-7.534746	1.409003	0.842701
1	-7.215570	0.997364	1.813014
1	-8.630811	1.523331	0.866009
1	-7.097062	2.413265	0.744544
6	2.750586	-0.048693	-0.185329
6	3.411502	-1.296888	-0.451308
6	4.809360	-1.306779	-0.574035
1	5.288114	-2.270807	-0.749084
6	5.603090	-0.158338	-0.505795
6	4.930263	1.046236	-0.334291
1	5.497362	1.976491	-0.314978
6	3.535740	1.143179	-0.167642
6	2.710308	-2.622598	-0.717507
1	1.617318	-2.489609	-0.635971
14	3.016221	-4.085259	0.509404
6	1.744684	-4.047401	1.907981
1	1.860989	-4.949546	2.531383

1	0.723471	-4.058970	1.496758
1	1.834339	-3.172583	2.565856
6	4.752032	-4.094175	1.258533
1	5.011214	-3.141251	1.743334
1	5.527461	-4.312926	0.507578
1	4.801680	-4.886995	2.023340
6	2.753990	-5.782694	-0.291939
1	2.961296	-6.548705	0.473996
1	3.412923	-5.987565	-1.148021
1	1.712435	-5.924495	-0.618687
14	2.943221	-3.079912	-2.583535
6	2.843423	-1.517085	-3.638659
1	2.983012	-1.779917	-4.700567
1	3.624717	-0.792726	-3.363513
1	1.867120	-1.015436	-3.548058
6	4.605412	-3.898358	-2.979476
1	4.842701	-4.752208	-2.327585
1	5.436733	-3.180504	-2.919146
1	4.575252	-4.273890	-4.016006
6	1.561108	-4.229596	-3.169881
1	0.570762	-3.849700	-2.876727
1	1.656900	-5.256845	-2.791986
1	1.581880	-4.278007	-4.271295
6	2.993360	2.549136	-0.025278
1	1.942555	2.513422	0.308535
14	3.845459	3.649403	1.314670
6	4.651713	2.617242	2.667371
1	5.508487	2.034698	2.297974
1	3.937091	1.913553	3.116094
1	5.015110	3.286326	3.465166
6	2.513375	4.724719	2.116720
1	2.970291	5.403127	2.855912
1	1.775316	4.103804	2.648116
1	1.972328	5.344027	1.385648
6	5.189637	4.813947	0.653833
1	5.587227	5.392049	1.505015
1	4.816955	5.537693	-0.086550
1	6.038840	4.275667	0.204448
14	2.863766	3.383750	-1.756735
6	2.049188	5.084032	-1.588156
1	2.662161	5.803721	-1.024766
1	1.071117	5.007011	-1.087846
1	1.876081	5.509853	-2.590058
6	1.793028	2.329810	-2.893750
1	1.660741	2.836398	-3.864059
1	0.797777	2.129298	-2.469602
1	2.266751	1.356245	-3.087382
6	4.525178	3.581176	-2.637949
1	4.991114	2.602724	-2.831295
1	5.246418	4.204821	-2.091396
1	4.345140	4.058922	-3.615832
6	7.132259	-0.250949	-0.625625
6	7.677413	-1.115655	0.526815
1	8.774369	-1.201459	0.459923
1	7.261315	-2.133826	0.507415
1	7.430078	-0.672140	1.503996
6	7.511744	-0.894885	-1.971885
1	7.120066	-0.307372	-2.817025
1	7.119470	-1.918383	-2.063251
1	8.607416	-0.952271	-2.076616
6	7.803337	1.126674	-0.552121
1	7.476497	1.787780	-1.369514
1	8.895400	1.013812	-0.636792

1 7.598697 1.634529 0.402867

Table S8
B3PW91/def2-SVP
 TS-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	1.589052	0.306922	-0.480818
1	0.212250	1.965354	-1.211446
34	0.146602	0.336965	1.290294
14	-1.525832	-0.002358	-0.187423
1	-0.592719	1.892685	-1.132764
6	0.677124	-0.590334	-1.780521
6	-0.729541	-0.718982	-1.648002
6	1.319775	-0.926450	-3.082653
6	1.912694	0.062908	-3.885588
1	1.942184	1.092534	-3.524106
6	2.424746	-0.242920	-5.147673
1	2.871400	0.549389	-5.754230
6	2.360825	-1.548342	-5.635665
1	2.754137	-1.787964	-6.626815
6	1.791724	-2.546829	-4.842217
1	1.738921	-3.574667	-5.210996
6	1.279352	-2.241048	-3.582217
1	0.818307	-3.025520	-2.977794
6	-1.570257	-1.194689	-2.787810
6	-1.557065	-0.559501	-4.042860
1	-0.936495	0.327057	-4.185370
6	-2.307247	-1.055724	-5.107442
1	-2.276437	-0.544830	-6.073423
6	-3.092638	-2.199417	-4.945621
1	-3.676501	-2.590633	-5.782726
6	-3.128530	-2.834335	-3.704201
1	-3.740603	-3.728650	-3.560943
6	-2.377700	-2.333291	-2.639004
1	-2.391938	-2.844439	-1.674716
6	3.398240	0.306470	0.084678
6	3.919309	1.539260	0.592827
6	5.187948	1.547443	1.189531
1	5.562438	2.499257	1.570028
6	5.964647	0.396211	1.348894
6	5.449491	-0.788766	0.825786
1	6.022505	-1.709688	0.922001
6	4.205318	-0.866425	0.171829
6	3.175850	2.856597	0.550493
1	2.144025	2.679988	0.183926
14	3.881025	4.039277	-0.792860
6	5.717470	4.423470	-0.573382
1	6.027492	5.136762	-1.355323
1	6.334050	3.518984	-0.686341
1	5.947266	4.878291	0.401653
6	2.919382	5.668517	-0.809620
1	3.064712	6.265500	0.103862
1	1.838193	5.499902	-0.937037
1	3.260699	6.281307	-1.660481
6	3.661066	3.240326	-2.487939
1	2.592245	3.121426	-2.726111
1	4.136571	2.248543	-2.538296
1	4.111433	3.872558	-3.271031
14	2.893489	3.634352	2.294383
6	4.253572	4.846329	2.821379
1	4.337852	5.709080	2.142349

1	5.246130	4.375375	2.895287
1	4.005799	5.239870	3.821407
6	1.260426	4.580046	2.290376
1	0.418605	3.911557	2.054408
1	1.251424	5.408681	1.567005
1	1.075661	5.006259	3.290259
6	2.789056	2.285633	3.609522
1	2.571174	2.740949	4.589858
1	3.728595	1.720112	3.697939
1	1.984037	1.568732	3.385509
6	3.810037	-2.214183	-0.378420
1	2.857962	-2.112447	-0.933716
14	5.038414	-2.828209	-1.736095
6	4.373483	-4.418671	-2.513060
1	3.331741	-4.310194	-2.848910
1	4.425500	-5.270230	-1.816356
1	4.983109	-4.676504	-3.394759
6	6.798953	-3.207091	-1.142629
1	7.324387	-3.718211	-1.967366
1	6.851016	-3.862456	-0.262044
1	7.360334	-2.286136	-0.924880
6	5.225385	-1.490163	-3.045776
1	5.938042	-1.816049	-3.821345
1	5.617779	-0.563806	-2.596800
1	4.272407	-1.252826	-3.537785
14	3.373118	-3.490050	1.000193
6	2.034532	-4.646395	0.339171
1	1.710199	-5.345481	1.127121
1	2.386967	-5.245093	-0.514060
1	1.150692	-4.077199	0.012383
6	4.829966	-4.557473	1.567744
1	4.486908	-5.217743	2.381810
1	5.665350	-3.958144	1.961893
1	5.218277	-5.201081	0.763515
6	2.712972	-2.582832	2.514920
1	1.834525	-1.968913	2.261800
1	3.474102	-1.914582	2.946987
1	2.414521	-3.306041	3.291613
6	7.318692	0.473916	2.070657
6	7.986353	-0.900097	2.208927
1	7.363106	-1.602890	2.783276
1	8.943829	-0.796720	2.742825
1	8.204000	-1.356226	1.231593
6	7.112755	1.047716	3.485750
1	6.679140	2.058417	3.463315
1	8.075901	1.112102	4.017509
1	6.440544	0.407559	4.078366
6	8.263599	1.396252	1.276759
1	8.431366	1.009844	0.259225
1	9.242453	1.468753	1.778250
1	7.860078	2.415694	1.185385
6	-3.338557	-0.006511	0.347465
6	-3.837521	-0.961550	1.286899
6	-5.192674	-0.918631	1.643566
1	-5.550752	-1.666240	2.354852
6	-6.090570	0.021313	1.127263
6	-5.578121	0.957520	0.230503
1	-6.237267	1.715660	-0.190960
6	-4.229351	0.981501	-0.168072
6	-2.983848	-2.023052	1.936031
1	-1.949322	-1.932046	1.549741
14	-3.462539	-3.830626	1.435536
6	-1.876459	-4.695446	0.886037

1	-2.081885	-5.734215	0.580239
1	-1.137363	-4.727434	1.701826
1	-1.403881	-4.180907	0.035046
6	-4.717360	-3.839796	0.022983
1	-4.458260	-3.139361	-0.783998
1	-5.722809	-3.568160	0.378953
1	-4.777762	-4.854542	-0.404849
6	-4.220225	-4.887988	2.811194
1	-4.390308	-5.900308	2.407282
1	-5.195243	-4.503905	3.148492
1	-3.567660	-4.991855	3.691392
14	-2.731034	-1.691776	3.820799
6	-2.373595	0.139031	4.105641
1	-2.204552	0.321082	5.179981
1	-3.232084	0.753734	3.792396
1	-1.486603	0.496378	3.562210
6	-4.225811	-2.080786	4.915088
1	-4.532334	-3.135220	4.894968
1	-5.097162	-1.460738	4.654142
1	-3.954904	-1.833547	5.955471
6	-1.262947	-2.726156	4.407459
1	-0.353771	-2.488281	3.833268
1	-1.447813	-3.808144	4.316447
1	-1.051241	-2.515702	5.468599
6	-3.813210	2.090836	-1.101593
1	-2.767148	1.913115	-1.422716
14	-4.777482	2.146303	-2.771070
6	-5.387845	0.421731	-3.219599
1	-6.133309	0.055111	-2.497685
1	-4.561837	-0.304633	-3.249193
1	-5.858760	0.438168	-4.216277
6	-3.603429	2.762998	-4.116591
1	-4.120908	2.772997	-5.090029
1	-2.728890	2.101870	-4.211365
1	-3.240822	3.783090	-3.919942
6	-6.281642	3.300003	-2.768636
1	-6.777942	3.223747	-3.750773
1	-6.009566	4.356968	-2.622672
1	-7.028981	3.032034	-2.005672
14	-3.674886	3.759279	-0.148987
6	-2.943593	5.084230	-1.282623
1	-3.624040	5.358488	-2.103476
1	-1.989145	4.757774	-1.725380
1	-2.744470	5.998248	-0.699228
6	-2.525863	3.523101	1.325703
1	-2.406261	4.472746	1.872550
1	-1.526494	3.182497	1.016175
1	-2.928330	2.777528	2.028998
6	-5.317923	4.391763	0.540973
1	-5.727502	3.702671	1.295450
1	-6.084856	4.557078	-0.229082
1	-5.135518	5.356951	1.042920
6	-7.563211	0.009551	1.565352
6	-8.172544	-1.380140	1.300941
1	-9.233081	-1.395710	1.600005
1	-7.659859	-2.171468	1.867821
1	-8.116614	-1.640897	0.232582
6	-7.640085	0.325258	3.071571
1	-7.212445	1.316209	3.290354
1	-7.092280	-0.415956	3.672374
1	-8.687882	0.323983	3.413425
6	-8.401557	1.049947	0.811131
1	-8.049997	2.076454	0.995560

1	-9.449194	0.998021	1.146081
1	-8.392525	0.873910	-0.275643

Table S9
B3PW91/def2-SVP
 TS-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.609798	0.418402	-0.348299
1	0.197806	2.191817	-0.823623
34	0.075036	0.114495	1.423966
32	-1.601402	0.056179	-0.169628
1	-0.606338	2.129933	-0.802500
6	0.668269	-0.318452	-1.842187
6	-0.731934	-0.412990	-1.782794
6	1.380722	-0.464975	-3.137623
6	2.244585	0.530388	-3.628846
1	2.403560	1.435142	-3.039439
6	2.867353	0.400547	-4.870863
1	3.524549	1.198035	-5.227686
6	2.646152	-0.730938	-5.656339
1	3.128131	-0.830434	-6.632140
6	1.802682	-1.735999	-5.178213
1	1.623526	-2.632310	-5.778031
6	1.179956	-1.606067	-3.938635
1	0.512125	-2.394003	-3.584791
6	-1.563119	-0.574702	-3.011221
6	-1.460673	0.323093	-4.089657
1	-0.773083	1.168084	-4.014737
6	-2.207364	0.136164	-5.251095
1	-2.108058	0.845624	-6.076869
6	-3.075615	-0.952576	-5.364605
1	-3.656460	-1.101290	-6.278491
6	-3.198105	-1.845380	-4.299784
1	-3.875462	-2.700158	-4.373736
6	-2.452272	-1.653026	-3.135340
1	-2.534431	-2.363285	-2.310751
6	3.504617	0.231362	0.177687
6	4.141544	1.421101	0.645445
6	5.513681	1.384152	0.932045
1	5.981759	2.302097	1.292239
6	6.288795	0.227932	0.790782
6	5.628678	-0.930075	0.384037
1	6.187146	-1.860407	0.294329
6	4.251420	-0.975020	0.089731
6	3.404466	2.713733	0.928935
1	2.337614	2.582723	0.652384
14	3.914164	4.193505	-0.182465
6	5.731031	4.700331	-0.047879
1	5.887634	5.607759	-0.655018
1	6.397784	3.920730	-0.446273
1	6.044638	4.931667	0.980779
6	2.848185	5.699898	0.232842
1	3.059390	6.108103	1.233261
1	1.772942	5.466133	0.180436
1	3.049353	6.500786	-0.497824
6	3.599062	3.751202	-1.990261
1	2.533149	3.539117	-2.169170
1	4.184008	2.868948	-2.293390
1	3.889849	4.589289	-2.645075
14	3.287899	3.065334	2.824049
6	4.691116	4.153335	3.482042

1	4.691066	5.159876	3.035599
1	5.683875	3.706129	3.317465
1	4.565255	4.277352	4.570617
6	1.645965	3.918698	3.200480
1	0.799361	3.295754	2.871143
1	1.553723	4.902739	2.718053
1	1.545257	4.067980	4.288254
6	3.323800	1.437453	3.776671
1	3.229232	1.632676	4.857667
1	4.260341	0.883982	3.609834
1	2.487038	0.785823	3.480329
6	3.671826	-2.330288	-0.243855
1	2.623780	-2.209041	-0.579719
14	4.537070	-3.223063	-1.723228
6	3.295494	-4.363626	-2.575904
1	2.979775	-5.195475	-1.929578
1	3.758020	-4.797380	-3.477907
1	2.398105	-3.814567	-2.895275
6	6.008076	-4.316970	-1.232234
1	6.419695	-4.766277	-2.151740
1	5.717311	-5.144908	-0.567524
1	6.827045	-3.763056	-0.748075
6	5.171089	-1.954728	-2.962065
1	5.609940	-2.468871	-3.832892
1	5.946437	-1.309255	-2.521752
1	4.359100	-1.307995	-3.325507
14	3.519577	-3.411348	1.349412
6	2.756070	-5.093706	0.940050
1	2.541948	-5.628028	1.880548
1	3.422748	-5.734486	0.343043
1	1.804967	-4.989189	0.394303
6	5.167735	-3.697622	2.232515
1	4.985702	-4.352758	3.101142
1	5.580823	-2.751555	2.614653
1	5.931959	-4.179746	1.606497
6	2.397246	-2.561575	2.600280
1	1.381360	-2.414435	2.205065
1	2.790537	-1.573312	2.883787
1	2.326911	-3.172195	3.515688
6	7.792671	0.262329	1.104937
6	8.470814	-1.091217	0.857301
1	8.053865	-1.885443	1.495158
1	9.545233	-1.016272	1.086516
1	8.378903	-1.409633	-0.192534
6	7.994942	0.639918	2.585104
1	7.569382	1.627254	2.818261
1	9.068800	0.673398	2.831494
1	7.516935	-0.096457	3.249995
6	8.477123	1.312837	0.210167
1	8.342730	1.072271	-0.856103
1	9.559088	1.348480	0.417238
1	8.074406	2.322214	0.379903
6	-3.495590	-0.029384	0.342703
6	-4.015769	-1.171681	1.016649
6	-5.384426	-1.195743	1.324787
1	-5.775176	-2.086477	1.822208
6	-6.254446	-0.141293	1.024892
6	-5.704330	0.979541	0.403762
1	-6.340109	1.832032	0.167857
6	-4.344987	1.071128	0.051296
6	-3.176563	-2.352877	1.439012
1	-2.129238	-2.172342	1.125422
14	-3.596898	-4.008082	0.530166

6	-1.968678	-4.705073	-0.131162
1	-2.141168	-5.637402	-0.693286
1	-1.275178	-4.935705	0.693379
1	-1.459398	-3.994456	-0.801129
6	-4.806896	-3.709704	-0.889109
1	-4.526940	-2.855582	-1.522047
1	-5.818730	-3.508247	-0.505310
1	-4.863189	-4.608799	-1.525124
6	-4.385456	-5.352504	1.605189
1	-4.505525	-6.258089	0.986949
1	-5.387251	-5.068430	1.963202
1	-3.775096	-5.629602	2.477908
14	-2.994940	-2.451424	3.357785
6	-2.584820	-0.743913	4.045626
1	-2.492202	-0.796108	5.143115
1	-3.385208	-0.024921	3.810077
1	-1.640738	-0.342448	3.648336
6	-4.552129	-3.011437	4.274618
1	-4.933384	-3.990126	3.952611
1	-5.362688	-2.273053	4.180041
1	-4.307988	-3.086998	5.347709
6	-1.586462	-3.644717	3.760101
1	-0.642219	-3.315915	3.298907
1	-1.790223	-4.672250	3.420794
1	-1.427065	-3.683169	4.850212
6	-3.877553	2.350181	-0.596825
1	-2.825893	2.216304	-0.923251
14	-4.778663	2.791511	-2.244709
6	-5.393985	1.220680	-3.083189
1	-6.171586	0.719073	-2.487309
1	-4.576001	0.502107	-3.243738
1	-5.825079	1.465802	-4.067814
6	-3.541154	3.650358	-3.385028
1	-4.023783	3.893242	-4.346015
1	-2.685357	2.992084	-3.599858
1	-3.153729	4.587760	-2.958853
6	-6.262778	3.949891	-2.031389
1	-6.702988	4.143330	-3.023946
1	-5.983510	4.924310	-1.602027
1	-7.056480	3.516144	-1.403317
14	-3.723417	3.774637	0.692517
6	-3.019907	5.321299	-0.138196
1	-3.706848	5.758536	-0.879057
1	-2.063558	5.110067	-0.642548
1	-2.827668	6.090554	0.627950
6	-2.535568	3.249882	2.057983
1	-2.439899	4.055906	2.804138
1	-1.530896	3.030470	1.666088
1	-2.892247	2.349119	2.580868
6	-5.363268	4.222020	1.519572
1	-5.750833	3.384918	2.119917
1	-6.143136	4.525461	0.806000
1	-5.191626	5.067898	2.206291
6	-7.745478	-0.242348	1.384290
6	-8.357629	-1.470723	0.684291
1	-9.430346	-1.553902	0.923137
1	-7.875751	-2.407837	1.000558
1	-8.258034	-1.394041	-0.409705
6	-7.893159	-0.395302	2.909996
1	-7.458323	0.467421	3.438535
1	-7.393931	-1.302631	3.280914
1	-8.957185	-0.463807	3.189083
6	-8.534878	0.998764	0.947776

1	-8.171984	1.913797	1.440365
1	-9.595288	0.878983	1.219241
1	-8.489116	1.153424	-0.141256

Table S10
B3PW91/def2-SVP
 TS-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	-1.744365	-0.014854	-0.336511
1	-0.689102	-1.725890	-1.264078
34	-0.145425	-0.303045	1.549649
50	1.701834	-0.535660	-0.320942
1	0.161779	-1.826898	-1.195550
6	-0.605600	1.055060	-1.806375
6	0.752215	0.909905	-1.717327
6	-1.280043	1.667475	-2.984174
6	-1.604899	0.897062	-4.113974
1	-1.391035	-0.174464	-4.110470
6	-2.172089	1.487093	-5.243312
1	-2.412011	0.869467	-6.112806
6	-2.422045	2.860296	-5.269530
1	-2.858127	3.324016	-6.157935
6	-2.110101	3.636382	-4.152510
1	-2.298325	4.713134	-4.164970
6	-1.552894	3.044823	-3.017821
1	-1.303554	3.657382	-2.147511
6	1.597994	1.355515	-2.858625
6	2.121309	0.422383	-3.772238
1	1.900544	-0.639828	-3.634964
6	2.885955	0.834606	-4.864223
1	3.271779	0.088704	-5.564146
6	3.152450	2.189075	-5.067090
1	3.751740	2.512637	-5.921750
6	2.642603	3.126057	-4.167039
1	2.842660	4.190885	-4.313380
6	1.874328	2.716069	-3.077850
1	1.479508	3.459534	-2.383154
6	-3.819555	-0.412902	0.151116
6	-4.209221	-1.754632	0.400910
6	-5.502447	-1.977565	0.899200
1	-5.798139	-3.010505	1.092754
6	-6.402017	-0.942528	1.177949
6	-5.983089	0.360439	0.905131
1	-6.653662	1.194810	1.103524
6	-4.711031	0.660178	0.379089
6	-3.318788	-2.948955	0.164723
1	-2.306294	-2.589657	-0.105159
14	-3.827803	-3.900720	-1.425979
6	-5.574323	-4.615922	-1.352537
1	-5.768045	-5.178909	-2.280873
1	-6.333556	-3.822198	-1.283918
1	-5.719045	-5.306687	-0.508406
6	-2.608285	-5.304119	-1.769341
1	-2.651458	-6.102763	-1.012815
1	-1.570210	-4.938513	-1.817905
1	-2.844664	-5.761020	-2.744579
6	-3.757603	-2.704626	-2.886309
1	-2.735375	-2.326154	-3.046163
1	-4.420121	-1.837846	-2.737053
1	-4.072058	-3.212715	-3.812901
14	-2.956996	-3.992238	1.747577

6	-4.146489	-5.447868	1.982034
1	-4.094055	-6.170837	1.153005
1	-5.195408	-5.129257	2.088488
1	-3.874343	-5.986315	2.905133
6	-1.202255	-4.672303	1.611445
1	-0.477009	-3.846994	1.528703
1	-1.070052	-5.336087	0.743972
1	-0.949065	-5.248635	2.516410
6	-3.056272	-2.889251	3.272122
1	-2.790342	-3.467503	4.172351
1	-4.065230	-2.474931	3.418269
1	-2.350154	-2.047858	3.189892
6	-4.379208	2.107423	0.107542
1	-3.367693	2.167495	-0.348559
14	-5.488341	2.838982	-1.292669
6	-4.952065	4.611107	-1.670489
1	-3.869725	4.686596	-1.851003
1	-5.215956	5.304156	-0.856194
1	-5.465990	4.961140	-2.580851
6	-7.339211	2.887408	-0.897867
1	-7.840711	3.456758	-1.698772
1	-7.578816	3.379813	0.055902
1	-7.781104	1.879865	-0.889369
6	-5.288909	1.757232	-2.821522
1	-5.908441	2.143814	-3.647234
1	-5.616185	0.726642	-2.611143
1	-4.247545	1.719808	-3.174821
14	-4.183723	3.152087	1.719872
6	-2.927953	4.529094	1.410918
1	-2.770551	5.101765	2.339877
1	-3.255014	5.237927	0.635744
1	-1.950691	4.120563	1.108044
6	-5.801655	3.941626	2.299832
1	-5.619480	4.484072	3.242361
1	-6.585835	3.194344	2.497442
1	-6.196260	4.667674	1.572182
6	-3.531177	2.050363	3.103029
1	-2.563312	1.595596	2.837713
1	-4.230555	1.234200	3.340622
1	-3.379623	2.646358	4.018003
6	-7.786849	-1.265821	1.761515
6	-8.613895	-0.002804	2.033572
1	-8.120359	0.663553	2.757767
1	-9.591100	-0.282141	2.457308
1	-8.806516	0.571791	1.115013
6	-7.617196	-2.023128	3.092479
1	-7.074222	-2.970932	2.962200
1	-8.601868	-2.261676	3.526134
1	-7.062062	-1.416845	3.825251
6	-8.563844	-2.147081	0.764777
1	-8.689502	-1.634383	-0.201760
1	-9.566414	-2.381383	1.158005
1	-8.051085	-3.101516	0.574253
6	3.734238	-0.036826	0.424682
6	4.026862	1.058112	1.281092
6	5.360817	1.273937	1.666962
1	5.570667	2.135900	2.305187
6	6.414463	0.443137	1.271795
6	6.088871	-0.652694	0.473346
1	6.872644	-1.339668	0.154958
6	4.776036	-0.916979	0.036210
6	2.981257	2.002677	1.822665
1	1.992810	1.697789	1.430606

14	3.142791	3.803372	1.161621
6	1.396577	4.425762	0.784911
1	1.425874	5.425082	0.320446
1	0.788888	4.498857	1.700312
1	0.878210	3.739535	0.096011
6	4.179214	3.820017	-0.413205
1	3.811838	3.096892	-1.156316
1	5.228601	3.567504	-0.197270
1	4.159044	4.822575	-0.871820
6	3.940883	5.035363	2.358207
1	3.990813	6.021661	1.866906
1	4.970256	4.752183	2.628760
1	3.364865	5.160024	3.288035
14	2.737304	1.774686	3.718508
6	2.618364	-0.066017	4.123473
1	2.493456	-0.204670	5.210250
1	3.541048	-0.586673	3.821927
1	1.771470	-0.559385	3.623281
6	4.148113	2.436846	4.793968
1	4.356859	3.505173	4.643685
1	5.080347	1.874820	4.631827
1	3.866362	2.298547	5.851568
6	1.142326	2.648744	4.233097
1	0.288912	2.297218	3.632174
1	1.213302	3.742517	4.121802
1	0.918517	2.438610	5.291891
6	4.575088	-2.152344	-0.818075
1	3.538389	-2.154477	-1.213817
14	5.632241	-2.183324	-2.426464
6	6.003391	-0.425440	-2.998174
1	6.635687	0.112795	-2.276252
1	5.080710	0.159015	-3.134542
1	6.534483	-0.450023	-3.964287
6	4.633228	-3.052824	-3.778759
1	5.196388	-3.045027	-4.726574
1	3.674979	-2.539912	-3.958131
1	4.412029	-4.101914	-3.531437
6	7.285434	-3.094910	-2.259481
1	7.818750	-3.040608	-3.223387
1	7.163696	-4.161043	-2.012448
1	7.942172	-2.643622	-1.499139
14	4.588834	-3.750617	0.251413
6	4.255120	-5.266782	-0.831332
1	5.062424	-5.463651	-1.553735
1	3.312544	-5.163518	-1.392503
1	4.161535	-6.159598	-0.191053
6	3.210870	-3.643243	1.536280
1	3.207142	-4.547653	2.166911
1	2.218640	-3.560913	1.064813
1	3.342240	-2.773102	2.198003
6	6.212301	-4.013831	1.181729
1	6.398030	-3.198586	1.897542
1	7.084118	-4.091951	0.515407
1	6.146153	-4.952666	1.756786
6	7.853607	0.749643	1.717024
6	8.249999	2.156497	1.229903
1	9.282386	2.393240	1.535117
1	7.594467	2.935827	1.646214
1	8.195890	2.224581	0.132063
6	7.937546	0.697324	3.254138
1	7.655032	-0.297738	3.632167
1	7.273354	1.436393	3.726072
1	8.964849	0.910078	3.592716

6	8.864206	-0.254779	1.148055
1	8.660379	-1.282039	1.487116
1	9.879562	0.006692	1.484778
1	8.870975	-0.251524	0.047092

Table S11
B3PW91/def2-SVP
 Prod-C

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.321009	0.321544	-0.172276
1	1.113824	1.400679	-0.219565
34	0.045577	-0.237304	1.246391
6	-1.335866	0.251161	-0.097021
1	-1.245723	1.347787	-0.091339
6	0.661337	-0.193490	-1.461684
6	-0.705186	-0.143818	-1.441734
6	1.436754	-0.421671	-2.704094
6	2.544588	0.374606	-3.048714
1	2.928927	1.105724	-2.337780
6	3.155686	0.256787	-4.297844
1	4.000943	0.904308	-4.544978
6	2.699795	-0.683232	-5.222196
1	3.179479	-0.774799	-6.199940
6	1.643281	-1.526884	-4.870984
1	1.294402	-2.290563	-5.570830
6	1.025442	-1.400894	-3.629481
1	0.193989	-2.058833	-3.372986
6	-1.546717	-0.080802	-2.671552
6	-1.188972	0.800098	-3.711606
1	-0.314446	1.441203	-3.588167
6	-1.915358	0.854364	-4.898978
1	-1.605504	1.542508	-5.689708
6	-3.028999	0.031366	-5.079521
1	-3.593775	0.062667	-6.014796
6	-3.429272	-0.809569	-4.041621
1	-4.316702	-1.437407	-4.155196
6	-2.708614	-0.850540	-2.846777
1	-3.050778	-1.497959	-2.041968
6	2.805704	0.242181	0.126283
6	3.472280	1.484945	0.398544
6	4.873414	1.518480	0.407938
1	5.354886	2.483136	0.574274
6	5.668130	0.380466	0.237783
6	4.994771	-0.832855	0.132152
1	5.568079	-1.758025	0.079303
6	3.591395	-0.945925	0.099312
6	2.761164	2.786931	0.758042
1	1.690940	2.591771	0.950745
14	2.744546	4.134240	-0.619011
6	4.407923	4.268923	-1.501106
1	4.330120	5.009382	-2.314319
1	4.720156	3.311303	-1.944426
1	5.209030	4.603683	-0.823563
6	2.296055	5.849874	0.045224
1	3.006449	6.239288	0.789489
1	1.290010	5.865670	0.492462
1	2.287751	6.555575	-0.802218
6	1.402845	3.749252	-1.897092
1	0.408941	3.705722	-1.422914
1	1.565558	2.803995	-2.433769
1	1.370222	4.555137	-2.649106

14	3.283801	3.406083	2.514000
6	4.862567	4.453986	2.546155
1	4.828009	5.304729	1.848874
1	5.762822	3.863919	2.317085
1	4.994346	4.865279	3.560859
6	1.882253	4.435046	3.258046
1	0.932160	3.877603	3.252987
1	1.720387	5.393388	2.744891
1	2.124194	4.659977	4.310184
6	3.533399	1.925021	3.653856
1	3.809129	2.269153	4.664382
1	4.326998	1.254515	3.292367
1	2.603942	1.340821	3.740981
6	3.041151	-2.354906	0.130741
1	1.949537	-2.345849	-0.041304
14	3.754284	-3.595985	-1.180734
6	2.348244	-4.722704	-1.746431
1	1.580748	-4.146880	-2.284853
1	1.860375	-5.243561	-0.908598
1	2.734191	-5.489427	-2.438074
6	5.149868	-4.722545	-0.556510
1	5.401870	-5.412721	-1.379472
1	4.886755	-5.337134	0.316188
1	6.067801	-4.163462	-0.316266
6	4.482257	-2.741088	-2.690750
1	4.821527	-3.511816	-3.402980
1	5.349272	-2.113815	-2.436348
1	3.748077	-2.107688	-3.202852
14	3.224380	-3.051531	1.931490
6	2.424441	-4.763581	2.035061
1	2.413799	-5.099911	3.084736
1	2.960054	-5.524656	1.448691
1	1.380575	-4.740831	1.686781
6	5.014718	-3.167798	2.536107
1	4.997168	-3.614219	3.544911
1	5.459992	-2.165596	2.631283
1	5.677162	-3.783416	1.913655
6	2.393897	-1.933663	3.202777
1	1.302938	-1.882544	3.084902
1	2.791942	-0.909448	3.148338
1	2.607193	-2.320088	4.213448
6	7.200274	0.493411	0.213605
6	7.879194	-0.867406	0.011629
1	7.653021	-1.567197	0.830653
1	8.972375	-0.738016	-0.017228
1	7.577346	-1.339304	-0.935960
6	7.698274	1.085894	1.545565
1	7.290763	2.091562	1.726057
1	8.797353	1.169590	1.543937
1	7.407907	0.449398	2.395997
6	7.619584	1.417214	-0.945698
1	7.281906	1.013613	-1.913121
1	8.716806	1.516062	-0.983074
1	7.197221	2.427354	-0.838742
6	-2.798861	-0.033387	0.207549
6	-3.324303	-1.332742	0.502427
6	-4.714257	-1.487885	0.630710
1	-5.087215	-2.491598	0.835446
6	-5.626387	-0.432582	0.542923
6	-5.087103	0.833590	0.341756
1	-5.749703	1.697725	0.303775
6	-3.711425	1.068918	0.165394
6	-2.485882	-2.564928	0.813928

1	-1.413210	-2.318881	0.716761
14	-2.680360	-4.122856	-0.311190
6	-1.571544	-4.007769	-1.837600
1	-1.513543	-4.998581	-2.317837
1	-0.549974	-3.717939	-1.549888
1	-1.928123	-3.292256	-2.590461
6	-4.450181	-4.439954	-0.898581
1	-4.866379	-3.587915	-1.457138
1	-5.138783	-4.673758	-0.071570
1	-4.440432	-5.310601	-1.575475
6	-2.093208	-5.700255	0.558892
1	-2.213736	-6.538439	-0.147493
1	-2.658635	-5.952123	1.467536
1	-1.025737	-5.648355	0.822545
14	-2.681433	-2.943993	2.706542
6	-2.796259	-1.327039	3.675529
1	-2.915651	-1.551182	4.748680
1	-3.658168	-0.722153	3.356202
1	-1.888013	-0.714110	3.564027
6	-4.236435	-3.942331	3.132987
1	-4.346583	-4.865906	2.544963
1	-5.153290	-3.347319	3.010010
1	-4.180151	-4.234865	4.194989
6	-1.194232	-3.888622	3.386985
1	-0.248495	-3.387465	3.135728
1	-1.135950	-4.926372	3.031562
1	-1.269655	-3.918166	4.486807
6	-3.334580	2.529731	-0.025660
1	-2.295161	2.632283	-0.379239
14	-4.282648	3.474080	-1.421853
6	-4.945151	2.305437	-2.739652
1	-5.706954	1.618176	-2.343390
1	-4.141748	1.697380	-3.178612
1	-5.406562	2.895424	-3.549135
6	-3.046361	4.641679	-2.250641
1	-3.545291	5.222543	-3.043790
1	-2.228293	4.073401	-2.722014
1	-2.600211	5.357696	-1.544340
6	-5.750825	4.511498	-0.820647
1	-6.191631	5.023228	-1.692643
1	-5.470721	5.288346	-0.093330
1	-6.545789	3.896184	-0.370656
14	-3.284897	3.459921	1.662230
6	-2.664552	5.230102	1.400386
1	-3.351537	5.848111	0.802915
1	-1.679631	5.243970	0.906463
1	-2.547416	5.721313	2.380499
6	-2.081545	2.602591	2.831877
1	-1.988873	3.185328	3.763475
1	-1.075151	2.486407	2.401070
1	-2.437153	1.596823	3.100895
6	-4.952009	3.516527	2.550587
1	-5.308883	2.503894	2.793036
1	-5.738160	4.031944	1.980731
1	-4.821081	4.057065	3.503061
6	-7.136312	-0.684843	0.678177
6	-7.590877	-1.652025	-0.431215
1	-8.672982	-1.847174	-0.353058
1	-7.072609	-2.620104	-0.368967
1	-7.393615	-1.229252	-1.428836
6	-7.438064	-1.307039	2.054059
1	-7.104759	-0.646742	2.869940
1	-6.939488	-2.278966	2.183644

1	-8.521010	-1.474154	2.172402
6	-7.953934	0.607478	0.550409
1	-7.701276	1.335375	1.336764
1	-9.027124	0.379875	0.646193
1	-7.807461	1.093492	-0.426562

Table S12
B3PW91/def2-SVP
 Prod-Si

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
14	1.586520	0.188507	-0.831085
1	1.421734	1.113457	-1.994182
34	0.210702	0.938880	0.861320
14	-1.531342	0.157551	-0.424382
1	-1.534338	1.089843	-1.586989
6	0.621324	-1.349277	-1.472827
6	-0.724415	-1.382809	-1.240555
6	1.233672	-2.268326	-2.475744
6	1.845267	-1.739189	-3.626103
1	1.936184	-0.656088	-3.740714
6	2.304149	-2.575352	-4.644802
1	2.759482	-2.137977	-5.537184
6	2.180642	-3.960153	-4.527518
1	2.537135	-4.615682	-5.326031
6	1.599874	-4.500419	-3.378682
1	1.499752	-5.583879	-3.273437
6	1.132431	-3.665452	-2.364519
1	0.663746	-4.099525	-1.479593
6	-1.618035	-2.362369	-1.925763
6	-1.799306	-2.328753	-3.318848
1	-1.288272	-1.562411	-3.906251
6	-2.598439	-3.276163	-3.958325
1	-2.719420	-3.236118	-5.044003
6	-3.233762	-4.276227	-3.220078
1	-3.854960	-5.021880	-3.722612
6	-3.075147	-4.311265	-1.833953
1	-3.571148	-5.085767	-1.243244
6	-2.282719	-3.357685	-1.193730
1	-2.152813	-3.399827	-0.110906
6	3.375704	0.365429	-0.192408
6	3.859470	1.712958	-0.088800
6	5.089325	1.952262	0.540510
1	5.435092	2.986479	0.594470
6	5.860445	0.944932	1.125745
6	5.387955	-0.358835	0.992354
1	5.962867	-1.182570	1.412800
6	4.192796	-0.680985	0.320389
6	3.134820	2.935858	-0.618012
1	2.104907	2.675122	-0.912996
14	3.898067	3.526376	-2.281958
6	5.721279	3.999989	-2.138320
1	6.073497	4.368002	-3.116476
1	6.340962	3.131391	-1.868313
1	5.901915	4.794295	-1.399329
6	2.935573	5.007056	-2.963372
1	3.027472	5.907350	-2.336378
1	1.863360	4.778229	-3.072920
1	3.322640	5.261910	-3.963976
6	3.786321	2.145064	-3.568528
1	2.742957	1.944728	-3.857696
1	4.225743	1.205504	-3.198457

1	4.335348	2.437948	-4.478874
14	2.806790	4.306938	0.699864
6	4.127706	5.666479	0.764148
1	4.226359	6.213587	-0.186147
1	5.123370	5.284393	1.039127
1	3.837842	6.399778	1.535297
6	1.154724	5.125775	0.291829
1	0.339163	4.385611	0.310761
1	1.155475	5.607147	-0.697661
1	0.921728	5.901015	1.040231
6	2.689646	3.560247	2.429103
1	2.408941	4.345255	3.150852
1	3.644237	3.122246	2.756329
1	1.924017	2.770801	2.473467
6	3.886837	-2.154501	0.178804
1	2.968384	-2.286057	-0.422429
14	5.229976	-3.032314	-0.899425
6	4.725233	-4.823078	-1.228027
1	3.704137	-4.896297	-1.629594
1	4.787599	-5.440370	-0.318012
1	5.410037	-5.263448	-1.971507
6	6.970570	-3.094498	-0.151092
1	7.579055	-3.762990	-0.783865
1	7.006425	-3.489416	0.874230
1	7.457136	-2.108012	-0.160132
6	5.409187	-2.100285	-2.527989
1	6.184955	-2.573704	-3.152225
1	5.714228	-1.058159	-2.342866
1	4.471639	-2.088183	-3.101400
14	3.448806	-3.003539	1.850457
6	2.264021	-4.435690	1.510505
1	1.954168	-4.904793	2.458395
1	2.723259	-5.214795	0.883965
1	1.353947	-4.083423	1.001714
6	4.932332	-3.713340	2.788834
1	4.577138	-4.116201	3.752144
1	5.698889	-2.955850	3.013840
1	5.414604	-4.540114	2.245006
6	2.605851	-1.750773	2.977784
1	1.733687	-1.289745	2.488278
1	3.294955	-0.938638	3.256903
1	2.263958	-2.238922	3.904938
6	7.162293	1.296649	1.861686
6	7.821315	0.067156	2.500182
1	7.159917	-0.416568	3.235532
1	8.738467	0.368787	3.029876
1	8.108846	-0.685512	1.750945
6	6.861824	2.310761	2.982171
1	6.434992	3.246228	2.591260
1	7.786763	2.569766	3.522530
1	6.148429	1.895509	3.711195
6	8.156708	1.917449	0.862215
1	8.390906	1.212924	0.048800
1	9.100384	2.178513	1.368466
1	7.758823	2.835690	0.405170
6	-3.288665	0.171132	0.317099
6	-3.581242	-0.234027	1.657674
6	-4.897025	-0.153036	2.136422
1	-5.081320	-0.480230	3.162386
6	-5.963155	0.321053	1.368880
6	-5.661868	0.731731	0.072861
1	-6.457643	1.116315	-0.563789
6	-4.368791	0.673056	-0.480082

6	-2.545948	-0.731792	2.639353
1	-1.557904	-0.774845	2.145952
14	-2.814691	-2.561704	3.202737
6	-1.169007	-3.458840	2.977366
1	-1.251658	-4.516436	3.276243
1	-0.376406	-2.997559	3.586622
1	-0.832183	-3.429735	1.929813
6	-4.141973	-3.413194	2.160075
1	-4.051430	-3.186045	1.088161
1	-5.152532	-3.107709	2.470481
1	-4.068250	-4.505654	2.292183
6	-3.334266	-2.808082	5.006474
1	-3.409949	-3.892803	5.192872
1	-4.320258	-2.370451	5.225589
1	-2.609609	-2.401727	5.728597
14	-2.235237	0.562889	4.041756
6	-2.176295	2.304652	3.313734
1	-1.970917	3.029980	4.118566
1	-3.147399	2.568085	2.865525
1	-1.401836	2.431694	2.543345
6	-3.574693	0.651523	5.378177
1	-3.690563	-0.271668	5.961648
1	-4.555853	0.925190	4.961633
1	-3.289147	1.453126	6.080322
6	-0.593550	0.150169	4.878156
1	0.234535	0.144017	4.152771
1	-0.616696	-0.833498	5.373529
1	-0.360703	0.902674	5.649294
6	-4.253051	1.189670	-1.901003
1	-3.267541	0.933028	-2.319847
14	-5.446058	0.352406	-3.163024
6	-5.825621	-1.413840	-2.624262
1	-6.393049	-1.442974	-1.682064
1	-4.901181	-1.992976	-2.478002
1	-6.423602	-1.922446	-3.398514
6	-4.571488	0.287385	-4.838880
1	-5.213555	-0.219510	-5.577968
1	-3.632750	-0.283809	-4.767830
1	-4.334600	1.286849	-5.232968
6	-7.094660	1.252004	-3.417261
1	-7.684213	0.701162	-4.169190
1	-6.963658	2.278815	-3.792048
1	-7.701693	1.299595	-2.499951
14	-4.231555	3.116724	-1.921344
6	-4.014996	3.753550	-3.691028
1	-4.877397	3.530037	-4.337766
1	-3.114222	3.333204	-4.166372
1	-3.894999	4.849453	-3.669679
6	-2.777515	3.759728	-0.903682
1	-2.821480	4.860246	-0.849738
1	-1.808007	3.485683	-1.346178
1	-2.796210	3.375065	0.127865
6	-5.796392	3.883830	-1.188764
1	-5.894284	3.646698	-0.118412
1	-6.716852	3.563187	-1.698030
1	-5.728908	4.980868	-1.280647
6	-7.380317	0.390403	1.958230
6	-7.789240	-0.994872	2.492811
1	-8.809656	-0.959199	2.907480
1	-7.121061	-1.342913	3.294432
1	-7.774895	-1.749667	1.691120
6	-7.394237	1.409477	3.113802
1	-7.108034	2.412440	2.760601

1	-6.697030	1.125816	3.916243
1	-8.401586	1.478976	3.555927
6	-8.421415	0.826000	0.918808
1	-8.221655	1.836517	0.531015
1	-9.421597	0.844876	1.379089
1	-8.463368	0.132148	0.064949

Table S13
B3PW91/def2-SVP
 Prod-Ge

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.639204	0.158299	-0.844912
1	1.469629	1.071024	-2.084491
34	0.220898	1.029467	0.858401
32	-1.582066	0.172370	-0.425255
1	-1.564029	1.083701	-1.672449
6	0.602740	-1.450445	-1.431896
6	-0.734927	-1.467591	-1.197580
6	1.220622	-2.421172	-2.378376
6	1.762717	-1.961388	-3.592025
1	1.795250	-0.888158	-3.796867
6	2.224412	-2.857198	-4.556660
1	2.626470	-2.475383	-5.498732
6	2.172434	-4.231949	-4.322037
1	2.531849	-4.934693	-5.077899
6	1.659055	-4.700721	-3.111752
1	1.613387	-5.775349	-2.916571
6	1.188175	-3.806599	-2.150139
1	0.768580	-4.185448	-1.216291
6	-1.629107	-2.491174	-1.809148
6	-1.835430	-2.534978	-3.198597
1	-1.345907	-1.794552	-3.835409
6	-2.631887	-3.526254	-3.771555
1	-2.772865	-3.546060	-4.855379
6	-3.239006	-4.493598	-2.969010
1	-3.858576	-5.273383	-3.419001
6	-3.053534	-4.453106	-1.586310
1	-3.526875	-5.202250	-0.946357
6	-2.263165	-3.456632	-1.012468
1	-2.112184	-3.438789	0.068433
6	3.494214	0.359561	-0.172984
6	3.996594	1.698186	-0.138421
6	5.236106	1.940634	0.472301
1	5.601665	2.969566	0.479174
6	5.990064	0.944249	1.097299
6	5.487225	-0.353526	1.033372
1	6.044875	-1.167051	1.494097
6	4.278551	-0.682324	0.388144
6	3.284432	2.905947	-0.714476
1	2.256151	2.637952	-1.008001
14	4.055752	3.439012	-2.393456
6	5.873034	3.937785	-2.260046
1	6.224429	4.276114	-3.249155
1	6.500636	3.084885	-1.959902
1	6.043760	4.758125	-1.547649
6	3.079178	4.880650	-3.134122
1	3.157175	5.802649	-2.537662
1	2.010398	4.634475	-3.239320
1	3.467467	5.105802	-4.141295
6	3.967595	2.000738	-3.617898
1	2.928892	1.773813	-3.904187

1	4.413437	1.084526	-3.199641
1	4.520382	2.254811	-4.537516
14	2.949660	4.316380	0.559811
6	4.270206	5.677124	0.587430
1	4.372300	6.194894	-0.378812
1	5.264436	5.302047	0.877278
1	3.978398	6.433607	1.335052
6	1.296723	5.117194	0.121146
1	0.485481	4.372980	0.162561
1	1.298398	5.565868	-0.883517
1	1.058087	5.915025	0.843523
6	2.828894	3.619873	2.309531
1	2.548078	4.425593	3.008036
1	3.783002	3.190762	2.650146
1	2.061978	2.833043	2.376365
6	3.918760	-2.149984	0.344746
1	2.984651	-2.284861	-0.231811
14	5.207718	-3.158119	-0.682002
6	4.704397	-4.978756	-0.763363
1	3.666531	-5.106434	-1.103579
1	4.816861	-5.482585	0.209271
1	5.357427	-5.501104	-1.482038
6	6.982630	-3.118062	-0.019675
1	7.569563	-3.852471	-0.597120
1	7.073848	-3.385867	1.042969
1	7.449611	-2.133808	-0.172227
6	5.290630	-2.448524	-2.425083
1	6.058105	-2.978169	-3.013461
1	5.562505	-1.381239	-2.401052
1	4.331795	-2.545842	-2.953572
14	3.479943	-2.865706	2.078960
6	2.260375	-4.292892	1.860619
1	1.931156	-4.661698	2.845608
1	2.700659	-5.140151	1.314657
1	1.362814	-3.964904	1.314434
6	4.969234	-3.531627	3.040664
1	4.625063	-3.882602	4.027903
1	5.738809	-2.764079	3.216218
1	5.445970	-4.386167	2.535900
6	2.671414	-1.517708	3.117087
1	1.789929	-1.093682	2.610181
1	3.371127	-0.690157	3.311586
1	2.347275	-1.923782	4.089190
6	7.309618	1.298636	1.800450
6	7.929317	0.092351	2.518056
1	7.255550	-0.316362	3.287073
1	8.859547	0.396978	3.022702
1	8.185920	-0.719197	1.820885
6	7.059298	2.397499	2.850725
1	6.662895	3.319571	2.400699
1	7.999713	2.658005	3.362873
1	6.340189	2.059925	3.613396
6	8.316142	1.811860	0.752878
1	8.516232	1.045353	-0.012165
1	9.274310	2.072093	1.231834
1	7.945958	2.710731	0.237559
6	-3.408926	0.222016	0.345032
6	-3.680724	-0.121209	1.702522
6	-4.997059	-0.033563	2.180943
1	-5.174114	-0.316566	3.221171
6	-6.070940	0.390889	1.394597
6	-5.779222	0.746670	0.079800
1	-6.580622	1.092178	-0.572429

6	-4.486323	0.676546	-0.473524
6	-2.630795	-0.560592	2.694583
1	-1.646987	-0.611176	2.193014
14	-2.864969	-2.367016	3.338520
6	-1.194257	-3.230965	3.174674
1	-1.256719	-4.281755	3.501067
1	-0.425868	-2.733472	3.786773
1	-0.836544	-3.221135	2.133589
6	-4.158435	-3.290604	2.315535
1	-4.046175	-3.119793	1.235096
1	-5.178642	-2.979808	2.587081
1	-4.076778	-4.373599	2.507191
6	-3.403283	-2.537825	5.145273
1	-3.454425	-3.612949	5.386984
1	-4.402105	-2.113707	5.330204
1	-2.697609	-2.075445	5.852234
14	-2.318265	0.796834	4.033247
6	-2.244713	2.497045	3.215913
1	-2.044296	3.265661	3.980764
1	-3.210704	2.737518	2.744227
1	-1.462056	2.577840	2.447051
6	-3.667067	0.954663	5.353904
1	-3.810483	0.052085	5.963434
1	-4.636937	1.237885	4.917481
1	-3.371618	1.770242	6.035715
6	-0.683759	0.415071	4.898261
1	0.146600	0.358976	4.177419
1	-0.719614	-0.538120	5.449421
1	-0.445184	1.208137	5.625775
6	-4.368124	1.120194	-1.917299
1	-3.365791	0.877886	-2.303978
14	-5.503754	0.160159	-3.142127
6	-5.818187	-1.583738	-2.499621
1	-6.397368	-1.576818	-1.564051
1	-4.873804	-2.115343	-2.307249
1	-6.384808	-2.163178	-3.247173
6	-4.604045	0.035168	-4.801117
1	-5.215508	-0.537307	-5.517936
1	-3.643653	-0.491970	-4.689513
1	-4.403351	1.020938	-5.246763
6	-7.183958	0.972667	-3.470151
1	-7.750898	0.339856	-4.173336
1	-7.088487	1.968563	-3.929794
1	-7.794401	1.075227	-2.559580
14	-4.400756	3.041713	-2.046457
6	-4.118542	3.576767	-3.839848
1	-4.949423	3.294767	-4.504971
1	-3.191719	3.145598	-4.250960
1	-4.020098	4.674123	-3.882566
6	-3.013550	3.773562	-0.995597
1	-3.061921	4.874657	-1.029600
1	-2.016567	3.471795	-1.351157
1	-3.099504	3.468990	0.059180
6	-6.017010	3.808013	-1.434241
1	-6.164959	3.625305	-0.358830
1	-6.903194	3.439400	-1.971432
1	-5.968648	4.900218	-1.580230
6	-7.488337	0.464181	1.983476
6	-7.880700	-0.908261	2.561980
1	-8.900300	-0.871159	2.978650
1	-7.205924	-1.224274	3.371414
1	-7.860176	-1.687082	1.783704
6	-7.514772	1.519601	3.105508

1	-7.240194	2.513912	2.719971
1	-6.815341	1.270685	3.917441
1	-8.523214	1.591714	3.544771
6	-8.534999	0.854323	0.931686
1	-8.344228	1.852180	0.508175
1	-9.534386	0.880922	1.393337
1	-8.573006	0.130632	0.102793

Table S14
B3PW91/def2-SVP
Prod-Sn

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
50	1.788423	-0.153344	-0.969000
1	1.658588	0.299207	-2.634868
34	0.258143	1.410967	0.373200
50	-1.712810	0.075108	-0.564552
1	-1.715474	0.504921	-2.237645
6	0.570359	-1.998458	-0.952589
6	-0.759865	-1.914253	-0.719000
6	1.202812	-3.254446	-1.439639
6	1.840798	-3.277566	-2.693470
1	1.915783	-2.355642	-3.277365
6	2.343539	-4.466297	-3.223006
1	2.820198	-4.459827	-4.206742
6	2.236615	-5.657212	-2.503128
1	2.629025	-6.589343	-2.917279
6	1.625653	-5.645536	-1.248062
1	1.537180	-6.571638	-0.673957
6	1.115607	-4.459335	-0.720900
1	0.627003	-4.466445	0.254955
6	-1.672787	-3.078220	-0.884034
6	-1.913997	-3.635799	-2.151748
1	-1.433004	-3.196018	-3.028751
6	-2.735034	-4.754367	-2.294953
1	-2.902986	-5.176425	-3.289313
6	-3.331342	-5.339719	-1.176830
1	-3.969870	-6.219431	-1.289689
6	-3.109312	-4.788846	0.086584
1	-3.572699	-5.235984	0.969927
6	-2.295741	-3.664637	0.229669
1	-2.115213	-3.247138	1.222930
6	3.801846	0.278944	-0.241816
6	4.358100	1.531492	-0.629086
6	5.565631	1.938713	-0.039819
1	5.981479	2.899617	-0.350570
6	6.227666	1.191812	0.939155
6	5.668030	-0.038867	1.280211
1	6.154465	-0.660517	2.030145
6	4.485262	-0.532939	0.694792
6	3.738202	2.466943	-1.645517
1	2.731445	2.109752	-1.923848
14	4.661837	2.370850	-3.330948
6	6.469654	2.911414	-3.234059
1	6.905926	2.876450	-4.246373
1	7.057940	2.233506	-2.597081
1	6.592276	3.935754	-2.852960
6	3.772603	3.435903	-4.616331
1	3.829094	4.511896	-4.390406
1	2.708801	3.162114	-4.701350
1	4.234795	3.282006	-5.605503
6	4.648853	0.584239	-3.946416

1	3.628642	0.239168	-4.175224
1	5.079910	-0.101043	-3.199842
1	5.247127	0.496950	-4.868477
14	3.344682	4.232731	-0.972262
6	4.693632	5.517310	-1.322923
1	4.871845	5.666307	-2.399212
1	5.655835	5.264797	-0.850262
1	4.372497	6.487164	-0.907356
6	1.745495	4.821671	-1.786348
1	0.919330	4.129696	-1.555601
1	1.831602	4.901397	-2.880661
1	1.467793	5.815872	-1.399217
6	3.082116	4.177888	0.894519
1	2.772135	5.172339	1.256117
1	3.997042	3.888121	1.432597
1	2.291545	3.459957	1.162340
6	4.034562	-1.912904	1.113043
1	3.119028	-2.183805	0.551331
14	5.286892	-3.261408	0.534487
6	4.663656	-4.980676	1.008747
1	3.645741	-5.163010	0.633923
1	4.666924	-5.140026	2.098388
1	5.324052	-5.742295	0.562103
6	7.034030	-3.090746	1.244120
1	7.608150	-3.982169	0.939176
1	7.063856	-3.039809	2.342488
1	7.557368	-2.210907	0.841445
6	5.451934	-3.147372	-1.339915
1	6.184028	-3.885058	-1.707688
1	5.801284	-2.146602	-1.639255
1	4.493922	-3.342684	-1.844615
14	3.463783	-2.004794	2.950715
6	2.102042	-3.308278	3.084844
1	1.705362	-3.340921	4.112443
1	2.461294	-4.316114	2.828919
1	1.264661	-3.064820	2.412232
6	4.840502	-2.467257	4.164809
1	4.422434	-2.485982	5.185142
1	5.665072	-1.737321	4.164147
1	5.265628	-3.463184	3.965601
6	2.765034	-0.335209	3.476594
1	1.930853	-0.020735	2.829359
1	3.532482	0.453036	3.435303
1	2.389666	-0.391476	4.511482
6	7.515868	1.729662	1.583065
6	8.038628	0.810716	2.694608
1	7.302174	0.686726	3.503658
1	8.947663	1.244450	3.139886
1	8.303768	-0.188113	2.316692
6	7.246604	3.115674	2.199239
1	6.920137	3.847692	1.445830
1	8.162137	3.510844	2.668667
1	6.465431	3.060746	2.973562
6	8.606978	1.853767	0.502431
1	8.819995	0.876481	0.041587
1	9.543756	2.234538	0.941280
1	8.310136	2.545103	-0.300346
6	-3.701496	0.443029	0.271565
6	-3.898203	0.676574	1.660758
6	-5.200385	0.917415	2.127751
1	-5.330926	1.078807	3.200407
6	-6.318967	0.951001	1.290112
6	-6.092211	0.747781	-0.069870

1	-6.931485	0.772191	-0.763994
6	-4.815909	0.492995	-0.609197
6	-2.788990	0.693099	2.683551
1	-1.826465	0.461578	2.188431
14	-2.937346	-0.710334	3.999317
6	-1.212104	-1.428625	4.266247
1	-1.238832	-2.242726	5.008867
1	-0.505809	-0.665518	4.627645
1	-0.801100	-1.839751	3.331162
6	-4.090305	-2.072599	3.379687
1	-3.874009	-2.362978	2.341071
1	-5.142056	-1.750009	3.411772
1	-3.991169	-2.966478	4.017728
6	-3.601508	-0.172263	5.688435
1	-3.644570	-1.058772	6.343325
1	-4.621037	0.239294	5.628213
1	-2.960219	0.572185	6.184758
14	-2.462197	2.473678	3.354922
6	-2.334467	3.682228	1.910909
1	-2.177920	4.703818	2.295471
1	-3.266290	3.684419	1.323489
1	-1.501716	3.449878	1.230124
6	-3.831467	3.163675	4.464254
1	-4.060903	2.534654	5.335040
1	-4.761329	3.331600	3.900095
1	-3.499993	4.145818	4.841763
6	-0.843495	2.466315	4.328116
1	-0.015500	2.069642	3.719839
1	-0.911041	1.865537	5.248871
1	-0.579222	3.494966	4.623513
6	-4.745447	0.302843	-2.109329
1	-3.732069	-0.026272	-2.396329
14	-5.830258	-1.145315	-2.772025
6	-6.003575	-2.469856	-1.442598
1	-6.543291	-2.092405	-0.560934
1	-5.020275	-2.832794	-1.105688
1	-6.561539	-3.333123	-1.841249
6	-4.952921	-1.903812	-4.265481
1	-5.533572	-2.760192	-4.646311
1	-3.955855	-2.278724	-3.985652
1	-4.829938	-1.189200	-5.093078
6	-7.571944	-0.644888	-3.324902
1	-8.103158	-1.548063	-3.669276
1	-7.563919	0.068211	-4.163773
1	-8.170289	-0.206538	-2.511106
14	-4.907894	1.987399	-3.031211
6	-4.695681	1.728829	-4.892731
1	-5.516232	1.144003	-5.336451
1	-3.747770	1.217705	-5.125180
1	-4.676521	2.707856	-5.399505
6	-3.555995	3.166985	-2.443666
1	-3.688570	4.152887	-2.919334
1	-2.548211	2.805744	-2.699244
1	-3.595588	3.315570	-1.353192
6	-6.562449	2.847109	-2.720543
1	-6.674731	3.124926	-1.661402
1	-7.429554	2.235499	-3.009740
1	-6.597279	3.777297	-3.312183
6	-7.718731	1.197422	1.874337
6	-8.039298	0.102539	2.909704
1	-9.044896	0.256576	3.333827
1	-7.324005	0.104361	3.745853
1	-8.014447	-0.897249	2.448681

6	-7.752006	2.576031	2.560681
1	-7.515854	3.380147	1.846305
1	-7.030188	2.640128	3.388499
1	-8.752768	2.774711	2.977672
6	-8.811464	1.170793	0.797676
1	-8.661452	1.951556	0.036214
1	-9.794734	1.348293	1.260559
1	-8.860513	0.197491	0.285276

Table S15
B3PW91/def2-SVP
Rea-O

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.000003	0.000115	-0.818771
32	-1.428732	-0.506140	0.166188
32	1.428832	0.506306	0.166163
6	-0.668779	-0.174386	1.921638
6	0.668829	0.174822	1.921633
6	-1.460089	-0.454236	3.139996
6	-2.142495	-1.673775	3.289921
1	-2.070929	-2.421169	2.494970
6	-2.872680	-1.956130	4.445696
1	-3.384290	-2.917535	4.538857
6	-2.943569	-1.021325	5.477853
1	-3.513106	-1.240773	6.384418
6	-2.275859	0.198421	5.341340
1	-2.326208	0.942475	6.140682
6	-1.539642	0.478058	4.192728
1	-1.018923	1.433019	4.104766
6	1.460141	0.454787	3.139966
6	2.142602	1.674312	3.289749
1	2.071093	2.421599	2.494693
6	2.872773	1.956780	4.445506
1	3.384428	2.918172	4.538557
6	2.943590	1.022104	5.477785
1	3.513117	1.241641	6.384335
6	2.275825	-0.197627	5.341413
1	2.326120	-0.941580	6.140853
6	1.539624	-0.477376	4.192818
1	1.018846	-1.432317	4.104969
6	-3.168215	0.268883	-0.390889
6	-4.233955	-0.612342	-0.705832
6	-5.490204	-0.066044	-1.031604
1	-6.297579	-0.760368	-1.262343
6	-5.734505	1.306727	-1.059117
6	-4.656195	2.150980	-0.772487
1	-4.802468	3.233401	-0.791917
6	-3.377654	1.674030	-0.446112
6	-4.107423	-2.118547	-0.724927
1	-3.100957	-2.393863	-0.341912
14	-4.059055	-2.787252	-2.530417
14	-5.305859	-3.017281	0.488235
6	-2.592804	-2.004384	-3.417326
1	-2.533399	-2.366952	-4.456833
1	-1.638347	-2.243219	-2.924769
1	-2.683452	-0.907758	-3.448731
6	-3.832523	-4.665252	-2.523939
1	-4.702853	-5.195515	-2.107737
1	-2.942136	-4.967636	-1.951046
1	-3.695959	-5.019547	-3.559147
6	-5.611965	-2.377676	-3.527248

1	-5.518315	-2.833892	-4.527091
1	-5.725431	-1.292231	-3.668482
1	-6.534323	-2.765110	-3.070117
6	-6.927266	-3.598668	-0.300296
1	-6.778513	-4.331483	-1.107977
1	-7.523861	-2.764606	-0.701614
1	-7.537384	-4.088074	0.477357
6	-5.761406	-1.877500	1.919317
1	-6.351023	-2.432461	2.667808
1	-6.365835	-1.023615	1.577459
1	-4.870030	-1.473439	2.421837
6	-4.423368	-4.546067	1.169532
1	-3.493927	-4.278851	1.696830
1	-4.162724	-5.260888	0.374526
1	-5.074441	-5.069875	1.888634
6	-2.291417	2.686781	-0.184319
1	-1.365347	2.156554	0.110004
14	-1.754505	3.543309	-1.822518
14	-2.634956	3.822483	1.334747
6	-1.394306	2.211143	-3.104162
1	-0.948323	2.652261	-4.010491
1	-2.329217	1.709761	-3.400890
1	-0.712000	1.441980	-2.712275
6	-3.052454	4.688921	-2.583513
1	-3.375709	5.498290	-1.914090
1	-3.942587	4.130344	-2.909945
1	-2.613723	5.154645	-3.482261
6	-0.198971	4.565145	-1.484809
1	0.224897	4.929941	-2.434424
1	0.573684	3.964632	-0.978833
1	-0.408486	5.446323	-0.857734
6	-3.786540	2.945172	2.542140
1	-3.904603	3.547513	3.458073
1	-3.400448	1.957029	2.834317
1	-4.785017	2.796432	2.103510
6	-3.429954	5.488003	0.910434
1	-3.616492	6.037912	1.848080
1	-4.398901	5.377980	0.398639
1	-2.782240	6.119391	0.282901
6	-0.984891	4.181452	2.183821
1	-0.306803	4.757254	1.535404
1	-0.469269	3.249448	2.463523
1	-1.144989	4.767091	3.103955
6	-7.116816	1.899101	-1.376776
6	-7.603551	2.722582	-0.168897
1	-7.690997	2.092718	0.730186
1	-6.916826	3.549078	0.067144
1	-8.593885	3.160370	-0.374996
6	-7.014202	2.814009	-2.611692
1	-8.000097	3.241464	-2.856928
1	-6.322966	3.653244	-2.445195
1	-6.658619	2.254859	-3.491344
6	-8.161166	0.814359	-1.669947
1	-8.309627	0.143459	-0.809794
1	-9.132406	1.282914	-1.892641
1	-7.884521	0.199952	-2.540467
6	3.168245	-0.268912	-0.390859
6	4.234058	0.612206	-0.705860
6	5.490267	0.065783	-1.031570
1	6.297692	0.760029	-1.262367
6	5.734467	-1.307010	-1.058955
6	4.656091	-2.151155	-0.772262
1	4.802284	-3.233590	-0.791580

6	3.377580	-1.674079	-0.445956
6	4.107635	2.118422	-0.725093
1	3.101215	2.393842	-0.342034
14	5.306237	3.017192	0.487885
14	4.059169	2.786951	-2.530650
6	5.761799	1.877547	1.919069
1	6.366133	1.023569	1.577277
1	4.870426	1.473620	2.421701
1	6.351513	2.432554	2.667451
6	4.423935	4.546138	1.169062
1	5.075115	5.069954	1.888062
1	3.494504	4.279080	1.696456
1	4.163311	5.260898	0.373995
6	6.927629	3.598355	-0.300843
1	7.537842	4.087840	0.476686
1	6.778855	4.331062	-1.108618
1	7.524140	2.764198	-0.702089
6	2.592760	2.004125	-3.417338
1	2.533321	2.366530	-4.456899
1	1.638369	2.243166	-2.924749
1	2.683261	0.907482	-3.448561
6	3.832803	4.664972	-2.524331
1	4.703225	5.195190	-2.108263
1	2.942502	4.967496	-1.951378
1	3.696174	5.019182	-3.559559
6	5.611949	2.377154	-3.527594
1	5.725332	1.291687	-3.668726
1	6.534382	2.764576	-3.070605
1	5.518222	2.833272	-4.527475
6	2.291242	-2.686714	-0.184112
1	1.365240	-2.156364	0.110200
14	2.634701	-3.822438	1.334955
14	1.754241	-3.543279	-1.822263
6	0.984623	-4.181215	2.184090
1	1.144670	-4.766916	3.104195
1	0.306444	-4.756902	1.535665
1	0.469130	-3.249157	2.463847
6	3.786449	-2.945286	2.542305
1	3.400495	-1.957091	2.834488
1	4.784932	-2.796677	2.103643
1	3.904461	-3.547639	3.458236
6	3.429444	-5.488056	0.910557
1	4.398413	-5.378179	0.398771
1	2.781613	-6.119284	0.282983
1	3.615873	-6.038057	1.848171
6	0.198614	-4.564959	-1.484529
1	-0.574015	-3.964354	-0.978622
1	0.408055	-5.446097	-0.857373
1	-0.225259	-4.929806	-2.434122
6	1.394159	-2.211151	-3.103978
1	0.948042	-2.652262	-4.010243
1	2.329109	-1.709909	-3.400818
1	0.711995	-1.441864	-2.712086
6	3.052090	-4.689073	-2.583143
1	2.613317	-5.154844	-3.481846
1	3.375259	-5.498408	-1.913635
1	3.942276	-4.130609	-2.909620
6	7.116741	-1.899516	-1.376529
6	8.161192	-0.814879	-1.669726
1	9.132400	-1.283528	-1.892366
1	8.309684	-0.143946	-0.809605
1	7.884623	-0.200495	-2.540288
6	7.603363	-2.722966	-0.168582

1	6.916553	-3.549385	0.067486
1	7.690839	-2.093056	0.730465
1	8.593662	-3.160859	-0.374623
6	7.014099	-2.814489	-2.611394
1	6.322788	-3.653658	-2.444877
1	7.999968	-3.242037	-2.856568
1	6.658595	-2.255359	-3.491092

Table S16
B3PW91/def2-SVP
 Rea-S

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
16	0.000053	-0.000052	-1.336787
32	-1.582871	-0.474479	0.137693
32	1.582842	0.474544	0.137822
6	-0.683188	-0.130269	1.805861
6	0.682963	0.130438	1.805930
6	-1.464344	-0.322648	3.054110
6	-2.208403	-1.496409	3.263530
1	-2.196082	-2.273716	2.494560
6	-2.921467	-1.700132	4.446482
1	-3.481027	-2.628540	4.586191
6	-2.910241	-0.731124	5.448881
1	-3.464707	-0.889895	6.377210
6	-2.178793	0.443198	5.254957
1	-2.163958	1.213426	6.030501
6	-1.462788	0.644380	4.077749
1	-0.893154	1.565188	3.944826
6	1.463953	0.322957	3.054254
6	2.207818	1.496832	3.263734
1	2.195508	2.274104	2.494727
6	2.920643	1.700728	4.446798
1	3.480050	2.629222	4.586547
6	2.909369	0.731785	5.449259
1	3.463647	0.890688	6.377678
6	2.178097	-0.442640	5.255287
1	2.163211	-1.212812	6.030885
6	1.462322	-0.643991	4.077968
1	0.892801	-1.564868	3.945019
6	-3.379319	0.206596	-0.339563
6	-4.390281	-0.745583	-0.631443
6	-5.688791	-0.285880	-0.922364
1	-6.453319	-1.033571	-1.132537
6	-6.024053	1.067897	-0.942792
6	-4.994572	1.983936	-0.697372
1	-5.211914	3.054390	-0.724526
6	-3.676809	1.596312	-0.409999
6	-4.151550	-2.237890	-0.673501
1	-3.121475	-2.440741	-0.307404
14	-4.069513	-2.882649	-2.488209
14	-5.256103	-3.257054	0.534229
6	-2.698408	-1.974610	-3.409716
1	-2.653084	-2.324006	-4.454631
1	-1.709813	-2.146612	-2.957194
1	-2.873674	-0.887955	-3.427964
6	-3.661213	-4.729785	-2.497714
1	-4.453744	-5.347801	-2.048722
1	-2.720619	-4.938010	-1.963588
1	-3.530283	-5.067742	-3.539048
6	-5.670921	-2.604615	-3.452673
1	-5.552142	-3.029038	-4.463735
1	-5.886269	-1.531395	-3.568696
1	-6.546582	-3.083927	-2.991230
6	-6.806305	-3.998725	-0.262039
1	-6.579149	-4.702018	-1.077792
1	-7.485945	-3.227985	-0.657884
1	-7.362991	-4.558415	0.508303
6	-5.832035	-2.176375	1.968371

1	-6.370193	-2.790270	2.709687
1	-6.514961	-1.384478	1.625246
1	-4.989802	-1.685279	2.478132
6	-4.220091	-4.687918	1.210653
1	-3.331579	-4.328227	1.753598
1	-3.871095	-5.358207	0.410493
1	-4.817333	-5.291194	1.913968
6	-2.645299	2.679868	-0.215287
1	-1.669982	2.202685	-0.000158
14	-2.274171	3.613250	-1.860619
14	-2.938547	3.758087	1.357128
6	-2.116974	2.382263	-3.279392
1	-1.887361	2.918602	-4.214988
1	-3.062945	1.837854	-3.427229
1	-1.322186	1.643563	-3.101552
6	-3.596796	4.852072	-2.410357
1	-3.770898	5.670347	-1.698360
1	-4.560037	4.359717	-2.614274
1	-3.260037	5.303266	-3.359175
6	-0.644365	4.546714	-1.645503
1	-0.316403	4.965400	-2.610865
1	0.149379	3.874450	-1.282166
1	-0.734081	5.384283	-0.935912
6	-3.990650	2.801688	2.593307
1	-4.069679	3.363048	3.538846
1	-3.563271	1.814362	2.821320
1	-5.008885	2.645015	2.205573
6	-3.816256	5.407655	1.049880
1	-3.999159	5.890192	2.024669
1	-4.792887	5.284714	0.556097
1	-3.212864	6.103396	0.446717
6	-1.248023	4.155067	2.106400
1	-0.656022	4.807876	1.446250
1	-0.660834	3.239958	2.280909
1	-1.364315	4.674023	3.071975
6	-7.451073	1.567338	-1.218951
6	-7.948392	2.373005	-0.003360
1	-7.961646	1.750756	0.905160
1	-7.310676	3.246545	0.198646
1	-8.972421	2.741330	-0.178241
6	-7.447605	2.471209	-2.466287
1	-8.465928	2.833307	-2.682075
1	-6.804432	3.353273	-2.331467
1	-7.086636	1.924361	-3.351393
6	-8.434394	0.415239	-1.464199
1	-8.507747	-0.254987	-0.593904
1	-9.441141	0.819319	-1.653458
1	-8.153454	-0.189512	-2.340170
6	3.379337	-0.206600	-0.339251
6	4.390323	0.745540	-0.631190
6	5.688809	0.285797	-0.922171
1	6.453319	1.033464	-1.132496
6	6.024055	-1.067980	-0.942533
6	4.994569	-1.983986	-0.697020
1	5.211881	-3.054447	-0.724151
6	3.676821	-1.596326	-0.409629
6	4.151632	2.237841	-0.673486
1	3.121505	2.440799	-0.307601
14	5.256053	3.257138	0.534245
14	4.069981	2.882300	-2.488318
6	5.831670	2.176668	1.968672
1	6.514572	1.384646	1.625792
1	4.989309	1.685747	2.478385

1	6.369773	2.790643	2.709962
6	4.220026	4.688193	1.210253
1	4.817196	5.291538	1.913572
1	3.331394	4.328661	1.753106
1	3.871227	5.358378	0.409923
6	6.806420	3.998601	-0.261895
1	7.363039	4.558327	0.508470
1	6.579398	4.701838	-1.077735
1	7.486065	3.227789	-0.657591
6	2.699048	1.974152	-3.409977
1	2.653902	2.323469	-4.454926
1	1.710367	2.146172	-2.957650
1	2.874339	0.887498	-3.428107
6	3.661762	4.729452	-2.498211
1	4.454288	5.347515	-2.049270
1	2.721132	4.937827	-1.964207
1	3.530943	5.067224	-3.539619
6	5.671583	2.604034	-3.452391
1	5.886925	1.530783	-3.568144
1	6.547167	3.083417	-2.990875
1	5.553015	3.028246	-4.463567
6	2.645319	-2.679875	-0.214881
1	1.670010	-2.202707	0.000319
14	2.938736	-3.758160	1.357447
14	2.274148	-3.613245	-1.860199
6	1.248317	-4.155001	2.107030
1	1.364742	-4.674140	3.072489
1	0.656069	-4.807602	1.446898
1	0.661316	-3.239825	2.281825
6	3.991181	-2.801924	2.593461
1	3.563965	-1.814552	2.821582
1	5.009365	-2.645358	2.205545
1	4.070319	-3.363321	3.538969
6	3.816211	-5.407807	1.049942
1	4.792783	-5.284956	0.556020
1	3.212634	-6.103422	0.446818
1	3.999194	-5.890439	2.024669
6	0.644369	-4.546764	-1.645078
1	-0.149400	-3.874572	-1.281668
1	0.734146	-5.384387	-0.935556
1	0.316399	-4.965401	-2.610459
6	2.116933	-2.382234	-3.278953
1	1.887224	-2.918541	-4.214544
1	3.062929	-1.837880	-3.426842
1	1.322210	-1.643482	-3.101050
6	3.596746	-4.852091	-2.409948
1	3.259951	-5.303288	-3.358751
1	3.770824	-5.670366	-1.697937
1	4.560003	-4.359779	-2.613887
6	7.451039	-1.567454	-1.218818
6	8.434325	-0.415380	-1.464319
1	9.441051	-0.819476	-1.653656
1	8.507780	0.254948	-0.594110
1	8.153269	0.189267	-2.340325
6	7.948520	-2.372999	-0.003212
1	7.310830	-3.246517	0.198968
1	7.961897	-1.750660	0.905244
1	8.972525	-2.741344	-0.178194
6	7.447402	-2.471450	-2.466063
1	6.804233	-3.353491	-2.331072
1	8.465692	-2.833585	-2.681945
1	7.086327	-1.924686	-3.351178

Table S17
B3PW91/def2-SVP
 Rea-Se (=Rea-Ge)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
34	-0.000007	0.000045	-1.456261
32	-1.623311	-0.457055	0.155455
32	1.623313	0.457110	0.155447
6	-0.689521	-0.106123	1.798786
6	0.689530	0.106171	1.798783
6	-1.472914	-0.233885	3.054596
6	-2.294262	-1.349857	3.288845
1	-2.341423	-2.137928	2.532228
6	-3.009513	-1.486088	4.480267
1	-3.629233	-2.372085	4.639555
6	-2.923133	-0.505588	5.467860
1	-3.478584	-0.612665	6.402967
6	-2.114927	0.612671	5.249673
1	-2.040207	1.391745	6.012865
6	-1.398286	0.746320	4.063636
1	-0.768744	1.624175	3.912582
6	1.472918	0.233947	3.054594
6	2.294244	1.349939	3.288840
1	2.341383	2.138011	2.532223
6	3.009494	1.486189	4.480260
1	3.629191	2.372202	4.639546
6	2.923141	0.505687	5.467854
1	3.478589	0.612780	6.402961
6	2.114964	-0.612593	5.249669
1	2.040268	-1.391671	6.012859
6	1.398321	-0.746259	4.063635
1	0.768808	-1.624136	3.912582
6	-3.447298	0.176269	-0.289709
6	-4.433732	-0.804677	-0.573271
6	-5.749115	-0.383337	-0.845672
1	-6.492875	-1.153580	-1.049574
6	-6.126269	0.959447	-0.853264
6	-5.121652	1.904905	-0.617128
1	-5.372213	2.968311	-0.636137
6	-3.788099	1.556689	-0.353100
6	-4.152649	-2.289505	-0.624696
1	-3.113370	-2.464402	-0.270928
14	-4.074854	-2.931669	-2.440653
14	-5.214511	-3.350941	0.587033
6	-2.744680	-1.988263	-3.387211
1	-2.729302	-2.317755	-4.439461
1	-1.740923	-2.161991	-2.969678
1	-2.931485	-0.903231	-3.379362
6	-3.604326	-4.764069	-2.453288
1	-4.364953	-5.409317	-1.988092
1	-2.647363	-4.936368	-1.935436
1	-3.479253	-5.100599	-3.495760
6	-5.696125	-2.699952	-3.383496
1	-5.580851	-3.123346	-4.395358
1	-5.939467	-1.632524	-3.498564
1	-6.553089	-3.199511	-2.908968
6	-6.724700	-4.170914	-0.209640
1	-6.464234	-4.856317	-1.030341
1	-7.443873	-3.433443	-0.599117
1	-7.249561	-4.762493	0.559202
6	-5.858064	-2.291507	2.008998

1	-6.353980	-2.930819	2.758286
1	-6.593784	-1.553875	1.654381
1	-5.053305	-1.734854	2.511314
6	-4.110919	-4.722489	1.278828
1	-3.246495	-4.312334	1.824862
1	-3.721059	-5.377756	0.484855
1	-4.679421	-5.352980	1.982058
6	-2.785470	2.670959	-0.182198
1	-1.792679	2.221109	0.012535
14	-2.484940	3.607955	-1.840997
14	-3.075352	3.745330	1.394394
6	-2.404703	2.379588	-3.270252
1	-2.204531	2.916258	-4.212378
1	-3.363900	1.849893	-3.381745
1	-1.614221	1.628286	-3.131010
6	-3.821652	4.855756	-2.334048
1	-3.928391	5.697153	-1.636081
1	-4.806988	4.380298	-2.455707
1	-3.542985	5.272438	-3.316826
6	-0.843780	4.535073	-1.700047
1	-0.569597	4.974482	-2.672969
1	-0.030454	3.857901	-1.394139
1	-0.896046	5.357397	-0.969055
6	-4.085135	2.767939	2.649032
1	-4.153111	3.325647	3.597505
1	-3.637592	1.787210	2.865526
1	-5.108695	2.596723	2.281751
6	-3.995897	5.374748	1.104047
1	-4.185335	5.843604	2.084303
1	-4.971721	5.233587	0.613668
1	-3.412284	6.090717	0.505107
6	-1.380125	4.185963	2.107313
1	-0.818340	4.849150	1.431110
1	-0.767235	3.286741	2.274625
1	-1.488956	4.708097	3.072024
6	-7.570869	1.417018	-1.108897
6	-8.073650	2.211224	0.111969
1	-8.052194	1.592364	1.022640
1	-7.461446	3.105735	0.300948
1	-9.111596	2.546019	-0.047487
6	-7.611301	2.316965	-2.358410
1	-8.642221	2.650938	-2.559112
1	-6.989540	3.216193	-2.236266
1	-7.249650	1.777180	-3.247541
6	-8.524397	0.236636	-1.337166
1	-8.564441	-0.434937	-0.465644
1	-9.545466	0.611156	-1.510001
1	-8.241105	-0.360608	-2.217536
6	3.447285	-0.176263	-0.289710
6	4.433748	0.804647	-0.573291
6	5.749117	0.383261	-0.845695
1	6.492903	1.153477	-1.049607
6	6.126223	-0.959535	-0.853292
6	5.121576	-1.904958	-0.617138
1	5.372097	-2.968372	-0.636157
6	3.788041	-1.556694	-0.353083
6	4.152716	2.289483	-0.624718
1	3.113423	2.464412	-0.271009
14	5.214549	3.350860	0.587081
14	4.075061	2.931673	-2.440678
6	5.857954	2.291387	2.009082
1	6.593651	1.553708	1.654515
1	5.053128	1.734785	2.511350

1	6.353860	2.930671	2.758400
6	4.110973	4.722453	1.278815
1	4.679456	5.352911	1.982090
1	3.246492	4.312336	1.824787
1	3.721200	5.377745	0.484822
6	6.724821	4.170773	-0.209495
1	7.249658	4.762332	0.559378
1	6.464428	4.856185	-1.030211
1	7.443989	3.433274	-0.598930
6	2.744884	1.988355	-3.387320
1	2.729582	2.317850	-4.439570
1	1.741116	2.162151	-2.969840
1	2.931617	0.903311	-3.379464
6	3.604627	4.764097	-2.453327
1	4.365257	5.409312	-1.988090
1	2.647644	4.936436	-1.935523
1	3.479622	5.100636	-3.495804
6	5.696376	2.699874	-3.383424
1	5.939663	1.632433	-3.498487
1	6.553341	3.199378	-2.908842
1	5.581186	3.123284	-4.395290
6	2.785393	-2.670939	-0.182142
1	1.792602	-2.221072	0.012560
14	3.075252	-3.745225	1.394511
14	2.484863	-3.607995	-1.840905
6	1.380018	-4.185862	2.107408
1	1.488837	-4.707974	3.072132
1	0.818254	-4.849071	1.431209
1	0.767114	-3.286644	2.274685
6	4.084971	-2.767736	2.649124
1	3.637390	-1.787009	2.865551
1	5.108535	-2.596507	2.281861
1	4.152937	-3.325385	3.597632
6	3.995869	-5.374623	1.104277
1	4.971697	-5.233428	0.613915
1	3.412312	-6.090655	0.505358
1	4.185307	-5.843416	2.084562
6	0.843629	-4.534982	-1.699954
1	0.030362	-3.857726	-1.394072
1	0.895811	-5.357295	-0.968944
1	0.569425	-4.974386	-2.672872
6	2.404755	-2.379697	-3.270228
1	2.204585	-2.916404	-4.212333
1	3.363988	-1.850065	-3.381714
1	1.614315	-1.628337	-3.131054
6	3.821502	-4.855907	-2.333874
1	3.542831	-5.272590	-3.316651
1	3.928163	-5.697297	-1.635887
1	4.806878	-4.380526	-2.455515
6	7.570803	-1.417159	-1.108945
6	8.524362	-0.236815	-1.337275
1	9.545414	-0.611373	-1.510132
1	8.564453	0.434776	-0.465769
1	8.241060	0.360418	-2.217649
6	8.073586	-2.211342	0.111934
1	7.461354	-3.105825	0.300957
1	8.052173	-1.592452	1.022586
1	9.111517	-2.546179	-0.047535
6	7.611178	-2.317148	-2.358431
1	6.989383	-3.216347	-2.236247
1	8.642080	-2.651168	-2.559140
1	7.249533	-1.777377	-3.247573

Table S18
B3PW91/def2-SVP
 Rea-Te

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
52	-0.000033	0.000037	-1.660935
32	-1.691431	-0.415505	0.166031
32	1.691408	0.415426	0.166026
6	-0.699442	-0.060967	1.765555
6	0.699476	0.060670	1.765535
6	-1.472899	-0.069575	3.035289
6	-2.399194	-1.084833	3.328381
1	-2.537050	-1.897999	2.610699
6	-3.108173	-1.095691	4.531193
1	-3.812057	-1.906350	4.735230
6	-2.908735	-0.088855	5.474771
1	-3.458321	-0.099494	6.419335
6	-1.993784	0.930308	5.199566
1	-1.827268	1.728740	5.927527
6	-1.286721	0.940127	4.000723
1	-0.572004	1.740686	3.805217
6	1.472977	0.069077	3.035244
6	2.399364	1.084223	3.328426
1	2.537243	1.897483	2.610854
6	3.108418	1.094854	4.531197
1	3.812381	1.905427	4.735304
6	2.908952	0.087905	5.474648
1	3.458596	0.098371	6.419181
6	1.993903	-0.931147	5.199356
1	1.827366	-1.729668	5.927213
6	1.286780	-0.940749	4.000547
1	0.572000	-1.741232	3.804963
6	-3.555394	0.124430	-0.245711
6	-4.493494	-0.909642	-0.510214
6	-5.827741	-0.560852	-0.791934
1	-6.531179	-1.372680	-0.977308
6	-6.271535	0.760503	-0.831016
6	-5.316889	1.758311	-0.606581
1	-5.620796	2.806614	-0.643816
6	-3.968870	1.484353	-0.329678
6	-4.147676	-2.381837	-0.521829
1	-3.093692	-2.500447	-0.189620
14	-4.090400	-3.099876	-2.308765
14	-5.132571	-3.435952	0.761549
6	-2.849179	-2.131930	-3.348550
1	-2.879887	-2.485916	-4.392445
1	-1.819280	-2.266697	-2.983182
1	-3.074450	-1.053913	-3.354548
6	-3.511446	-4.900104	-2.250338
1	-4.222832	-5.565150	-1.737384
1	-2.535170	-4.993802	-1.748330
1	-3.389233	-5.279073	-3.278475
6	-5.747072	-3.012543	-3.213957
1	-5.629557	-3.476366	-4.207692
1	-6.059212	-1.968905	-3.372731
1	-6.559175	-3.540867	-2.694098
6	-6.599040	-4.393319	0.038300
1	-6.310982	-5.118923	-0.737371
1	-7.361344	-3.722800	-0.388641
1	-7.082460	-4.957720	0.853369
6	-5.841198	-2.335406	2.121009

1	-6.225491	-2.958842	2.945412
1	-6.676726	-1.728636	1.740265
1	-5.095362	-1.639928	2.531494
6	-3.940352	-4.695946	1.516183
1	-3.087915	-4.208677	2.015621
1	-3.532602	-5.376680	0.752913
1	-4.459122	-5.312200	2.268809
6	-3.034787	2.656510	-0.157694
1	-2.017580	2.266879	0.041690
14	-2.797785	3.629689	-1.807728
14	-3.406274	3.681607	1.436397
6	-2.758150	2.432467	-3.266988
1	-2.627499	2.996179	-4.205579
1	-3.700122	1.866820	-3.341134
1	-1.931683	1.711106	-3.189688
6	-4.156770	4.881590	-2.224959
1	-4.189477	5.741142	-1.541558
1	-5.158214	4.425263	-2.250121
1	-3.954347	5.270200	-3.237297
6	-1.157441	4.564691	-1.719004
1	-0.945191	5.049562	-2.685948
1	-0.322559	3.881890	-1.494252
1	-1.169925	5.352985	-0.949757
6	-4.292611	2.586440	2.687110
1	-4.363304	3.102245	3.658583
1	-3.773000	1.631163	2.849027
1	-5.315380	2.359578	2.348060
6	-4.502638	5.206874	1.192341
1	-4.756063	5.607095	2.188632
1	-5.450933	4.980654	0.680874
1	-3.997016	6.010712	0.636504
6	-1.757290	4.294533	2.127794
1	-1.284277	5.027170	1.455227
1	-1.047866	3.465723	2.271669
1	-1.907208	4.785929	3.103005
6	-7.733597	1.141131	-1.111269
6	-8.283766	1.956213	0.074734
1	-8.242279	1.373321	1.008163
1	-7.716195	2.885054	0.235123
1	-9.334604	2.235813	-0.105190
6	-7.802942	1.990454	-2.394613
1	-8.845566	2.271721	-2.614884
1	-7.220449	2.919415	-2.304036
1	-7.411116	1.433075	-3.259756
6	-8.629889	-0.089485	-1.302038
1	-8.643723	-0.732249	-0.408142
1	-9.666259	0.230862	-1.491798
1	-8.314357	-0.702669	-2.160137
6	3.555383	-0.124400	-0.245838
6	4.493428	0.909742	-0.510259
6	5.827684	0.561045	-0.792042
1	6.531081	1.372927	-0.977335
6	6.271533	-0.760286	-0.831293
6	5.316942	-1.758163	-0.606925
1	5.620899	-2.806445	-0.644261
6	3.968922	-1.484296	-0.329932
6	4.147527	2.381926	-0.521666
1	3.093525	2.500395	-0.189465
14	5.132293	3.435903	0.761931
14	4.090248	3.100224	-2.308496
6	5.840990	2.335160	2.121195
1	6.676509	1.728465	1.740315
1	5.095183	1.639604	2.531604

1	6.225309	2.958472	2.945681
6	3.939963	4.695658	1.516777
1	4.458687	5.311817	2.269511
1	3.087559	4.208238	2.016125
1	3.532169	5.376496	0.753621
6	6.598679	4.393555	0.038876
1	7.082021	4.957878	0.854044
1	6.310531	5.119258	-0.736670
1	7.361070	3.723206	-0.388175
6	2.849077	2.132377	-3.348433
1	2.879804	2.486486	-4.392286
1	1.819165	2.267075	-2.983074
1	3.074376	1.054367	-3.354555
6	3.511225	4.900422	-2.249828
1	4.222590	5.565417	-1.736779
1	2.534945	4.994021	-1.747809
1	3.389001	5.279529	-3.277912
6	5.746930	3.013104	-3.213693
1	6.059131	1.969512	-3.372639
1	6.559004	3.541388	-2.693746
1	5.629394	3.477088	-4.207351
6	3.034909	-2.656505	-0.157902
1	2.017707	-2.266910	0.041580
14	3.406594	-3.681568	1.436164
14	2.797796	-3.629684	-1.807921
6	1.757726	-4.294653	2.127698
1	1.907763	-4.785919	3.102956
1	1.284791	-5.027441	1.455239
1	1.048182	-3.465937	2.271516
6	4.292941	-2.586329	2.686809
1	3.773266	-1.631099	2.848793
1	5.315658	-2.359377	2.347662
1	4.363773	-3.102145	3.658266
6	4.503102	-5.206721	1.192029
1	5.451334	-4.980388	0.680497
1	3.997538	-6.010619	0.636229
1	4.756649	-5.606915	2.188301
6	1.157431	-4.564640	-1.719111
1	0.322563	-3.881809	-1.494398
1	1.169914	-5.352877	-0.949806
1	0.945160	-5.049580	-2.686016
6	2.758126	-2.432455	-3.267172
1	2.627257	-2.996128	-4.205755
1	3.700170	-1.866943	-3.341442
1	1.931775	-1.710976	-3.189742
6	4.156705	-4.881646	-2.225218
1	3.954281	-5.270149	-3.237597
1	4.189300	-5.741265	-1.541892
1	5.158195	-4.425417	-2.250299
6	7.733604	-1.140812	-1.111631
6	8.629819	0.089873	-1.302309
1	9.666203	-0.230395	-1.492129
1	8.643640	0.732554	-0.408352
1	8.314227	0.703121	-2.160340
6	8.283860	-1.955977	0.074275
1	7.716345	-2.884864	0.234598
1	8.242378	-1.373175	1.007760
1	9.334707	-2.235505	-0.105715
6	7.802955	-1.990005	-2.395062
1	7.220522	-2.919009	-2.304557
1	8.845589	-2.271186	-2.615398
1	7.411065	-1.432563	-3.260136

Table S19
B3PW91/def2-SVP
 TS-O

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-1.449966	0.299545	-0.958137
1	0.181405	0.130223	-2.529938
8	-0.100337	-0.604711	-0.047355
32	1.358590	0.380111	0.011553
1	0.963799	0.218106	-2.403949
6	-0.681113	2.069689	-0.725615
6	0.668886	2.096241	-0.367263
6	-1.351081	3.270453	-1.273686
6	-1.915164	3.260367	-2.563755
1	-1.866008	2.343668	-3.156060
6	-2.499423	4.406543	-3.104681
1	-2.922826	4.369894	-4.111943
6	-2.536675	5.592545	-2.370847
1	-2.987494	6.492650	-2.796222
6	-1.991041	5.616011	-1.085048
1	-2.016710	6.537698	-0.497545
6	-1.406624	4.473242	-0.542615
1	-0.974671	4.508746	0.459752
6	1.529316	3.306205	-0.369886
6	1.649126	4.131979	-1.502821
1	1.109831	3.868975	-2.414925
6	2.433647	5.283554	-1.469369
1	2.509955	5.908842	-2.362850
6	3.117756	5.641408	-0.305169
1	3.728773	6.547307	-0.280786
6	3.013915	4.831113	0.825662
1	3.541867	5.098423	1.744772
6	2.229155	3.677464	0.790563
1	2.130005	3.059112	1.686420
6	-3.205747	-0.335069	-0.267376
6	-3.661434	-1.568584	-0.819843
6	-4.867992	-2.116380	-0.360600
1	-5.199204	-3.058066	-0.802833
6	-5.631261	-1.530912	0.653244
6	-5.175882	-0.314885	1.160982
1	-5.742408	0.181067	1.947034
6	-4.006261	0.324903	0.703589
6	-2.912345	-2.344734	-1.883286
1	-1.901999	-1.903673	-2.006151
14	-3.684755	-2.090429	-3.624984
6	-5.495267	-2.622954	-3.718430
1	-5.866536	-2.454600	-4.743264
1	-6.120674	-2.025359	-3.037537
1	-5.647384	-3.686375	-3.481006
6	-2.693662	-3.041297	-4.927176
1	-2.757960	-4.133160	-4.802858
1	-1.628764	-2.758987	-4.908103
1	-3.081571	-2.800566	-5.930841
6	-3.612158	-0.260968	-4.087964
1	-2.569916	0.086627	-4.165209
1	-4.125795	0.369028	-3.345098
1	-4.098571	-0.098143	-5.064198
14	-2.521826	-4.162408	-1.377454
6	-3.804517	-5.425813	-1.972585
1	-3.888706	-5.461917	-3.069743
1	-4.809289	-5.238900	-1.562598

1	-3.496436	-6.429222	-1.633767
6	-0.851967	-4.652119	-2.108938
1	-0.048862	-4.009183	-1.717647
1	-0.835278	-4.586176	-3.207189
1	-0.611985	-5.692125	-1.832675
6	-2.413775	-4.303720	0.501135
1	-2.035322	-5.300866	0.780735
1	-3.394644	-4.164477	0.979021
1	-1.729546	-3.549097	0.916560
6	-3.684555	1.671699	1.309110
1	-2.806447	2.095577	0.787542
14	-5.057445	2.983584	0.983167
6	-4.536297	4.655515	1.697673
1	-3.538074	4.958836	1.351019
1	-4.537478	4.653758	2.799205
1	-5.251745	5.427570	1.369397
6	-6.756605	2.599926	1.732590
1	-7.384516	3.499368	1.613436
1	-6.728282	2.359533	2.805564
1	-7.263796	1.778262	1.205447
6	-5.325803	3.141980	-0.874971
1	-6.140286	3.855572	-1.082388
1	-5.609314	2.171176	-1.312035
1	-4.422909	3.497937	-1.391778
14	-3.054627	1.514630	3.116380
6	-1.825881	2.909428	3.463935
1	-1.417164	2.812513	4.482976
1	-2.290664	3.903402	3.384221
1	-0.982504	2.873165	2.755725
6	-4.419029	1.591809	4.426194
1	-3.971721	1.442649	5.423159
1	-5.175228	0.803938	4.284896
1	-4.936094	2.563849	4.439449
6	-2.167388	-0.137768	3.302791
1	-1.378281	-0.252894	2.542995
1	-2.866024	-0.979761	3.179853
1	-1.709675	-0.213510	4.301694
6	-6.911739	-2.220323	1.150424
6	-7.558591	-1.474163	2.324394
1	-6.879302	-1.401471	3.187864
1	-8.459137	-2.013799	2.656770
1	-7.870144	-0.455768	2.048512
6	-6.579139	-3.648733	1.621851
1	-6.164220	-4.266182	0.811515
1	-7.487576	-4.153165	1.989453
1	-5.843964	-3.633254	2.441687
6	-7.930330	-2.286537	-0.003679
1	-8.189103	-1.277294	-0.360462
1	-8.859316	-2.778771	0.328134
1	-7.540127	-2.854587	-0.861462
6	3.142991	-0.368566	0.295723
6	3.457649	-0.870435	1.591535
6	4.767782	-1.304059	1.840725
1	4.994725	-1.678264	2.840935
6	5.781032	-1.262578	0.877504
6	5.433562	-0.791943	-0.387534
1	6.187405	-0.755290	-1.172428
6	4.140095	-0.345062	-0.718406
6	2.461673	-0.973696	2.718834
1	1.502805	-0.508431	2.405750
14	2.955790	0.036781	4.287027
6	1.385666	0.723431	5.077996
1	1.644074	1.331335	5.960616

1	0.705059	-0.075285	5.409270
1	0.831925	1.368417	4.378314
6	4.071056	1.483490	3.809221
1	3.628107	2.103500	3.015657
1	5.051501	1.140268	3.446524
1	4.239730	2.127158	4.688339
6	3.873843	-0.964841	5.604454
1	4.121707	-0.294699	6.444592
1	4.820922	-1.389215	5.236384
1	3.266556	-1.788157	6.010849
14	1.936983	-2.813304	2.992013
6	1.341033	-3.491376	1.341925
1	0.884117	-4.485012	1.475301
1	2.186412	-3.602744	0.645116
1	0.601697	-2.825420	0.871138
6	3.343649	-3.934666	3.575480
1	3.797120	-3.621191	4.526714
1	4.139406	-4.013202	2.819625
1	2.932087	-4.947636	3.722325
6	0.545542	-2.895851	4.265058
1	-0.305191	-2.258700	3.979924
1	0.877689	-2.597401	5.271840
1	0.175969	-3.932177	4.334895
6	3.915112	0.093626	-2.142734
1	2.906720	0.541778	-2.228511
14	5.063399	1.527867	-2.736253
6	5.511343	2.625825	-1.273113
1	6.093026	2.078600	-0.515651
1	4.612087	3.029295	-0.783130
1	6.118194	3.479631	-1.616524
6	4.124408	2.554102	-4.013551
1	4.745115	3.407172	-4.333736
1	3.196308	2.961782	-3.585632
1	3.863465	1.974565	-4.911479
6	6.677509	0.960013	-3.551736
1	7.259793	1.856427	-3.823941
1	6.508622	0.388499	-4.477805
1	7.310652	0.352371	-2.886715
14	3.808472	-1.440322	-3.309849
6	3.383299	-0.889234	-5.066956
1	4.197422	-0.318693	-5.539856
1	2.473084	-0.269461	-5.090262
1	3.196223	-1.777539	-5.692709
6	2.451917	-2.594137	-2.694985
1	2.404263	-3.493335	-3.330837
1	1.460931	-2.118309	-2.709924
1	2.648324	-2.923897	-1.663548
6	5.403636	-2.453993	-3.358118
1	5.620287	-2.904175	-2.377355
1	6.283136	-1.874713	-3.673975
1	5.272243	-3.279813	-4.077408
6	7.205320	-1.716251	1.233543
6	7.741151	-0.843413	2.384899
1	8.764289	-1.150787	2.655593
1	7.119757	-0.927419	3.288917
1	7.771412	0.218717	2.095513
6	7.177833	-3.190730	1.678241
1	6.792884	-3.839927	0.876323
1	6.544623	-3.340634	2.564981
1	8.193445	-3.533658	1.934023
6	8.170339	-1.589581	0.047701
1	7.859181	-2.210827	-0.806075
1	9.174921	-1.924801	0.348947

1 8.261664 -0.548836 -0.299273

Table S20

B3PW91/def2-SVP

TS-S

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-1.607144	-0.426826	-0.694752
1	-0.067113	-1.782523	-1.583559
16	-0.174729	-0.551498	1.060577
32	1.497744	0.084344	-0.184047
1	0.735018	-1.669130	-1.504420
6	-0.680399	0.868604	-1.791343
6	0.694326	1.042279	-1.610633
6	-1.335413	1.352737	-3.034050
6	-1.949493	0.461398	-3.932984
1	-1.962215	-0.605748	-3.698781
6	-2.505709	0.913363	-5.130510
1	-2.969186	0.195738	-5.812612
6	-2.464284	2.268484	-5.459510
1	-2.893129	2.622725	-6.400211
6	-1.869553	3.167747	-4.571663
1	-1.832828	4.232894	-4.815290
6	-1.313949	2.718284	-3.375156
1	-0.841388	3.430104	-2.695048
6	1.557785	1.745854	-2.601129
6	1.626315	1.344238	-3.946983
1	1.047064	0.478974	-4.275439
6	2.406452	2.045754	-4.864632
1	2.442988	1.714875	-5.905857
6	3.136342	3.166004	-4.460558
1	3.744076	3.717538	-5.182422
6	3.084491	3.573830	-3.127429
1	3.650088	4.449011	-2.797309
6	2.305569	2.867626	-2.209291
1	2.248576	3.202371	-1.171050
6	-3.435120	-0.359121	0.079730
6	-3.959809	-1.614603	0.507581
6	-5.176569	-1.635580	1.205118
1	-5.562800	-2.606179	1.521959
6	-5.885503	-0.477030	1.535525
6	-5.364529	0.732976	1.079445
1	-5.888912	1.660307	1.304555
6	-4.174421	0.827482	0.330574
6	-3.278742	-2.945178	0.265270
1	-2.270621	-2.760753	-0.158513
14	-4.123838	-3.922536	-1.156408
6	-5.949590	-4.288686	-0.837867
1	-6.350266	-4.875481	-1.681331
1	-6.538383	-3.361319	-0.769125
1	-6.115602	-4.870660	0.081257
6	-3.219595	-5.556292	-1.460331
1	-3.303159	-6.253389	-0.612551
1	-2.148997	-5.393837	-1.663426
1	-3.651769	-6.056434	-2.342906
6	-4.007190	-2.903149	-2.741809
1	-2.956087	-2.758293	-3.038465
1	-4.465674	-1.909526	-2.619421
1	-4.523685	-3.416202	-3.569896
14	-2.885737	-3.925114	1.877485
6	-4.249336	-5.140461	2.387974
1	-4.425894	-5.921311	1.631633

1	-5.211044	-4.644489	2.593095
1	-3.940966	-5.648511	3.317075
6	-1.301794	-4.919244	1.615801
1	-0.454685	-4.252491	1.393454
1	-1.386161	-5.650064	0.797861
1	-1.054170	-5.473866	2.535994
6	-2.600941	-2.735812	3.312664
1	-2.311199	-3.300622	4.214223
1	-3.503186	-2.152735	3.549762
1	-1.791340	-2.025926	3.082844
6	-3.768285	2.202575	-0.141947
1	-2.864560	2.110056	-0.772702
14	-5.060810	2.966441	-1.350430
6	-4.421273	4.618267	-2.012792
1	-3.415956	4.522726	-2.448501
1	-4.389737	5.395507	-1.233340
1	-5.095953	4.976532	-2.807888
6	-6.771087	3.303940	-0.606200
1	-7.353923	3.874552	-1.349117
1	-6.748570	3.896263	0.319874
1	-7.321024	2.371640	-0.408829
6	-5.346753	1.775659	-2.782676
1	-6.108386	2.183302	-3.467887
1	-5.712764	0.804904	-2.412011
1	-4.430808	1.595697	-3.363469
14	-3.169834	3.346940	1.284913
6	-1.817129	4.480051	0.608134
1	-1.403914	5.106955	1.414726
1	-2.190433	5.150220	-0.180595
1	-0.990824	3.886040	0.186780
6	-4.520488	4.440442	2.038780
1	-4.080640	5.019697	2.867979
1	-5.352866	3.853279	2.457319
1	-4.938323	5.163064	1.320902
6	-2.451958	2.304258	2.681143
1	-1.624865	1.670804	2.324536
1	-3.214416	1.641439	3.119047
1	-2.069573	2.958145	3.482178
6	-7.175614	-0.575110	2.364888
6	-7.788762	0.800509	2.656728
1	-7.099251	1.445346	3.223079
1	-8.699996	0.680071	3.263284
1	-8.074923	1.330884	1.736076
6	-6.864871	-1.253799	3.712856
1	-6.464927	-2.270063	3.580870
1	-7.779403	-1.333430	4.323000
1	-6.124152	-0.674303	4.285882
6	-8.213661	-1.414457	1.596062
1	-8.454375	-0.953107	0.625473
1	-9.148620	-1.496076	2.174228
1	-7.853169	-2.435457	1.401117
6	3.356382	-0.085020	0.423665
6	3.800540	0.641445	1.566230
6	5.140772	0.510257	1.959670
1	5.470729	1.087009	2.826549
6	6.058208	-0.306757	1.291057
6	5.585024	-1.025109	0.193891
1	6.260942	-1.683295	-0.350398
6	4.256636	-0.943189	-0.264307
6	2.921829	1.556045	2.383123
1	1.907486	1.578783	1.936446
14	3.462325	3.411547	2.304205
6	1.901329	4.453692	2.096328

1	2.154696	5.525818	2.059242
1	1.198647	4.303424	2.930609
1	1.367653	4.203742	1.166371
6	4.613977	3.704365	0.836724
1	4.238721	3.252161	-0.092802
1	5.612600	3.280785	1.022573
1	4.734277	4.787648	0.669431
6	4.375509	4.051135	3.833759
1	4.617572	5.114812	3.670555
1	5.326503	3.523960	4.007075
1	3.775581	3.988481	4.754409
14	2.567909	0.851685	4.146273
6	1.991401	-0.937281	4.017213
1	1.783229	-1.333671	5.024869
1	2.771677	-1.568692	3.563871
1	1.077575	-1.043908	3.414668
6	4.069146	0.823178	5.298046
1	4.543559	1.803170	5.444688
1	4.833408	0.114796	4.943820
1	3.731569	0.466268	6.285831
6	1.210100	1.894540	4.944796
1	0.301160	1.913049	4.323250
1	1.524842	2.934869	5.122404
1	0.935462	1.462047	5.920866
6	3.882349	-1.801174	-1.446930
1	2.857493	-1.534427	-1.773110
14	4.931960	-1.477194	-3.032928
6	5.502934	0.318221	-3.060216
1	6.178980	0.543597	-2.221487
1	4.649887	1.011622	-3.002042
1	6.042720	0.527403	-3.998404
6	3.846605	-1.797092	-4.545972
1	4.416345	-1.581474	-5.464909
1	2.963002	-1.141393	-4.541792
1	3.499246	-2.839255	-4.604754
6	6.461449	-2.582415	-3.196934
1	6.999426	-2.299478	-4.117166
1	6.200150	-3.648238	-3.285414
1	7.167391	-2.472304	-2.359484
14	3.682244	-3.643277	-0.912257
6	3.029828	-4.666668	-2.362782
1	3.763354	-4.760839	-3.178638
1	2.106256	-4.236504	-2.781630
1	2.792740	-5.685295	-2.013754
6	2.442563	-3.738942	0.503056
1	2.288153	-4.789554	0.798863
1	1.464912	-3.316523	0.228196
1	2.804449	-3.191756	1.387303
6	5.281472	-4.431837	-0.284284
1	5.640727	-3.934653	0.629644
1	6.095831	-4.428527	-1.022688
1	5.071160	-5.483166	-0.025132
6	7.517583	-0.380514	1.767076
6	8.146365	1.024289	1.691944
1	9.195833	0.993996	2.026924
1	7.615737	1.747104	2.329481
1	8.130498	1.410658	0.660813
6	7.558170	-0.883097	3.222474
1	7.107895	-1.884295	3.309211
1	7.016786	-0.211503	3.904909
1	8.599449	-0.946789	3.577877
6	8.363144	-1.329547	0.908111
1	7.984026	-2.362489	0.938871

1	9.398122	-1.347874	1.283464
1	8.401319	-1.008740	-0.144288

Table S21

B3PW91/def2-SVP

TS-Se (= TS-Ge)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.609798	0.418402	-0.348299
1	0.197806	2.191817	-0.823623
34	0.075036	0.114495	1.423966
32	-1.601402	0.056179	-0.169628
1	-0.606338	2.129933	-0.802500
6	0.668269	-0.318452	-1.842187
6	-0.731934	-0.412990	-1.782794
6	1.380722	-0.464975	-3.137623
6	2.244585	0.530388	-3.628846
1	2.403560	1.435142	-3.039439
6	2.867353	0.400547	-4.870863
1	3.524549	1.198035	-5.227686
6	2.646152	-0.730938	-5.656339
1	3.128131	-0.830434	-6.632140
6	1.802682	-1.735999	-5.178213
1	1.623526	-2.632310	-5.778031
6	1.179956	-1.606067	-3.938635
1	0.512125	-2.394003	-3.584791
6	-1.563119	-0.574702	-3.011221
6	-1.460673	0.323093	-4.089657
1	-0.773083	1.168084	-4.014737
6	-2.207364	0.136164	-5.251095
1	-2.108058	0.845624	-6.076869
6	-3.075615	-0.952576	-5.364605
1	-3.656460	-1.101290	-6.278491
6	-3.198105	-1.845380	-4.299784
1	-3.875462	-2.700158	-4.373736
6	-2.452272	-1.653026	-3.135340
1	-2.534431	-2.363285	-2.310751
6	3.504617	0.231362	0.177687
6	4.141544	1.421101	0.645445
6	5.513681	1.384152	0.932045
1	5.981759	2.302097	1.292239
6	6.288795	0.227932	0.790782
6	5.628678	-0.930075	0.384037
1	6.187146	-1.860407	0.294329
6	4.251420	-0.975020	0.089731
6	3.404466	2.713733	0.928935
1	2.337614	2.582723	0.652384
14	3.914164	4.193505	-0.182465
6	5.731031	4.700331	-0.047879
1	5.887634	5.607759	-0.655018
1	6.397784	3.920730	-0.446273
1	6.044638	4.931667	0.980779
6	2.848185	5.699898	0.232842
1	3.059390	6.108103	1.233261
1	1.772942	5.466133	0.180436
1	3.049353	6.500786	-0.497824
6	3.599062	3.751202	-1.990261
1	2.533149	3.539117	-2.169170
1	4.184008	2.868948	-2.293390
1	3.889849	4.589289	-2.645075
14	3.287899	3.065334	2.824049
6	4.691116	4.153335	3.482042

1	4.691066	5.159876	3.035599
1	5.683875	3.706129	3.317465
1	4.565255	4.277352	4.570617
6	1.645965	3.918698	3.200480
1	0.799361	3.295754	2.871143
1	1.553723	4.902739	2.718053
1	1.545257	4.067980	4.288254
6	3.323800	1.437453	3.776671
1	3.229232	1.632676	4.857667
1	4.260341	0.883982	3.609834
1	2.487038	0.785823	3.480329
6	3.671826	-2.330288	-0.243855
1	2.623780	-2.209041	-0.579719
14	4.537070	-3.223063	-1.723228
6	3.295494	-4.363626	-2.575904
1	2.979775	-5.195475	-1.929578
1	3.758020	-4.797380	-3.477907
1	2.398105	-3.814567	-2.895275
6	6.008076	-4.316970	-1.232234
1	6.419695	-4.766277	-2.151740
1	5.717311	-5.144908	-0.567524
1	6.827045	-3.763056	-0.748075
6	5.171089	-1.954728	-2.962065
1	5.609940	-2.468871	-3.832892
1	5.946437	-1.309255	-2.521752
1	4.359100	-1.307995	-3.325507
14	3.519577	-3.411348	1.349412
6	2.756070	-5.093706	0.940050
1	2.541948	-5.628028	1.880548
1	3.422748	-5.734486	0.343043
1	1.804967	-4.989189	0.394303
6	5.167735	-3.697622	2.232515
1	4.985702	-4.352758	3.101142
1	5.580823	-2.751555	2.614653
1	5.931959	-4.179746	1.606497
6	2.397246	-2.561575	2.600280
1	1.381360	-2.414435	2.205065
1	2.790537	-1.573312	2.883787
1	2.326911	-3.172195	3.515688
6	7.792671	0.262329	1.104937
6	8.470814	-1.091217	0.857301
1	8.053865	-1.885443	1.495158
1	9.545233	-1.016272	1.086516
1	8.378903	-1.409633	-0.192534
6	7.994942	0.639918	2.585104
1	7.569382	1.627254	2.818261
1	9.068800	0.673398	2.831494
1	7.516935	-0.096457	3.249995
6	8.477123	1.312837	0.210167
1	8.342730	1.072271	-0.856103
1	9.559088	1.348480	0.417238
1	8.074406	2.322214	0.379903
6	-3.495590	-0.029384	0.342703
6	-4.015769	-1.171681	1.016649
6	-5.384426	-1.195743	1.324787
1	-5.775176	-2.086477	1.822208
6	-6.254446	-0.141293	1.024892
6	-5.704330	0.979541	0.403762
1	-6.340109	1.832032	0.167857
6	-4.344987	1.071128	0.051296
6	-3.176563	-2.352877	1.439012
1	-2.129238	-2.172342	1.125422
14	-3.596898	-4.008082	0.530166

6	-1.968678	-4.705073	-0.131162
1	-2.141168	-5.637402	-0.693286
1	-1.275178	-4.935705	0.693379
1	-1.459398	-3.994456	-0.801129
6	-4.806896	-3.709704	-0.889109
1	-4.526940	-2.855582	-1.522047
1	-5.818730	-3.508247	-0.505310
1	-4.863189	-4.608799	-1.525124
6	-4.385456	-5.352504	1.605189
1	-4.505525	-6.258089	0.986949
1	-5.387251	-5.068430	1.963202
1	-3.775096	-5.629602	2.477908
14	-2.994940	-2.451424	3.357785
6	-2.584820	-0.743913	4.045626
1	-2.492202	-0.796108	5.143115
1	-3.385208	-0.024921	3.810077
1	-1.640738	-0.342448	3.648336
6	-4.552129	-3.011437	4.274618
1	-4.933384	-3.990126	3.952611
1	-5.362688	-2.273053	4.180041
1	-4.307988	-3.086998	5.347709
6	-1.586462	-3.644717	3.760101
1	-0.642219	-3.315915	3.298907
1	-1.790223	-4.672250	3.420794
1	-1.427065	-3.683169	4.850212
6	-3.877553	2.350181	-0.596825
1	-2.825893	2.216304	-0.923251
14	-4.778663	2.791511	-2.244709
6	-5.393985	1.220680	-3.083189
1	-6.171586	0.719073	-2.487309
1	-4.576001	0.502107	-3.243738
1	-5.825079	1.465802	-4.067814
6	-3.541154	3.650358	-3.385028
1	-4.023783	3.893242	-4.346015
1	-2.685357	2.992084	-3.599858
1	-3.153729	4.587760	-2.958853
6	-6.262778	3.949891	-2.031389
1	-6.702988	4.143330	-3.023946
1	-5.983510	4.924310	-1.602027
1	-7.056480	3.516144	-1.403317
14	-3.723417	3.774637	0.692517
6	-3.019907	5.321299	-0.138196
1	-3.706848	5.758536	-0.879057
1	-2.063558	5.110067	-0.642548
1	-2.827668	6.090554	0.627950
6	-2.535568	3.249882	2.057983
1	-2.439899	4.055906	2.804138
1	-1.530896	3.030470	1.666088
1	-2.892247	2.349119	2.580868
6	-5.363268	4.222020	1.519572
1	-5.750833	3.384918	2.119917
1	-6.143136	4.525461	0.806000
1	-5.191626	5.067898	2.206291
6	-7.745478	-0.242348	1.384290
6	-8.357629	-1.470723	0.684291
1	-9.430346	-1.553902	0.923137
1	-7.875751	-2.407837	1.000558
1	-8.258034	-1.394041	-0.409705
6	-7.893159	-0.395302	2.909996
1	-7.458323	0.467421	3.438535
1	-7.393931	-1.302631	3.280914
1	-8.957185	-0.463807	3.189083
6	-8.534878	0.998764	0.947776

1	-8.171984	1.913797	1.440365
1	-9.595288	0.878983	1.219241
1	-8.489116	1.153424	-0.141256

Table S22
B3PW91/def2-SVP
 TS-Te

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	-1.689400	0.430128	0.388825
1	-0.243162	2.123523	0.738968
52	-0.181031	-0.001034	-1.646079
32	1.612866	0.059164	0.110352
1	0.568338	2.054994	0.685172
6	-0.656348	-0.349002	1.822208
6	0.739178	-0.425386	1.731891
6	-1.309541	-0.536194	3.145853
6	-2.051191	0.484874	3.764291
1	-2.176486	1.438811	3.248979
6	-2.593486	0.313483	5.038675
1	-3.157264	1.130290	5.497005
6	-2.411510	-0.886624	5.726465
1	-2.830152	-1.019710	6.727137
6	-1.692803	-1.918337	5.118465
1	-1.547997	-2.867137	5.641955
6	-1.151468	-1.747511	3.845705
1	-0.577979	-2.555519	3.386241
6	1.586818	-0.591153	2.950297
6	1.498760	0.302870	4.033083
1	0.812891	1.149834	3.969924
6	2.256076	0.109755	5.186594
1	2.166528	0.816453	6.015789
6	3.122701	-0.981302	5.286984
1	3.711923	-1.135704	6.194518
6	3.233818	-1.868534	4.216434
1	3.910687	-2.724424	4.279731
6	2.477313	-1.669680	3.060057
1	2.553475	-2.375235	2.231037
6	-3.602907	0.187658	-0.093919
6	-4.276570	1.345543	-0.586973
6	-5.584145	1.207757	-1.076995
1	-6.080307	2.104037	-1.454077
6	-6.252406	-0.019340	-1.135806
6	-5.572171	-1.132808	-0.644852
1	-6.048518	-2.112338	-0.677858
6	-4.270854	-1.066393	-0.109735
6	-3.653107	2.723805	-0.661056
1	-2.603619	2.657966	-0.306612
14	-4.413685	3.971059	0.587327
6	-6.274405	4.232514	0.385407
1	-6.600707	5.008020	1.098578
1	-6.835829	3.314595	0.616476
1	-6.559687	4.567734	-0.622759
6	-3.548802	5.648017	0.442284
1	-3.739075	6.150453	-0.518362
1	-2.458123	5.552822	0.565731
1	-3.914460	6.314976	1.240634
6	-4.122122	3.344411	2.343400
1	-3.048431	3.355582	2.588779
1	-4.496930	2.318079	2.478718
1	-4.636890	3.992845	3.071515
14	-3.452049	3.368289	-2.468646

6	-4.890719	4.451945	-3.056947
1	-5.020095	5.359808	-2.448057
1	-5.848774	3.908809	-3.065263
1	-4.691300	4.776017	-4.092036
6	-1.861284	4.381371	-2.577381
1	-0.989174	3.766568	-2.303559
1	-1.874259	5.265398	-1.922793
1	-1.708569	4.732345	-3.611284
6	-3.311635	1.922631	-3.672738
1	-3.168300	2.303665	-4.697418
1	-4.212425	1.290887	-3.664856
1	-2.448900	1.282505	-3.431629
6	-3.667353	-2.356657	0.386212
1	-2.691725	-2.132071	0.858432
14	-4.667950	-3.128822	1.842488
6	-3.624610	-4.502457	2.618281
1	-2.632814	-4.133701	2.920096
1	-3.480185	-5.352736	1.933215
1	-4.125888	-4.887608	3.521426
6	-6.350354	-3.881903	1.398786
1	-6.744371	-4.365623	2.308927
1	-6.314753	-4.644847	0.609317
1	-7.079735	-3.111894	1.105226
6	-5.039739	-1.789704	3.111586
1	-5.582189	-2.218768	3.970092
1	-5.675662	-1.006990	2.668155
1	-4.127752	-1.310087	3.492222
14	-3.187750	-3.568949	-1.040310
6	-1.474777	-4.256870	-0.646979
1	-1.141440	-4.949342	-1.436982
1	-1.464474	-4.806097	0.307523
1	-0.739067	-3.440408	-0.575278
6	-4.360562	-5.037810	-1.276111
1	-3.974872	-5.655026	-2.104987
1	-5.378795	-4.721308	-1.551494
1	-4.430284	-5.685863	-0.389269
6	-3.143322	-2.669483	-2.698509
1	-2.468598	-1.801108	-2.674012
1	-4.142259	-2.309043	-2.988493
1	-2.786431	-3.354792	-3.485117
6	-7.667008	-0.099048	-1.731375
6	-8.212208	-1.532660	-1.749764
1	-7.581687	-2.205281	-2.351474
1	-9.220305	-1.541987	-2.192793
1	-8.295130	-1.956055	-0.737407
6	-7.642094	0.420789	-3.181607
1	-7.307946	1.467298	-3.239293
1	-8.649471	0.369265	-3.625852
1	-6.964681	-0.182158	-3.806445
6	-8.622258	0.770371	-0.891814
1	-8.657890	0.422905	0.152614
1	-9.644971	0.724476	-1.300417
1	-8.315009	1.826663	-0.883589
6	3.537693	0.034025	-0.320253
6	4.133487	-1.094981	-0.953536
6	5.506283	-1.052609	-1.240030
1	5.949953	-1.932109	-1.712642
6	6.316637	0.048940	-0.945726
6	5.698011	1.149533	-0.354244
1	6.286601	2.034728	-0.115965
6	4.327012	1.181188	-0.036554
6	3.375316	-2.336160	-1.358349
1	2.315478	-2.219635	-1.056758

14	3.907839	-3.939436	-0.410764
6	2.338043	-4.761741	0.244447
1	2.588258	-5.672647	0.812671
1	1.669292	-5.055531	-0.579660
1	1.762398	-4.098176	0.908177
6	5.069453	-3.527158	1.021039
1	4.731596	-2.666014	1.614874
1	6.081257	-3.292966	0.656547
1	5.149908	-4.400195	1.690067
6	4.809063	-5.241023	-1.448671
1	5.020373	-6.106122	-0.797647
1	5.774422	-4.879505	-1.835047
1	4.213531	-5.608601	-2.298266
14	3.226626	-2.482683	-3.278099
6	2.857900	-0.788090	-4.023601
1	2.750872	-0.880502	-5.117126
1	3.685088	-0.088583	-3.825030
1	1.934026	-0.332669	-3.637353
6	4.783318	-3.078628	-4.174493
1	5.091840	-4.098230	-3.907889
1	5.636604	-2.402937	-4.010347
1	4.569808	-3.068719	-5.256760
6	1.812625	-3.675195	-3.662199
1	0.869526	-3.334810	-3.205867
1	2.016720	-4.693573	-3.295239
1	1.653929	-3.741411	-4.750971
6	3.788661	2.452510	0.572173
1	2.735737	2.284201	0.875034
14	4.632768	2.954588	2.232397
6	5.292406	1.420603	3.104499
1	6.102517	0.943169	2.532585
1	4.500253	0.671639	3.255379
1	5.690518	1.693887	4.095581
6	3.335838	3.776769	3.333438
1	3.784524	4.047966	4.303275
1	2.499140	3.090242	3.534359
1	2.924764	4.694351	2.886721
6	6.072146	4.171262	2.036860
1	6.489465	4.384055	3.035377
1	5.760317	5.132866	1.600687
1	6.891574	3.768241	1.421344
14	3.619743	3.845558	-0.748759
6	2.810838	5.368668	0.027051
1	3.448248	5.851449	0.783780
1	1.848565	5.117708	0.501028
1	2.608231	6.115008	-0.758745
6	2.518856	3.242101	-2.154657
1	2.427562	4.026467	-2.924269
1	1.505010	2.990656	-1.807849
1	2.937398	2.345585	-2.637973
6	5.266721	4.357494	-1.523511
1	5.711893	3.530852	-2.098096
1	6.007756	4.706861	-0.790057
1	5.079677	5.184727	-2.228735
6	7.815506	0.019608	-1.283795
6	8.475316	-1.190112	-0.595206
1	9.553790	-1.218242	-0.820199
1	8.043532	-2.143873	-0.933217
1	8.357528	-1.136560	0.498339
6	7.987645	-0.102183	-2.809993
1	7.524227	0.750726	-3.330015
1	7.528792	-1.022332	-3.201389
1	9.056712	-0.123517	-3.077318

6	8.541649	1.288176	-0.817414
1	8.148938	2.193119	-1.305594
1	9.611304	1.218378	-1.069311
1	8.467678	1.426167	0.272383

Table S23
B3PW91/def2-SVP
 Prod-O

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.436438	-0.221555	-0.922859
1	1.280898	0.206910	-2.404489
8	0.101017	0.633264	-0.026854
32	-1.454713	-0.132084	-0.559624
1	-1.548510	0.297991	-2.043035
6	0.591798	-2.035106	-0.927380
6	-0.748329	-1.985513	-0.700270
6	1.250165	-3.269107	-1.427466
6	1.915222	-3.252692	-2.666403
1	2.006166	-2.310935	-3.214874
6	2.418008	-4.426839	-3.228512
1	2.914745	-4.390020	-4.201643
6	2.283015	-5.642111	-2.556020
1	2.674276	-6.562635	-2.996431
6	1.647632	-5.669883	-1.312959
1	1.540670	-6.614503	-0.773328
6	1.137435	-4.498528	-0.755109
1	0.626848	-4.537327	0.208399
6	-1.652333	-3.153393	-0.868364
6	-1.870453	-3.724886	-2.133733
1	-1.371845	-3.296577	-3.006569
6	-2.694119	-4.841045	-2.280625
1	-2.846018	-5.272886	-3.273402
6	-3.313511	-5.411861	-1.167411
1	-3.953265	-6.290425	-1.282841
6	-3.112676	-4.848458	0.093807
1	-3.594931	-5.283600	0.973040
6	-2.298481	-3.724729	0.239050
1	-2.138413	-3.293274	1.229265
6	3.202975	0.402245	-0.293249
6	3.543726	1.748500	-0.634682
6	4.740496	2.291404	-0.143320
1	4.980915	3.319656	-0.421407
6	5.609456	1.593008	0.699243
6	5.277549	0.269800	0.980669
1	5.936973	-0.326958	1.609241
6	4.121936	-0.359049	0.475948
6	2.708187	2.650605	-1.520822
1	1.708077	2.213371	-1.680067
14	3.441512	2.751878	-3.299422
6	5.195205	3.455739	-3.337203
1	5.523646	3.529976	-4.387425
1	5.902772	2.793067	-2.815974
1	5.271147	4.458659	-2.892904
6	2.330883	3.814890	-4.402406
1	2.317773	4.874161	-4.103469
1	1.291789	3.448679	-4.401506
1	2.697177	3.769639	-5.441411
6	3.541395	1.035919	-4.087814
1	2.545098	0.625241	-4.312067
1	4.069292	0.318523	-3.440356
1	4.098816	1.103741	-5.036969

14	2.256152	4.342673	-0.711007
6	3.445953	5.763847	-1.111778
1	3.493171	5.993019	-2.187560
1	4.472480	5.579696	-0.758538
1	3.085520	6.671911	-0.599598
6	0.547508	4.854295	-1.329506
1	-0.208424	4.090477	-1.092941
1	0.530133	5.023839	-2.416572
1	0.236693	5.792519	-0.841137
6	2.208134	4.160933	1.165124
1	1.758753	5.059773	1.618235
1	3.215093	4.033851	1.588936
1	1.606717	3.289794	1.462403
6	3.981424	-1.833182	0.778369
1	3.069581	-2.229721	0.295177
14	5.388446	-2.840086	-0.078923
6	5.040827	-4.686193	0.100791
1	4.036760	-4.950405	-0.262737
1	5.128962	-5.021396	1.146607
1	5.773861	-5.259241	-0.490604
6	7.138928	-2.540381	0.581941
1	7.805673	-3.268642	0.089270
1	7.241268	-2.683383	1.666785
1	7.511130	-1.537032	0.327251
6	5.455366	-2.360594	-1.902794
1	6.237037	-2.941892	-2.419228
1	5.702634	-1.292691	-2.010185
1	4.501414	-2.548030	-2.415250
14	3.691999	-2.196171	2.647272
6	2.576637	-3.711503	2.814420
1	2.390009	-3.930551	3.878421
1	3.020357	-4.608769	2.357432
1	1.601605	-3.535727	2.334905
6	5.261668	-2.529443	3.651413
1	4.977871	-2.657400	4.709477
1	5.981972	-1.698195	3.604369
1	5.778180	-3.449414	3.336818
6	2.829053	-0.707094	3.413271
1	1.902209	-0.470860	2.869101
1	3.469258	0.187607	3.381125
1	2.569898	-0.904626	4.465752
6	6.867120	2.279117	1.254798
6	7.649590	1.372682	2.214015
1	7.042463	1.072421	3.082103
1	8.530957	1.909852	2.597727
1	8.013160	0.459826	1.718801
6	6.461520	3.549548	2.025909
1	5.939749	4.274119	1.383482
1	7.353730	4.051584	2.434157
1	5.794431	3.306414	2.867742
6	7.794268	2.664095	0.086246
1	8.101641	1.774116	-0.484983
1	8.705415	3.156778	0.463096
1	7.305588	3.358609	-0.613205
6	-3.158224	0.328873	0.326104
6	-3.267608	0.526503	1.731815
6	-4.510854	0.876408	2.280794
1	-4.562670	1.023806	3.362177
6	-5.667036	1.036321	1.511949
6	-5.537717	0.838766	0.138861
1	-6.410900	0.946404	-0.503536
6	-4.323503	0.487661	-0.481429
6	-2.106657	0.406773	2.688411

1	-1.207223	0.066272	2.140606
14	-2.369405	-0.926773	4.056624
6	-0.765081	-1.902008	4.249304
1	-0.880069	-2.684132	5.017474
1	0.071598	-1.254814	4.551436
1	-0.478831	-2.396378	3.307915
6	-3.748407	-2.132283	3.587127
1	-3.658741	-2.493374	2.552210
1	-4.742607	-1.670754	3.681262
1	-3.716738	-3.004954	4.260628
6	-2.820834	-0.242313	5.763567
1	-2.939657	-1.089706	6.459462
1	-3.772141	0.312191	5.757880
1	-2.043786	0.417921	6.178537
14	-1.556558	2.162516	3.268165
6	-1.395987	3.237850	1.732163
1	-0.975647	4.224607	1.982841
1	-2.384274	3.397659	1.273174
1	-0.743477	2.754861	0.989346
6	-2.770347	3.048240	4.419716
1	-2.952024	2.524596	5.368902
1	-3.738479	3.231078	3.929891
1	-2.340394	4.034755	4.663343
6	0.103095	2.034890	4.158408
1	0.872203	1.578334	3.517995
1	0.035726	1.440788	5.083479
1	0.455486	3.041420	4.436932
6	-4.381223	0.310275	-1.985935
1	-3.428959	-0.102103	-2.355282
14	-5.636744	-1.028161	-2.579047
6	-5.848794	-2.347307	-1.250784
1	-6.280623	-1.932088	-0.327668
1	-4.885379	-2.812926	-0.992432
1	-6.520110	-3.142716	-1.614346
6	-4.926492	-1.847618	-4.128222
1	-5.611485	-2.633929	-4.486120
1	-3.959687	-2.326806	-3.907339
1	-4.775539	-1.135156	-4.953045
6	-7.355137	-0.361613	-3.018635
1	-7.987545	-1.205743	-3.340968
1	-7.330392	0.363348	-3.846950
1	-7.860459	0.114888	-2.164132
14	-4.469968	2.008892	-2.888872
6	-4.449503	1.752879	-4.763250
1	-5.353674	1.247012	-5.135187
1	-3.574296	1.164229	-5.081686
1	-4.389273	2.732648	-5.265450
6	-2.959642	3.044264	-2.431214
1	-3.044715	4.052332	-2.869424
1	-2.025860	2.595283	-2.802492
1	-2.866578	3.161235	-1.340439
6	-5.997297	3.024334	-2.431472
1	-5.985842	3.306963	-1.367756
1	-6.942971	2.502571	-2.639075
1	-5.993470	3.955900	-3.021919
6	-7.000479	1.408778	2.178820
6	-7.364413	0.343363	3.230306
1	-8.323816	0.591574	3.712750
1	-6.605352	0.270872	4.023546
1	-7.464253	-0.651426	2.768508
6	-6.859399	2.779210	2.867770
1	-6.594447	3.563070	2.141061
1	-6.082365	2.766714	3.646227

1	-7.807735	3.068514	3.349198
6	-8.151998	1.494531	1.168624
1	-7.971544	2.261557	0.400040
1	-9.084273	1.764227	1.688967
1	-8.324989	0.533395	0.660326

Table S24
B3PW91/def2-SVP
 Prod-S

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.606092	-0.064229	-0.911724
1	1.416360	0.563022	-2.315263
16	0.217649	1.030834	0.490446
32	-1.539260	0.011254	-0.470403
1	-1.560797	0.624941	-1.887439
6	0.614332	-1.790314	-1.133985
6	-0.719536	-1.767173	-0.875070
6	1.241671	-2.933339	-1.851779
6	1.876364	-2.712870	-3.087686
1	1.967703	-1.694474	-3.474436
6	2.355753	-3.778523	-3.850022
1	2.828954	-3.581205	-4.815482
6	2.228936	-5.088223	-3.385775
1	2.602300	-5.923909	-3.982951
6	1.623270	-5.320205	-2.149612
1	1.520544	-6.341390	-1.773367
6	1.135643	-4.256624	-1.390876
1	0.649263	-4.453418	-0.434182
6	-1.624014	-2.900685	-1.212192
6	-1.838961	-3.289387	-2.545486
1	-1.340946	-2.741804	-3.349068
6	-2.656270	-4.378205	-2.848716
1	-2.804950	-4.667149	-3.892435
6	-3.273872	-5.102473	-1.827652
1	-3.909237	-5.959108	-2.066220
6	-3.077420	-4.720329	-0.499582
1	-3.557817	-5.276728	0.309395
6	-2.268373	-3.624684	-0.196976
1	-2.110202	-3.338344	0.844574
6	3.431961	0.355762	-0.265700
6	3.851121	1.706262	-0.479137
6	5.038978	2.151597	0.118748
1	5.337443	3.185982	-0.062607
6	5.820592	1.352394	0.955645
6	5.409938	0.031787	1.120460
1	5.996259	-0.635478	1.750002
6	4.259655	-0.503479	0.507437
6	3.100198	2.718483	-1.321057
1	2.101404	2.331211	-1.581044
14	3.923192	2.922973	-3.047278
6	5.711384	3.524855	-2.953550
1	6.106247	3.634635	-3.977440
1	6.351646	2.800233	-2.427776
1	5.811582	4.498939	-2.452162
6	2.929377	4.127439	-4.115695
1	2.961201	5.160486	-3.736731
1	1.872418	3.825904	-4.191379
1	3.344379	4.137613	-5.137220
6	3.945581	1.256633	-3.940673
1	2.928545	0.914287	-4.187974
1	4.429617	0.476832	-3.332040

1	4.508375	1.345112	-4.884731
14	2.635140	4.344989	-0.394279
6	3.891924	5.749760	-0.603745
1	4.029999	6.046588	-1.654934
1	4.881717	5.502503	-0.188665
1	3.523673	6.635444	-0.059298
6	0.975899	4.943978	-1.069118
1	0.189054	4.198513	-0.872802
1	1.003291	5.134789	-2.152436
1	0.679905	5.882488	-0.572168
6	2.443716	4.021275	1.453533
1	2.064216	4.928800	1.951807
1	3.397612	3.746007	1.927400
1	1.726732	3.206543	1.636957
6	4.020333	-1.978917	0.727226
1	3.132044	-2.301284	0.153482
14	5.437997	-3.028863	-0.057713
6	5.045780	-4.869593	0.104846
1	4.061271	-5.116884	-0.316818
1	5.069098	-5.207431	1.152999
1	5.802113	-5.453416	-0.445490
6	7.157246	-2.772866	0.696793
1	7.821011	-3.551523	0.283946
1	7.183387	-2.865579	1.792076
1	7.586509	-1.798512	0.419781
6	5.592031	-2.563495	-1.878575
1	6.450372	-3.082980	-2.335569
1	5.757286	-1.479712	-1.986252
1	4.689889	-2.831472	-2.446842
14	3.551600	-2.407115	2.545419
6	2.379777	-3.889223	2.529350
1	2.063033	-4.136561	3.555430
1	2.847627	-4.785454	2.095161
1	1.473418	-3.663298	1.946829
6	5.019755	-2.847524	3.656374
1	4.642478	-3.039575	4.674763
1	5.755430	-2.031546	3.730299
1	5.546834	-3.755400	3.325094
6	2.675196	-0.928935	3.317466
1	1.784524	-0.640763	2.737439
1	3.338253	-0.051060	3.360973
1	2.356811	-1.165368	4.345663
6	7.068941	1.933125	1.638240
6	7.738840	0.925410	2.580899
1	7.057870	0.599787	3.382434
1	8.614996	1.389209	3.060395
1	8.092881	0.030408	2.047768
6	6.672757	3.169498	2.467511
1	6.229833	3.961288	1.845528
1	7.557935	3.596512	2.966214
1	5.939272	2.904894	3.245203
6	8.090409	2.344675	0.560772
1	8.391761	1.479372	-0.050282
1	8.997285	2.762674	1.027614
1	7.683783	3.108570	-0.118851
6	-3.329379	0.290906	0.331940
6	-3.552646	0.336151	1.740302
6	-4.842843	0.612677	2.219322
1	-4.983617	0.633926	3.302617
6	-5.937058	0.848363	1.383629
6	-5.694767	0.808653	0.012764
1	-6.514964	0.986742	-0.681696
6	-4.429352	0.539109	-0.542625

6	-2.484495	0.112605	2.784323
1	-1.520624	-0.105811	2.289177
14	-2.789676	-1.464383	3.857142
6	-1.161053	-2.414306	3.947447
1	-1.258220	-3.298137	4.598730
1	-0.353365	-1.784857	4.351029
1	-0.839098	-2.761925	2.953974
6	-4.113917	-2.563395	3.077096
1	-3.937148	-2.745637	2.007104
1	-5.112556	-2.109919	3.165483
1	-4.138884	-3.536598	3.595274
6	-3.347385	-1.155072	5.639899
1	-3.440667	-2.132104	6.143318
1	-4.330699	-0.663200	5.698250
1	-2.628665	-0.554830	6.218467
14	-2.071035	1.739931	3.739641
6	-1.913782	3.175712	2.526433
1	-1.647966	4.094262	3.075492
1	-2.871436	3.356694	2.013253
1	-1.142414	3.002409	1.762173
6	-3.378282	2.297158	4.993305
1	-3.585176	1.566197	5.786901
1	-4.329477	2.560583	4.506301
1	-3.002430	3.213962	5.478718
6	-0.441987	1.490709	4.661254
1	0.363452	1.188992	3.974275
1	-0.520872	0.726548	5.450885
1	-0.134858	2.432839	5.144278
6	-4.363574	0.557949	-2.056580
1	-3.384997	0.186018	-2.399965
14	-5.568720	-0.674040	-2.921167
6	-5.898325	-2.149610	-1.796180
1	-6.393310	-1.846682	-0.861365
1	-4.963189	-2.665995	-1.530072
1	-6.550492	-2.875430	-2.309346
6	-4.733635	-1.298864	-4.498820
1	-5.374825	-2.048614	-4.991034
1	-3.773076	-1.785000	-4.267717
1	-4.543946	-0.493624	-5.224164
6	-7.240288	0.063589	-3.423364
1	-7.834450	-0.722311	-3.919175
1	-7.138648	0.894869	-4.138124
1	-7.829324	0.423076	-2.565283
14	-4.377154	2.367864	-2.718171
6	-4.136491	2.368888	-4.595089
1	-4.985049	1.917768	-5.132220
1	-3.222396	1.827491	-4.887260
1	-4.035490	3.407305	-4.951628
6	-2.959392	3.345540	-1.945247
1	-2.997074	4.391584	-2.291892
1	-1.973702	2.938919	-2.216915
1	-3.027136	3.355324	-0.846077
6	-5.966807	3.307668	-2.312879
1	-6.091501	3.433509	-1.226679
1	-6.871753	2.826322	-2.711065
1	-5.901703	4.315480	-2.756369
6	-7.325870	1.130208	1.978318
6	-7.745570	-0.046148	2.880333
1	-8.740675	0.139690	3.316149
1	-7.043227	-0.196826	3.713594
1	-7.795065	-0.986016	2.308561
6	-7.268382	2.421676	2.816125
1	-7.006424	3.288565	2.189550

1	-6.522659	2.353622	3.621648
1	-8.246226	2.622492	3.283401
6	-8.397320	1.307623	0.894669
1	-8.173789	2.154544	0.228290
1	-9.372723	1.508236	1.364709
1	-8.508699	0.403727	0.276104

Table S25

B3PW91/def2-SVP

Prod-Se (= Prod-Ge)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.639204	0.158299	-0.844912
1	1.469629	1.071024	-2.084491
34	0.220898	1.029467	0.858401
32	-1.582066	0.172370	-0.425255
1	-1.564029	1.083701	-1.672449
6	0.602740	-1.450445	-1.431896
6	-0.734927	-1.467591	-1.197580
6	1.220622	-2.421172	-2.378376
6	1.762717	-1.961388	-3.592025
1	1.795250	-0.888158	-3.796867
6	2.224412	-2.857198	-4.556660
1	2.626470	-2.475383	-5.498732
6	2.172434	-4.231949	-4.322037
1	2.531849	-4.934693	-5.077899
6	1.659055	-4.700721	-3.111752
1	1.613387	-5.775349	-2.916571
6	1.188175	-3.806599	-2.150139
1	0.768580	-4.185448	-1.216291
6	-1.629107	-2.491174	-1.809148
6	-1.835430	-2.534978	-3.198597
1	-1.345907	-1.794552	-3.835409
6	-2.631887	-3.526254	-3.771555
1	-2.772865	-3.546060	-4.855379
6	-3.239006	-4.493598	-2.969010
1	-3.858576	-5.273383	-3.419001
6	-3.053534	-4.453106	-1.586310
1	-3.526875	-5.202250	-0.946357
6	-2.263165	-3.456632	-1.012468
1	-2.112184	-3.438789	0.068433
6	3.494214	0.359561	-0.172984
6	3.996594	1.698186	-0.138421
6	5.236106	1.940634	0.472301
1	5.601665	2.969566	0.479174
6	5.990064	0.944249	1.097299
6	5.487225	-0.353526	1.033372
1	6.044875	-1.167051	1.494097
6	4.278551	-0.682324	0.388144
6	3.284432	2.905947	-0.714476
1	2.256151	2.637952	-1.008001
14	4.055752	3.439012	-2.393456
6	5.873034	3.937785	-2.260046
1	6.224429	4.276114	-3.249155
1	6.500636	3.084885	-1.959902
1	6.043760	4.758125	-1.547649
6	3.079178	4.880650	-3.134122
1	3.157175	5.802649	-2.537662
1	2.010398	4.634475	-3.239320
1	3.467467	5.105802	-4.141295
6	3.967595	2.000738	-3.617898
1	2.928892	1.773813	-3.904187

1	4.413437	1.084526	-3.199641
1	4.520382	2.254811	-4.537516
14	2.949660	4.316380	0.559811
6	4.270206	5.677124	0.587430
1	4.372300	6.194894	-0.378812
1	5.264436	5.302047	0.877278
1	3.978398	6.433607	1.335052
6	1.296723	5.117194	0.121146
1	0.485481	4.372980	0.162561
1	1.298398	5.565868	-0.883517
1	1.058087	5.915025	0.843523
6	2.828894	3.619873	2.309531
1	2.548078	4.425593	3.008036
1	3.783002	3.190762	2.650146
1	2.061978	2.833043	2.376365
6	3.918760	-2.149984	0.344746
1	2.984651	-2.284861	-0.231811
14	5.207718	-3.158119	-0.682002
6	4.704397	-4.978756	-0.763363
1	3.666531	-5.106434	-1.103579
1	4.816861	-5.482585	0.209271
1	5.357427	-5.501104	-1.482038
6	6.982630	-3.118062	-0.019675
1	7.569563	-3.852471	-0.597120
1	7.073848	-3.385867	1.042969
1	7.449611	-2.133808	-0.172227
6	5.290630	-2.448524	-2.425083
1	6.058105	-2.978169	-3.013461
1	5.562505	-1.381239	-2.401052
1	4.331795	-2.545842	-2.953572
14	3.479943	-2.865706	2.078960
6	2.260375	-4.292892	1.860619
1	1.931156	-4.661698	2.845608
1	2.700659	-5.140151	1.314657
1	1.362814	-3.964904	1.314434
6	4.969234	-3.531627	3.040664
1	4.625063	-3.882602	4.027903
1	5.738809	-2.764079	3.216218
1	5.445970	-4.386167	2.535900
6	2.671414	-1.517708	3.117087
1	1.789929	-1.093682	2.610181
1	3.371127	-0.690157	3.311586
1	2.347275	-1.923782	4.089190
6	7.309618	1.298636	1.800450
6	7.929317	0.092351	2.518056
1	7.255550	-0.316362	3.287073
1	8.859547	0.396978	3.022702
1	8.185920	-0.719197	1.820885
6	7.059298	2.397499	2.850725
1	6.662895	3.319571	2.400699
1	7.999713	2.658005	3.362873
1	6.340189	2.059925	3.613396
6	8.316142	1.811860	0.752878
1	8.516232	1.045353	-0.012165
1	9.274310	2.072093	1.231834
1	7.945958	2.710731	0.237559
6	-3.408926	0.222016	0.345032
6	-3.680724	-0.121209	1.702522
6	-4.997059	-0.033563	2.180943
1	-5.174114	-0.316566	3.221171
6	-6.070940	0.390889	1.394597
6	-5.779222	0.746670	0.079800
1	-6.580622	1.092178	-0.572429

6	-4.486323	0.676546	-0.473524
6	-2.630795	-0.560592	2.694583
1	-1.646987	-0.611176	2.193014
14	-2.864969	-2.367016	3.338520
6	-1.194257	-3.230965	3.174674
1	-1.256719	-4.281755	3.501067
1	-0.425868	-2.733472	3.786773
1	-0.836544	-3.221135	2.133589
6	-4.158435	-3.290604	2.315535
1	-4.046175	-3.119793	1.235096
1	-5.178642	-2.979808	2.587081
1	-4.076778	-4.373599	2.507191
6	-3.403283	-2.537825	5.145273
1	-3.454425	-3.612949	5.386984
1	-4.402105	-2.113707	5.330204
1	-2.697609	-2.075445	5.852234
14	-2.318265	0.796834	4.033247
6	-2.244713	2.497045	3.215913
1	-2.044296	3.265661	3.980764
1	-3.210704	2.737518	2.744227
1	-1.462056	2.577840	2.447051
6	-3.667067	0.954663	5.353904
1	-3.810483	0.052085	5.963434
1	-4.636937	1.237885	4.917481
1	-3.371618	1.770242	6.035715
6	-0.683759	0.415071	4.898261
1	0.146600	0.358976	4.177419
1	-0.719614	-0.538120	5.449421
1	-0.445184	1.208137	5.625775
6	-4.368124	1.120194	-1.917299
1	-3.365791	0.877886	-2.303978
14	-5.503754	0.160159	-3.142127
6	-5.818187	-1.583738	-2.499621
1	-6.397368	-1.576818	-1.564051
1	-4.873804	-2.115343	-2.307249
1	-6.384808	-2.163178	-3.247173
6	-4.604045	0.035168	-4.801117
1	-5.215508	-0.537307	-5.517936
1	-3.643653	-0.491970	-4.689513
1	-4.403351	1.020938	-5.246763
6	-7.183958	0.972667	-3.470151
1	-7.750898	0.339856	-4.173336
1	-7.088487	1.968563	-3.929794
1	-7.794401	1.075227	-2.559580
14	-4.400756	3.041713	-2.046457
6	-4.118542	3.576767	-3.839848
1	-4.949423	3.294767	-4.504971
1	-3.191719	3.145598	-4.250960
1	-4.020098	4.674123	-3.882566
6	-3.013550	3.773562	-0.995597
1	-3.061921	4.874657	-1.029600
1	-2.016567	3.471795	-1.351157
1	-3.099504	3.468990	0.059180
6	-6.017010	3.808013	-1.434241
1	-6.164959	3.625305	-0.358830
1	-6.903194	3.439400	-1.971432
1	-5.968648	4.900218	-1.580230
6	-7.488337	0.464181	1.983476
6	-7.880700	-0.908261	2.561980
1	-8.900300	-0.871159	2.978650
1	-7.205924	-1.224274	3.371414
1	-7.860176	-1.687082	1.783704
6	-7.514772	1.519601	3.105508

1	-7.240194	2.513912	2.719971
1	-6.815341	1.270685	3.917441
1	-8.523214	1.591714	3.544771
6	-8.534999	0.854323	0.931686
1	-8.344228	1.852180	0.508175
1	-9.534386	0.880922	1.393337
1	-8.573006	0.130632	0.102793

Table S26
B3PW91/def2-SVP
 Prod-Te

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
32	1.701862	0.346408	-0.752289
1	1.543490	1.522818	-1.745769
52	0.257140	0.896151	1.313329
32	-1.638658	0.302582	-0.326837
1	-1.596073	1.488832	-1.314661
6	0.594343	-1.048241	-1.675022
6	-0.746694	-1.094061	-1.460435
6	1.197773	-1.792808	-2.817757
6	1.760695	-1.084324	-3.894266
1	1.821765	0.005968	-3.850123
6	2.207949	-1.749632	-5.036041
1	2.627111	-1.174574	-5.865806
6	2.118892	-3.139806	-5.120176
1	2.465719	-3.661827	-6.015478
6	1.585512	-3.857389	-4.048407
1	1.511547	-4.946711	-4.102298
6	1.131755	-3.192845	-2.909093
1	0.698560	-3.762628	-2.084931
6	-1.641142	-1.928551	-2.313521
6	-1.820691	-1.632720	-3.675709
1	-1.313350	-0.765966	-4.105456
6	-2.609946	-2.448065	-4.486156
1	-2.728310	-2.204230	-5.545128
6	-3.239326	-3.574042	-3.952524
1	-3.853359	-4.215960	-4.589161
6	-3.082934	-3.869701	-2.597561
1	-3.574228	-4.745745	-2.166329
6	-2.297981	-3.050230	-1.785538
1	-2.168214	-3.296532	-0.730103
6	3.578897	0.315218	-0.099950
6	4.161309	1.591097	0.187440
6	5.387161	1.637082	0.868277
1	5.814351	2.621618	1.070170
6	6.054223	0.498108	1.326725
6	5.481992	-0.730854	1.007179
1	5.974193	-1.648651	1.324248
6	4.285492	-0.858763	0.274486
6	3.560857	2.928911	-0.202099
1	2.516684	2.797072	-0.529351
14	4.406629	3.606653	-1.792700
6	6.269278	3.844452	-1.587916
1	6.681746	4.270267	-2.517866
1	6.777050	2.884705	-1.407898
1	6.526773	4.528357	-0.765799
6	3.631056	5.251914	-2.315673
1	3.813556	6.063562	-1.595104
1	2.542091	5.159283	-2.455209
1	4.062775	5.564067	-3.281074

6	4.148173	2.393109	-3.218561
1	3.092005	2.355037	-3.528004
1	4.462947	1.372655	-2.950736
1	4.740664	2.710407	-4.092736
14	3.351996	4.191477	1.240957
6	4.802722	5.396398	1.447674
1	4.971646	6.023916	0.558940
1	5.749512	4.886496	1.686470
1	4.578434	6.074205	2.288340
6	1.794039	5.205139	0.902226
1	0.913463	4.547769	0.819837
1	1.866288	5.797261	-0.022396
1	1.610786	5.905500	1.733696
6	3.130287	3.310238	2.895751
1	2.985367	4.059737	3.691579
1	4.001474	2.694150	3.162773
1	2.244072	2.657319	2.888109
6	3.866511	-2.267342	-0.079961
1	2.934885	-2.238688	-0.674985
14	5.130349	-3.061477	-1.307597
6	4.550579	-4.786101	-1.821520
1	3.527635	-4.770757	-2.224633
1	4.585570	-5.504369	-0.987482
1	5.215061	-5.168956	-2.613789
6	6.893144	-3.255201	-0.642236
1	7.471693	-3.816482	-1.395721
1	6.958377	-3.811356	0.303930
1	7.388116	-2.281749	-0.509315
6	5.275010	-1.963030	-2.831349
1	5.994290	-2.397343	-3.545135
1	5.638974	-0.960955	-2.554446
1	4.311830	-1.847705	-3.348307
14	3.401704	-3.353984	1.441102
6	2.076664	-4.588084	0.900674
1	1.741858	-5.192348	1.759288
1	2.442386	-5.277757	0.125559
1	1.194639	-4.064267	0.501518
6	4.842856	-4.341865	2.174044
1	4.474096	-4.892186	3.055941
1	5.667919	-3.697254	2.515555
1	5.256470	-5.084828	1.474748
6	2.714385	-2.267054	2.817824
1	1.862954	-1.661485	2.469356
1	3.481201	-1.574491	3.198161
1	2.370813	-2.890401	3.659716
6	7.357796	0.632405	2.129267
6	7.883628	-0.723959	2.616023
1	7.156671	-1.234465	3.266544
1	8.804716	-0.577460	3.201504
1	8.129138	-1.397836	1.781614
6	7.113132	1.518694	3.365204
1	6.783725	2.531437	3.089910
1	8.039232	1.620936	3.954080
1	6.342467	1.081521	4.019228
6	8.434781	1.281455	1.239107
1	8.632893	0.667615	0.346415
1	9.381041	1.389827	1.794025
1	8.132842	2.282342	0.896090
6	-3.507783	0.158600	0.340529
6	-3.847188	-0.500206	1.560527
6	-5.185119	-0.514526	1.984252
1	-5.411874	-1.041796	2.913778
6	-6.219898	0.103643	1.278935

6	-5.863855	0.763648	0.105699
1	-6.631792	1.268112	-0.479385
6	-4.546713	0.811735	-0.390195
6	-2.855995	-1.186853	2.470732
1	-1.843711	-1.124640	2.030971
14	-3.131982	-3.093945	2.623570
6	-1.452273	-3.920209	2.377779
1	-1.538223	-5.016881	2.445794
1	-0.731719	-3.591030	3.142886
1	-1.017694	-3.676106	1.396403
6	-4.350943	-3.712577	1.318213
1	-4.177558	-3.272598	0.325772
1	-5.387208	-3.472917	1.601185
1	-4.273652	-4.809353	1.231364
6	-3.805320	-3.704773	4.284859
1	-3.882055	-4.804165	4.234653
1	-4.812692	-3.317779	4.503466
1	-3.151035	-3.461051	5.135851
14	-2.641934	-0.225342	4.133936
6	-2.537617	1.632276	3.804975
1	-2.427534	2.166297	4.763505
1	-3.463800	1.989316	3.327424
1	-1.694438	1.928823	3.163670
6	-4.065830	-0.398565	5.370877
1	-4.260465	-1.429368	5.695269
1	-5.003410	0.028347	4.984185
1	-3.794790	0.184078	6.267786
6	-1.063683	-0.834233	4.975954
1	-0.189607	-0.744151	4.312219
1	-1.144293	-1.887488	5.289061
1	-0.863462	-0.236115	5.879992
6	-4.369944	1.591556	-1.677570
1	-3.357531	1.432740	-2.081434
14	-5.471348	0.978582	-3.135376
6	-5.852271	-0.856406	-2.933046
1	-6.481644	-1.049725	-2.051424
1	-4.929663	-1.446328	-2.822791
1	-6.387110	-1.228947	-3.822349
6	-4.496944	1.217119	-4.738830
1	-5.082785	0.845124	-5.595458
1	-3.552427	0.651871	-4.711716
1	-4.256557	2.273274	-4.932370
6	-7.119291	1.893822	-3.336119
1	-7.654247	1.465122	-4.200140
1	-6.987056	2.968833	-3.534341
1	-7.779267	1.788120	-2.460946
14	-4.390146	3.488243	-1.340201
6	-4.079959	4.440178	-2.946297
1	-4.898895	4.328874	-3.673577
1	-3.145047	4.121476	-3.434472
1	-3.984169	5.514882	-2.719298
6	-3.020059	3.942606	-0.123299
1	-3.086136	5.015006	0.124924
1	-2.015773	3.755666	-0.532935
1	-3.109568	3.377647	0.817774
6	-6.012851	4.094254	-0.583147
1	-6.172961	3.663256	0.416978
1	-6.893415	3.865996	-1.201199
1	-5.961633	5.189900	-0.466997
6	-7.664312	0.044580	1.798970
6	-8.093496	-1.426246	1.958531
1	-9.131233	-1.486207	2.324684
1	-7.458378	-1.965528	2.677011

1	-8.040997	-1.960319	0.996903
6	-7.741372	0.752414	3.165073
1	-7.434384	1.806721	3.082299
1	-7.092289	0.271943	3.912038
1	-8.772057	0.727729	3.555102
6	-8.653082	0.730195	0.846983
1	-8.428583	1.800122	0.718847
1	-9.673808	0.655481	1.253381
1	-8.659239	0.259051	-0.148104
