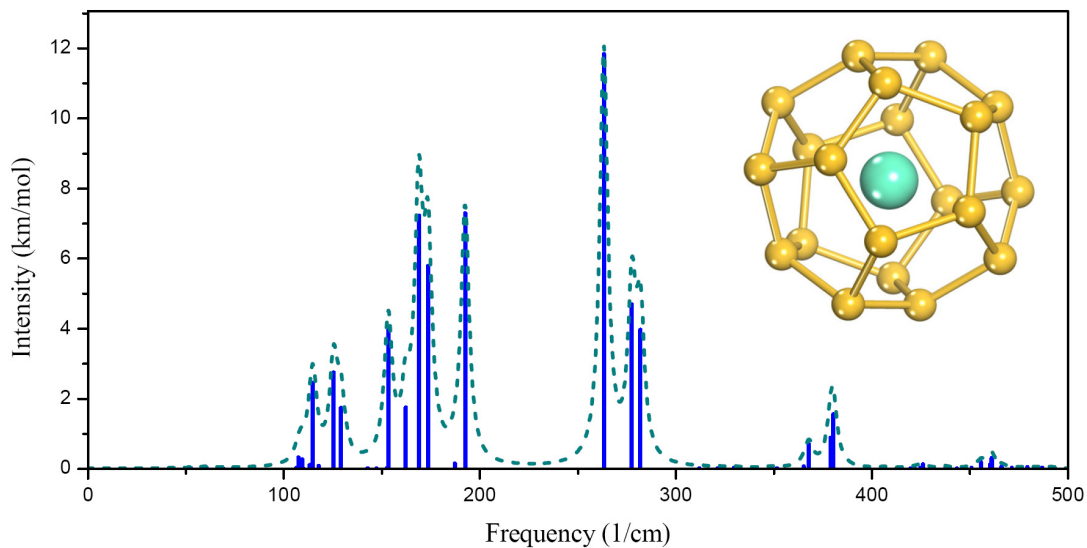
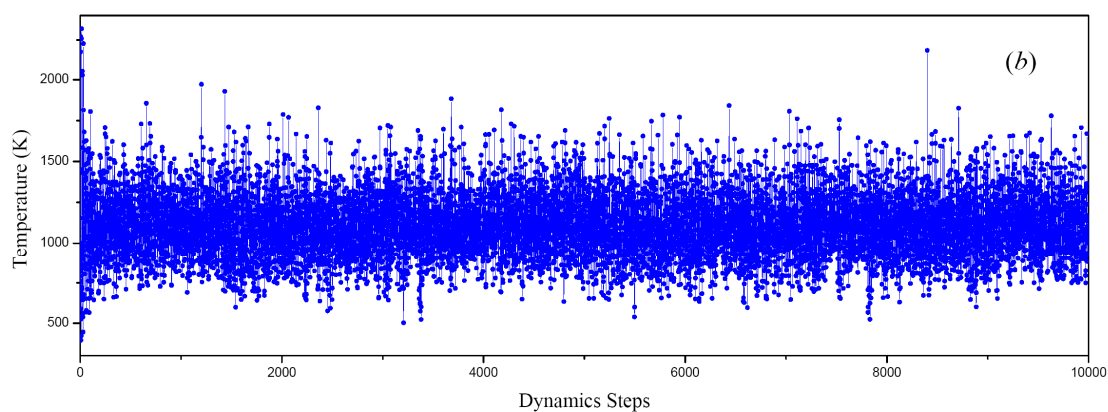
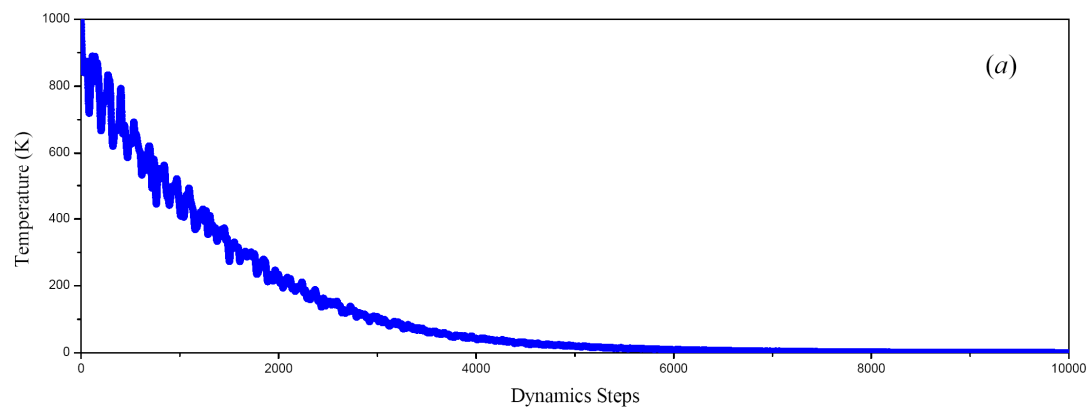


Part I: Frequency Analysis of D_{2h} -Eu@Si₂₀



The frequency spectrum of D_{2h} -Eu@Si₂₀ obtained at the PW91 level. The insert is the stable D_{2h} -Eu@Si₂₀ fullerene cage. Large ball: Eu atom, small ball: Si atom.

Part II: *Ab Initio* Molecular Dynamics



The temperature vs dynamics steps of the molecular dynamics imposed on (a) I_h -Eu@Si₂₀ with a Gaussian thermostat and an initial temperature of 1000 K and (b) D_{2h} -Eu@Si₂₀ with a Massive Nosé-Hoover thermostat and an average temperature of 1000 K at the PW91 level. The *ab initio* molecular dynamics is in the constant-NVT ensemble, a time step of 1.0 femtosecond, 10000 dynamics steps.

Part III: xyz Coordinates for Stationary Points

1. For structures in Table 1

RbSi ₂₀						
Cage	PW91			BLYP		
Si	2.669	-1.094	-1.565	2.705	-1.107	-1.584
Si	2.988	1.089	-0.788	3.029	1.107	-0.798
Si	0.808	-1.087	-2.983	0.821	-1.103	-3.024
Si	-0.015	1.099	-3.087	-0.017	1.113	-3.131
Si	1.333	2.447	-1.730	1.350	2.479	-1.756
Si	-0.840	-2.441	-2.024	-0.852	-2.474	-2.050
Si	-2.685	-1.090	-1.531	-2.722	-1.103	-1.553
Si	-2.177	1.096	-2.192	-2.206	1.113	-2.221
Si	-0.002	-3.277	-0.005	-0.003	-3.322	-0.005
Si	-1.333	-2.447	1.730	-1.350	-2.479	1.756
Si	-2.988	-1.089	0.788	-3.029	-1.107	0.798
Si	2.165	-2.443	0.279	2.194	-2.478	0.282
Si	2.177	-1.096	2.192	2.206	-1.113	2.221
Si	0.016	-1.099	3.087	0.017	-1.113	3.131
Si	2.686	1.090	1.531	2.722	1.103	1.553
Si	0.840	2.441	2.024	0.852	2.474	2.050
Si	-0.808	1.087	2.983	-0.820	1.103	3.024
Si	-2.668	1.094	1.564	-2.704	1.107	1.584
Si	-2.165	2.444	-0.280	-2.194	2.478	-0.282
Si	0.002	3.277	0.005	0.003	3.322	0.005
Rb	0.000	0.000	0.000	0.000	-0.000	0.000
No.1	PW91			BLYP		
Si	2.162	1.390	-2.063	2.203	1.410	-2.045
Si	-1.223	4.382	1.850	-1.258	4.474	1.878
Si	-0.174	1.685	-1.670	-0.165	1.728	-1.761
Si	-2.237	0.850	1.173	-2.306	0.914	1.139
Si	-0.455	2.146	2.008	-0.540	2.190	2.104
Si	-1.410	3.673	-2.003	-1.413	3.761	-2.021
Si	1.629	2.236	0.099	1.649	2.320	0.113
Si	1.784	1.383	2.310	1.728	1.378	2.312
Si	0.117	4.026	-0.131	0.122	4.131	-0.131
Si	-2.184	2.992	0.153	-2.249	3.098	0.157
Si	-0.800	-0.404	-0.404	-0.833	-0.400	-0.452
Si	2.677	-2.379	0.483	2.721	-2.449	0.511
Si	-1.363	-2.795	-0.223	-1.379	-2.846	-0.196
Si	1.654	-0.790	-1.221	1.745	-0.853	-1.258
Si	-0.292	-4.262	-1.865	-0.369	-4.303	-1.896
Si	-0.265	-1.806	-2.378	-0.244	-1.844	-2.408
Si	0.906	-4.090	0.288	0.940	-4.226	0.270
Si	-0.054	-2.562	1.807	0.005	-2.678	1.843
Si	2.057	-3.080	-1.822	2.147	-3.166	-1.864
Si	1.121	-0.584	1.178	1.092	-0.636	1.151
Rb	-3.655	-2.014	2.432	-3.599	-2.007	2.556
No.2	PW91			BLYP		
Si	-1.520	3.485	2.953	-1.573	3.531	2.977
Si	-1.122	2.791	-1.308	-1.096	2.835	-1.345
Si	-3.417	2.122	-0.812	-3.433	2.172	-0.847
Si	-0.607	1.464	2.060	-0.628	1.498	2.062
Si	-1.287	5.107	-0.502	-1.332	5.179	-0.499
Si	0.922	2.142	0.129	0.999	2.305	0.182
Si	1.722	0.798	2.006	1.727	0.821	2.043
Si	-0.041	4.005	1.184	-0.049	4.142	1.239
Si	-2.660	3.721	0.824	-2.753	3.804	0.830
Si	-0.713	-1.190	-0.586	-0.728	-1.218	-0.567
Si	2.969	-2.525	-0.416	3.004	-2.545	-0.490
Si	-0.724	-2.640	1.430	-0.715	-2.725	1.451
Si	1.466	-1.138	-1.730	1.425	-1.217	-1.822
No.3	PW91			BLYP		
Si	-0.866	2.093	-1.508	-0.931	2.087	-1.640
Si	-2.960	1.582	1.796	-3.035	1.634	1.793
Si	-0.682	1.555	1.209	-0.732	1.588	1.259
Si	-1.510	4.359	-1.463	-1.603	4.381	-1.465
Si	1.399	2.028	-0.202	1.374	2.142	-0.144
Si	1.481	0.977	1.964	1.452	0.980	1.998
Si	0.155	3.996	0.282	0.098	4.138	0.249
Si	-2.268	3.637	0.712	-2.274	3.817	0.871
Si	-0.947	-1.343	-0.176	-0.966	-1.399	-0.238
Si	3.193	-1.785	-0.525	3.239	-1.847	-0.509
Si	-1.784	-3.662	-0.343	-1.793	-3.751	-0.423
Si	1.016	-0.895	-1.530	1.057	-0.937	-1.570
Si	0.460	-4.546	-0.474	0.484	-4.669	-0.486
Si	-0.438	-2.713	-2.289	-0.381	-2.792	-2.382
Si	2.125	-3.506	0.940	2.139	-3.589	0.983
Si	-0.190	-2.992	1.653	-0.215	-3.063	1.671
Si	1.898	-3.311	-1.954	1.973	-3.429	-1.974
Si	1.223	-1.147	0.931	1.217	-1.185	0.943
Si	-2.324	0.587	-0.357	-2.310	0.593	-0.351
Si	1.223	1.298	-2.461	1.241	1.345	-2.440
Rb	-0.208	3.790	3.795	-0.036	3.958	3.854
No.4	PW91			BLYP		
Si	-4.011	1.789	-0.068	-3.982	1.806	-0.093
Si	-0.451	1.769	1.769	-0.460	1.807	1.861
Si	-1.371	5.180	-0.206	-1.346	5.258	-0.300
Si	1.566	1.866	0.139	1.599	1.971	0.169
Si	1.729	0.873	2.331	1.779	0.913	2.359
Si	0.334	3.784	0.420	0.344	3.890	0.502
Si	-2.458	3.327	0.719	-2.513	3.473	0.702
Si	-1.020	-1.228	-0.024	-1.000	-1.266	0.059
Si	2.931	-2.147	-0.215	2.974	-2.205	-0.236
Si	-1.028	-3.311	1.148	-1.087	-3.460	1.077
Si	1.118	-0.880	-1.321	1.148	-0.904	-1.349
Si	-0.003	-4.322	-0.721	0.028	-4.429	-0.783
Si	-0.745	-2.459	-2.142	-0.790	-2.479	-2.125
Si	2.399	-4.676	-0.474	2.441	-4.755	-0.434
Si	1.336	-3.517	1.420	1.314	-3.594	1.459
Si	1.619	-3.038	-2.299	1.623	-3.070	-2.395
Si	1.147	-1.134	1.145	1.223	-1.164	1.175
Si	-2.215	0.646	0.715	-2.200	0.654	0.757
Si	1.722	1.243	-2.123	1.657	1.297	-2.113
Si	-1.007	4.009	2.525	-1.056	4.053	2.598
Rb	-1.593	2.229	-2.742	-1.697	2.204	-2.891
No.5	PW91			BLYP		
Si	-0.818	1.392	1.683	-0.833	1.442	1.761
Si	-0.722	4.140	-0.665	-0.788	4.262	-0.661
Si	1.259	2.120	0.272	1.378	2.170	0.293
Si	1.347	0.746	2.306	1.371	0.754	2.314
Si	1.311	4.524	0.617	1.259	4.592	0.670
Si	-2.569	4.368	0.695	-2.644	4.505	0.715

Part III: xyz Coordinates for Stationary Points

Si	-1.090	-1.328	-0.185	-1.057	-1.345	-0.226
Si	2.966	-2.028	-0.367	3.011	-2.091	-0.400
Si	-0.734	-3.239	1.251	-0.735	-3.272	1.279
Si	1.027	-0.879	-1.395	1.089	-0.890	-1.428
Si	0.100	-4.465	-0.655	0.113	-4.605	-0.613
Si	-0.814	-2.768	-2.100	-0.928	-2.954	-2.038
Si	2.536	-4.614	-0.742	2.568	-4.671	-0.844
Si	1.646	-3.556	1.325	1.702	-3.649	1.379
Si	1.558	-3.015	-2.366	1.471	-3.070	-2.441
Si	1.075	-1.238	1.025	1.119	-1.298	1.046
Si	-2.433	0.573	0.128	-2.382	0.605	0.108
Si	1.247	1.390	-2.070	1.301	1.443	-2.062
Si	-0.655	3.774	1.837	-0.748	3.858	1.892
Si	-0.886	1.813	-1.195	-0.887	1.918	-1.257
Rb	-5.355	2.294	0.601	-5.383	2.297	0.511
No.6	PW91			BLYP		
Si	-1.138	4.465	-1.330	-1.220	4.508	-1.399
Si	1.592	1.842	0.277	1.625	1.951	0.256
Si	1.939	0.708	2.313	1.900	0.769	2.309
Si	0.363	3.758	0.548	0.364	3.876	0.474
Si	-2.447	3.371	0.383	-2.497	3.509	0.454
Si	-1.011	-1.206	-0.037	-1.000	-1.227	-0.050
Si	2.902	-2.179	-0.401	2.938	-2.241	-0.388
Si	-1.049	-3.328	1.060	-1.150	-3.440	0.924
Si	1.042	-0.858	-1.417	1.085	-0.899	-1.473
Si	-0.041	-4.288	-0.833	0.018	-4.408	-0.898
Si	-0.840	-2.403	-2.199	-0.841	-2.472	-2.236
Si	2.353	-4.685	-0.606	2.412	-4.767	-0.486
Si	1.318	-3.524	1.288	1.243	-3.578	1.355
Si	1.530	-2.999	-2.458	1.590	-3.059	-2.540
Si	1.229	-1.139	1.049	1.264	-1.160	1.060
Si	-2.250	0.765	-0.275	-2.250	0.773	-0.267
Si	1.558	1.383	-2.086	1.571	1.413	-2.122
Si	-1.265	4.975	1.606	-1.218	5.048	1.695
Si	-0.552	2.112	-1.164	-0.592	2.155	-1.231
Si	-3.962	1.689	0.897	-3.914	1.705	0.998
Rb	-1.274	1.539	3.387	-1.332	1.542	3.568
No.7	PW91			BLYP		
Si	0.634	2.069	0.445	0.751	2.119	0.477
Si	1.122	0.689	2.393	1.135	0.690	2.434
Si	0.304	4.417	0.979	0.276	4.476	0.991
Si	-1.779	3.811	-0.192	-1.860	3.891	-0.203
Si	-1.207	-1.569	0.045	-1.185	-1.614	0.045
Si	2.896	-1.683	-0.597	2.947	-1.733	-0.584
Si	-0.417	-3.503	1.256	-0.471	-3.639	1.200
Si	0.705	-0.851	-1.369	0.750	-0.877	-1.388
Si	0.418	-4.528	-0.757	0.437	-4.665	-0.812
Si	-0.900	-2.906	-1.957	-0.916	-2.994	-1.971
Si	2.830	-4.266	-1.054	2.876	-4.333	-1.056
Si	1.987	-3.459	1.142	1.985	-3.565	1.197
Si	1.444	-2.808	-2.528	1.464	-2.853	-2.602
Si	1.063	-1.248	1.017	1.106	-1.303	1.051
Si	-2.889	-0.007	0.606	-2.856	0.016	0.612
Si	0.409	1.418	-1.900	0.456	1.446	-1.870
Si	-1.420	3.360	2.251	-1.479	3.443	2.288
Si	-1.639	1.490	-0.763	-1.664	1.556	-0.809
Si	-3.512	3.831	1.350	-3.577	4.008	1.384
Si	-1.180	0.982	1.958	-1.199	1.035	2.050
Rb	1.131	4.761	-2.325	1.022	4.895	-2.433
No.8	PW91			BLYP		
Si	0.501	0.316	3.028	0.553	0.336	3.042
Si	0.300	3.210	-0.324	0.313	3.413	-0.371
Si	-2.183	3.747	0.517	-2.225	3.875	0.542
Si	-1.310	-1.272	-0.255	-1.275	-1.297	-0.245
Si	2.733	-1.795	0.055	2.785	-1.866	0.062
Si	-1.053	-3.373	0.894	-1.114	-3.483	0.822
Si	0.906	-0.553	-1.101	0.976	-0.595	-1.134
Si	0.147	-4.256	-0.993	0.151	-4.388	-1.043
Si	-0.660	-2.392	-2.289	-0.684	-2.471	-2.306
Si	2.549	-4.336	-0.694	2.570	-4.441	-0.668
Si	1.319	-3.541	1.313	1.284	-3.648	1.360
Si	1.745	-2.510	-2.231	1.779	-2.584	-2.301
Si	0.629	-1.229	1.256	0.678	-1.282	1.280
Si	-2.389	0.803	-0.132	-2.374	0.802	-0.116
Si	1.074	1.648	-2.054	1.071	1.693	-2.067
Si	-0.309	3.903	1.921	-0.344	3.983	1.964
Si	-1.300	1.970	-1.865	-1.309	2.013	-1.859
Si	-3.450	1.950	1.638	-3.505	1.982	1.616
Si	-1.036	1.606	1.780	-1.083	1.664	1.918
Si	-1.409	4.301	-1.640	-1.496	4.374	-1.680
Rb	3.190	1.803	1.174	3.244	1.921	1.183
No.9	PW91			BLYP		
Si	0.984	4.484	0.587	0.806	4.791	0.462
Si	-2.839	3.619	0.863	-3.029	3.789	0.662
Si	-1.159	-1.302	-0.318	-1.023	-1.330	-0.079
Si	2.668	-2.132	0.222	2.811	-2.387	0.125
Si	-1.358	-3.408	0.770	-1.297	-3.578	0.760
Si	1.072	-0.904	-1.154	1.187	-0.953	-1.057
Si	-0.021	-4.375	-0.958	-0.062	-4.483	-1.114
Si	-0.518	-2.464	-2.388	-0.614	-2.395	-2.306
Si	2.285	-4.701	-0.285	2.294	-4.910	-0.580
Si	0.925	-3.559	1.402	1.039	-3.902	1.319
Si	1.852	-2.988	-2.141	1.789	-2.987	-2.316
Si	0.685	-1.127	1.340	0.938	-1.445	1.482
Si	-2.066	0.888	-0.361	-1.984	0.868	-0.166
Si	1.521	1.376	-1.662	1.609	1.391	-1.525
Si	-0.869	3.905	2.009	-1.146	4.350	1.889
Si	-0.818	2.103	-1.977	-0.789	2.007	-1.908
Si	-3.704	1.411	1.246	-3.781	1.535	1.271
Si	-1.392	1.525	2.040	-1.547	1.958	2.191
Si	-1.016	4.146	-0.717	-1.103	4.191	-0.904
Si	0.258	2.133	0.234	0.301	2.312	0.332
Rb	3.508	1.367	1.249	3.599	1.175	1.462
No.10	PW91			BLYP		
Si	-1.803	3.606	0.473	-1.941	3.752	0.513
Si	-1.200	-1.331	-0.372	-1.138	-1.362	-0.276
Si	2.886	-1.975	-0.382	2.925	-2.070	-0.348
Si	-0.875	-2.992	1.331	-1.057	-3.302	1.166
Si	0.935	-1.035	-1.628	0.986	-1.088	-1.653
Si	0.035	-4.418	-0.364	0.088	-4.542	-0.518
Si	-0.813	-2.964	-2.111	-0.800	-2.919	-2.192
Si	2.464	-4.603	-0.293	2.516	-4.661	-0.156
Si	1.497	-3.184	1.500	1.337	-3.268	1.550
Si	1.585	-3.282	-2.222	1.677	-3.352	-2.325
Si	0.979	-0.954	0.791	1.078	-0.953	0.832
Si	-2.170	0.809	-0.303	-2.166	0.788	-0.217
Si	1.239	1.188	-2.439	1.219	1.185	-2.471
Si	-2.195	3.152	2.762	-2.187	3.270	2.830
Si	-0.917	2.008	-1.958	-0.953	1.996	-1.937
Si	-3.672	2.217	0.899	-3.736	2.218	0.955
Si	-1.068	1.373	1.726	-1.047	1.479	1.794
Si	-0.246	4.226	-1.205	-0.349	4.262	-1.242
Si	1.047	2.329	-0.348	1.140	2.433	-0.403
Si	1.305	1.181	1.787	1.352	1.267	1.782
Rb	0.987	4.649	2.360	1.053	4.865	2.318
No.11	PW91			BLYP		
Si	-1.065	-1.110	-0.222	-1.032	-1.134	-0.285
Si	2.898	-2.194	-0.276	2.954	-2.260	-0.282
Si	-0.926	-3.058	1.225	-0.954	-3.104	1.204
Si	1.115	-0.800	-1.319	1.198	-0.824	-1.347
Si	-0.165	-4.324	-0.704	-0.153	-4.459	-0.694
Si	-0.909	-2.563	-2.132	-0.978	-2.716	-2.126

Part III: xyz Coordinates for Stationary Points

Si	2.247	-4.701	-0.797	2.283	-4.770	-0.858
Si	1.422	-3.651	1.324	1.443	-3.738	1.388
Si	1.435	-2.949	-2.346	1.418	-3.003	-2.421
Si	1.036	-1.296	1.090	1.080	-1.347	1.104
Si	-2.129	0.955	-0.088	-2.103	0.967	-0.110
Si	1.650	1.434	-1.960	1.713	1.481	-1.930
Si	-1.605	3.931	1.510	-1.603	4.059	1.601
Si	-0.423	2.339	-1.075	-0.430	2.388	-1.171
Si	-2.810	1.870	2.150	-2.869	1.945	2.158
Si	-0.574	1.508	1.710	-0.634	1.494	1.786
Si	-0.872	4.631	-0.818	-0.907	4.701	-0.856
Si	1.688	1.839	0.387	1.688	1.953	0.441
Si	1.493	0.608	2.452	1.485	0.621	2.485
Si	0.663	3.914	0.839	0.645	4.050	0.816
Rb	-4.171	3.619	-0.952	-4.248	3.697	-0.907
No.12	PW91			BLYP		
Si	1.887	-1.014	0.498	1.837	-1.053	0.531
Si	-0.633	-4.919	-1.008	-0.641	-4.986	-1.016
Si	0.431	-1.063	-1.592	0.380	-1.123	-1.654
Si	1.384	-4.200	-0.090	1.425	-4.362	-0.128
Si	0.646	-3.250	-2.418	0.716	-3.318	-2.521
Si	1.236	-2.907	1.928	1.336	-3.063	1.910
Si	-0.891	-3.492	1.030	-0.874	-3.578	1.082
Si	2.637	-2.498	-1.321	2.669	-2.556	-1.295
Si	-0.560	-1.233	0.562	-0.636	-1.290	0.512
Si	-1.875	0.708	0.751	-1.758	0.766	0.808
Si	0.566	1.034	-2.728	0.567	1.049	-2.734
Si	-0.288	4.054	1.718	-0.258	4.163	1.765
Si	-0.882	1.923	-1.015	-0.966	2.000	-1.069
Si	-1.687	2.128	2.755	-1.786	2.207	2.801
Si	0.293	1.506	1.566	0.347	1.650	1.806
Si	-1.665	4.191	-0.632	-1.687	4.311	-0.722
Si	1.652	1.869	-0.787	1.627	1.962	-0.776
Si	2.616	1.113	1.268	2.639	1.109	1.263
Si	0.646	4.002	-0.420	0.640	4.114	-0.429
Si	-2.574	4.296	1.727	-2.569	4.430	1.742
Rb	-2.937	-2.251	-1.793	-3.008	-2.434	-1.880
No.13	PW91			BLYP		
Si	-1.012	-3.074	1.299	-1.033	-3.139	1.270
Si	1.029	-0.902	-1.334	1.127	-0.906	-1.355
Si	-0.122	-4.315	-0.644	-0.162	-4.470	-0.648
Si	-0.950	-2.821	-2.304	-1.033	-2.932	-2.289
Si	2.166	-4.735	-0.755	2.158	-4.725	-0.771
Si	1.360	-3.547	1.370	1.347	-3.624	1.484
Si	1.422	-2.989	-2.313	1.370	-3.024	-2.409
Si	0.844	-1.278	1.029	0.951	-1.316	1.030
Si	-2.092	0.872	-0.364	-2.064	0.881	-0.382
Si	1.594	1.315	-1.956	1.647	1.379	-1.949
Si	-1.074	4.057	2.508	-1.115	4.144	2.535
Si	-0.589	2.221	-1.531	-0.600	2.278	-1.588
Si	-3.481	1.806	1.226	-3.516	1.795	1.189
Si	-1.089	1.696	1.881	-1.159	1.724	2.018
Si	-1.072	4.551	-1.397	-1.138	4.637	-1.404
Si	1.176	1.823	0.349	1.181	1.932	0.360
Si	0.992	0.635	2.429	1.003	0.666	2.419
Si	0.235	3.969	0.529	0.208	4.087	0.534
Si	-2.322	3.835	0.535	-2.403	3.918	0.565
Si	-1.205	-1.302	-0.376	-1.144	-1.306	-0.409
Rb	4.192	-1.815	-0.179	4.375	-1.999	-0.199
No.14	PW91			BLYP		
Si	-1.669	0.559	-0.244	-1.674	0.571	-0.259
Si	1.644	1.668	-2.207	1.671	1.678	-2.222
Si	-0.957	3.807	2.613	-0.957	3.912	2.639
Si	-0.640	2.164	-1.561	-0.661	2.194	-1.611
Si	-3.006	1.156	1.545	-3.036	1.180	1.532
Si	-0.602	1.486	1.981	-0.646	1.533	2.151
Si	-1.541	4.341	-1.245	-1.575	4.403	-1.250
Si	1.371	1.989	0.116	1.380	2.042	0.125
Si	1.695	0.817	2.157	1.689	0.831	2.173
Si	0.086	3.933	0.481	0.091	4.022	0.478
Si	-2.384	3.371	0.788	-2.440	3.463	0.837
Si	-0.396	-1.425	-0.315	-0.392	-1.442	-0.364
Si	3.136	-2.059	-0.564	3.190	-2.068	-0.547
Si	1.577	-0.612	-1.576	1.623	-0.668	-1.662
Si	0.821	-4.126	-0.248	0.806	-4.271	-0.278
Si	-1.024	-3.410	-1.552	-1.010	-3.464	-1.613
Si	2.731	-4.199	-1.591	2.784	-4.245	-1.575
Si	-0.034	-2.894	1.640	-0.036	-2.962	1.608
Si	1.035	-2.726	-2.520	1.084	-2.811	-2.618
Si	1.669	-1.386	1.178	1.678	-1.415	1.217
Rb	-3.514	-2.453	1.125	-3.569	-2.482	1.239
No.15	PW91			BLYP		
Si	-1.919	0.523	0.539	-1.851	0.536	0.562
Si	1.646	1.226	-1.708	1.670	1.249	-1.714
Si	-1.390	3.906	2.519	-1.420	3.962	2.549
Si	-0.561	1.940	-1.069	-0.612	2.009	-1.229
Si	-3.051	1.776	-1.060	-3.122	1.738	-0.982
Si	-0.657	1.674	2.117	-0.654	1.690	2.222
Si	-0.835	4.366	-1.373	-0.859	4.474	-1.356
Si	1.465	1.923	0.586	1.449	2.005	0.577
Si	1.519	0.808	2.683	1.599	0.856	2.686
Si	0.210	3.934	0.716	0.206	4.040	0.744
Si	-2.311	3.652	0.317	-2.370	3.712	0.315
Si	-0.598	-1.339	0.104	-0.628	-1.430	0.158
Si	1.734	-1.020	-0.871	1.771	-1.030	-0.870
Si	-0.426	-3.371	1.314	-0.471	-3.479	1.380
Si	-0.669	-4.936	-0.513	-0.692	-5.005	-0.528
Si	-0.161	-2.864	-1.703	-0.216	-2.890	-1.750
Si	1.561	-4.261	-0.181	1.571	-4.379	-0.190
Si	1.787	-3.522	2.108	1.798	-3.572	2.111
Si	2.196	-2.972	-2.130	2.176	-3.023	-2.138
Si	1.499	-1.247	1.458	1.544	-1.251	1.480
Rb	-1.041	-0.198	-3.850	-0.890	-0.215	-4.027
No.16	PW91			BLYP		
Si	-1.924	0.349	-0.184	-1.842	0.383	-0.115
Si	1.630	1.491	-2.133	1.658	1.507	-2.149
Si	-1.645	3.662	1.641	-1.651	3.711	1.694
Si	-0.583	1.928	-1.285	-0.618	1.972	-1.383
Si	-3.013	1.439	1.731	-3.120	1.448	1.693
Si	-0.639	1.329	1.645	-0.733	1.356	1.887
Si	-1.807	4.001	-1.130	-1.819	4.076	-1.223
Si	1.555	2.093	0.150	1.504	2.166	0.142
Si	1.630	1.161	2.349	1.649	1.176	2.357
Si	0.133	4.012	0.165	0.102	4.102	0.139
Si	-3.680	3.576	0.550	-3.706	3.667	0.581
Si	-0.330	-1.419	-0.106	-0.324	-1.482	-0.140
Si	3.339	-1.856	-0.294	3.405	-1.845	-0.288
Si	-0.619	-3.726	0.501	-0.604	-3.799	0.590
Si	1.656	-0.879	-1.640	1.721	-0.908	-1.726
Si	0.040	-2.404	-2.365	0.085	-2.447	-2.423
Si	3.215	-4.206	0.264	3.236	-4.243	0.197
Si	1.419	-3.159	1.600	1.492	-3.241	1.637
Si	1.261	-3.915	-0.953	1.191	-4.078	-0.977
Si	1.743	-0.852	1.110	1.777	-0.906	1.158
Rb	-3.387	-2.626	-1.611	-3.407	-2.618	-1.647
No.17	PW91			BLYP		
Si	-1.895	0.587	0.143	-1.884	0.600	0.153
Si	1.407	1.303	-2.178	1.356	1.334	-2.266
Si	-0.842	4.271	2.366	-0.782	4.384	2.399
Si	-0.820	1.940	-1.429	-0.904	1.989	-1.475
Si	-3.045	1.542	1.899	-3.028	1.540	1.950
Si	-0.602	1.873	2.062	-0.592	1.945	2.257

Part III: xyz Coordinates for Stationary Points

Si	-1.640	4.181	-1.482	-1.759	4.262	-1.439
Si	1.300	2.039	0.070	1.281	2.135	-0.004
Si	1.673	1.167	2.257	1.714	1.190	2.167
Si	0.080	4.052	0.184	0.057	4.172	0.152
Si	-2.374	3.581	0.728	-2.416	3.680	0.843
Si	-0.734	-1.422	0.010	-0.760	-1.449	-0.084
Si	3.100	-2.319	0.068	3.152	-2.529	0.266
Si	-1.072	-3.737	0.083	-1.154	-3.794	0.078
Si	1.150	-0.908	-1.337	1.168	-0.923	-1.401
Si	0.492	-4.859	-1.597	0.548	-4.848	-1.650
Si	1.527	-4.117	0.344	1.506	-4.292	0.398
Si	0.161	-2.908	1.972	0.124	-2.933	1.970
Si	2.056	-2.965	-1.970	2.210	-2.998	-1.901
Si	1.394	-0.929	1.188	1.420	-0.964	1.144
Rb	-1.321	-2.368	-3.383	-1.262	-2.498	-3.558
No.18	PW91			BLYP		
Si	-2.135	1.000	-0.321	-2.117	0.987	-0.321
Si	1.525	1.380	-2.017	1.547	1.415	-2.040
Si	-0.969	4.170	2.508	-0.972	4.271	2.530
Si	-0.652	2.317	-1.539	-0.683	2.350	-1.590
Si	-3.424	1.896	1.368	-3.451	1.887	1.361
Si	-1.018	1.807	1.916	-1.074	1.850	2.088
Si	-1.142	4.644	-1.394	-1.214	4.706	-1.402
Si	1.169	1.893	0.274	1.180	1.983	0.269
Si	1.088	0.753	2.376	1.106	0.791	2.369
Si	0.252	4.056	0.473	0.243	4.162	0.460
Si	-2.290	3.924	0.588	-2.356	3.997	0.638
Si	-1.258	-1.175	-0.341	-1.217	-1.205	-0.376
Si	2.499	-2.312	-0.226	2.580	-2.358	-0.215
Si	-1.126	-3.197	0.933	-1.152	-3.222	0.966
Si	0.888	-0.849	-1.439	0.963	-0.878	-1.484
Si	0.450	-4.334	-0.660	0.384	-4.434	-0.683
Si	-0.898	-2.773	-2.084	-0.891	-2.803	-2.169
Si	1.250	-3.500	1.595	1.257	-3.573	1.601
Si	1.552	-2.925	-2.459	1.596	-2.998	-2.482
Si	0.694	-1.217	1.088	0.739	-1.252	1.110
Rb	3.541	-5.559	-0.637	3.526	-5.676	-0.628
No.19	PW91			BLYP		
Si	-2.063	0.906	-0.449	-2.063	0.906	-0.449
Si	1.661	1.497	-2.069	1.661	1.497	-2.069
Si	-1.051	4.152	2.515	-1.051	4.152	2.515
Si	-0.618	2.346	-1.633	-0.618	2.346	-1.633
Si	-3.469	1.777	1.187	-3.469	1.777	1.187
Si	-1.107	1.742	2.003	-1.107	1.742	2.003
Si	-1.178	4.688	-1.416	-1.178	4.688	-1.416
Si	1.220	1.985	0.253	1.220	1.985	0.253
Si	1.101	0.738	2.301	1.101	0.738	2.301
Si	0.226	4.129	0.477	0.226	4.129	0.477
Si	-2.382	3.912	0.578	-2.382	3.912	0.578
Si	-1.092	-1.260	-0.554	-1.092	-1.260	-0.554
Si	2.815	-2.210	-0.205	2.815	-2.210	-0.205
Si	-0.964	-2.903	1.223	-0.964	-2.903	1.223
Si	1.172	-0.746	-1.373	1.172	-0.746	-1.373
Si	0.055	-4.268	-0.650	0.055	-4.268	-0.650
Si	-1.001	-2.969	-2.347	-1.001	-2.969	-2.347
Si	2.416	-4.583	-1.042	2.416	-4.583	-1.042
Si	1.451	-2.921	-2.458	1.451	-2.921	-2.458
Si	0.883	-1.398	1.161	0.883	-1.398	1.161
Rb	1.923	-4.616	2.496	1.923	-4.616	2.496
No.20	PW91			BLYP		
Si	-1.983	0.748	-0.053	-2.007	0.766	-0.075
Si	1.503	1.300	-1.971	1.504	1.322	-2.016
Si	-1.006	4.208	2.456	-0.984	4.290	2.491
Si	-0.703	2.095	-1.474	-0.740	2.134	-1.531
Si	-3.267	1.621	1.652	-3.304	1.655	1.641
Si	-0.843	1.818	2.044	-0.892	1.850	2.198
Si	-1.446	4.356	-1.459	-1.479	4.436	-1.452
Si	1.246	1.992	0.266	1.251	2.047	0.243
Si	1.384	0.990	2.425	1.395	1.005	2.408
Si	0.103	4.053	0.349	0.115	4.140	0.346
Si	-2.401	3.673	0.637	-2.446	3.786	0.694
Si	-0.964	-1.395	-0.151	-1.006	-1.412	-0.185
Si	2.781	-2.165	-0.135	2.835	-2.176	-0.135
Si	-1.512	-3.541	0.807	-1.512	-3.591	0.794
Si	1.177	-1.045	-1.548	1.214	-1.061	-1.593
Si	0.044	-4.007	-0.870	0.032	-4.144	-0.902
Si	-0.686	-2.239	-2.385	-0.663	-2.304	-2.411
Si	2.151	-4.517	0.131	2.182	-4.563	0.133
Si	0.738	-3.254	1.562	0.753	-3.345	1.616
Si	1.196	-0.960	1.104	1.207	-1.027	1.147
Rb	2.486	-3.733	-3.387	2.543	-3.810	-3.411
No.21	PW91			BLYP		
Si	-1.300	0.677	0.360	-1.313	0.652	0.355
Si	2.161	1.300	-1.548	2.192	1.336	-1.542
Si	-1.757	4.750	1.542	-1.809	4.810	1.566
Si	-0.275	1.394	-1.698	-0.280	1.374	-1.738
Si	-3.462	1.328	1.063	-3.496	1.352	1.076
Si	-1.709	2.426	2.221	-1.759	2.456	2.289
Si	-1.447	3.511	-2.161	-1.482	3.544	-2.182
Si	1.061	2.116	0.365	1.069	2.220	0.360
Si	0.321	1.068	2.343	0.343	1.160	2.363
Si	-0.251	4.036	-0.146	-0.273	4.151	-0.163
Si	-2.701	3.318	-0.100	-2.781	3.399	-0.103
Si	0.092	-1.064	1.109	0.140	-1.028	1.202
Si	3.261	-2.787	-0.630	3.284	-2.841	-0.630
Si	-0.565	-3.315	1.505	-0.586	-3.334	1.498
Si	1.946	-0.820	-0.386	1.976	-0.833	-0.373
Si	-1.026	-3.117	-0.800	-1.069	-3.148	-0.829
Si	-0.168	-1.045	-1.709	-0.121	-1.101	-1.808
Si	0.287	-4.748	-1.989	0.268	-4.807	-2.004
Si	1.242	-4.025	0.042	1.240	-4.128	0.054
Si	1.562	-2.651	-2.285	1.624	-2.718	-2.355
Rb	2.725	-2.354	2.901	2.831	-2.516	2.962
CsSi ₂₀						
Cage	PW91			BLYP		
Si	2.852	-1.191	-1.666	2.797	-1.159	-1.638
Si	2.710	0.987	-0.718	2.882	1.066	-0.761
Si	0.883	-1.143	-3.049	0.840	-1.118	-3.039
Si	0.020	1.053	-2.939	0.007	1.120	-3.090
Si	1.440	2.630	-1.857	1.443	2.650	-1.877
Si	-0.872	-2.418	-2.056	-0.871	-2.467	-2.064
Si	-2.868	-1.173	-1.634	-2.868	-1.166	-1.640
Si	-2.176	1.077	-2.099	-2.202	1.082	-2.190
Si	0.008	-3.040	0.031	-0.012	-3.251	0.016
Si	-1.440	-2.630	1.857	-1.443	-2.650	1.877
Si	-2.710	-0.986	0.718	-2.882	-1.066	0.761
Si	2.325	-2.577	0.267	2.246	-2.520	0.273
Si	2.177	-1.077	2.099	2.202	-1.082	2.190
Si	-0.020	-1.053	2.939	-0.007	-1.120	3.090
Si	2.868	1.173	1.634	2.868	1.166	1.640
Si	0.873	2.418	2.057	0.871	2.467	2.064
Si	-0.883	1.143	3.048	-0.840	1.118	3.039
Si	-2.852	1.191	1.666	-2.796	1.159	1.638
Si	-2.325	2.577	-0.267	-2.245	2.520	-0.273
Si	-0.008	3.040	-0.031	0.012	3.251	-0.016
Cs	0.000	0.000	0.000	0.000	-0.000	0.000
No.1	PW91			BLYP		
Cs	-3.692	-0.158	-2.178	-4.015	-0.449	-1.778
Si	0.903	1.345	-2.076	0.842	1.336	-2.020
Si	-0.455	4.386	2.568	-0.363	4.600	2.573
Si	-0.995	2.117	-0.793	-1.097	2.339	-0.884

Part III: xyz Coordinates for Stationary Points

Si	-2.430	1.287	0.947	-2.639	1.794	0.912
Si	-0.417	1.971	1.976	-0.579	2.149	2.068
Si	-1.308	4.544	-1.154	-1.045	4.823	-1.202
Si	1.458	2.116	0.106	1.377	2.118	0.178
Si	1.802	1.127	2.242	1.591	1.050	2.303
Si	0.480	4.234	0.372	0.688	4.364	0.409
Si	-2.099	3.749	0.983	-2.048	4.159	0.906
Si	-1.101	-1.455	0.472	-1.185	-1.812	0.456
Si	2.870	-1.979	-0.293	2.892	-1.973	-0.238
Si	-0.755	-3.866	0.452	-0.640	-4.198	0.338
Si	0.752	-0.865	-1.188	0.660	-0.954	-1.203
Si	0.167	-4.856	-1.593	0.447	-5.020	-1.753
Si	-0.903	-2.537	-1.747	-0.871	-2.748	-1.851
Si	1.886	-4.181	-0.012	2.080	-4.284	-0.067
Si	0.964	-3.189	1.949	1.011	-3.388	1.918
Si	1.676	-2.853	-2.245	1.814	-2.833	-2.296
Si	1.195	-0.934	1.212	1.077	-1.069	1.231
No.2	PW91			BLYP		
Si	-1.789	0.776	0.160	-1.837	0.778	0.151
Cs	1.878	2.120	-3.462	1.971	2.127	-3.451
Si	-1.541	3.488	2.951	-1.599	3.538	2.979
Si	-1.142	2.753	-1.312	-1.114	2.808	-1.331
Si	-3.436	2.091	-0.808	-3.455	2.152	-0.838
Si	-0.625	1.461	2.072	-0.649	1.500	2.071
Si	-1.309	5.077	-0.526	-1.353	5.160	-0.511
Si	0.896	2.121	0.126	0.977	2.288	0.183
Si	1.706	0.802	2.016	1.706	0.822	2.054
Si	-0.063	3.994	1.174	-0.072	4.133	1.236
Si	-2.679	3.704	0.815	-2.775	3.797	0.828
Si	-0.717	-1.203	-0.569	-0.736	-1.234	-0.549
Si	2.967	-2.507	-0.401	3.007	-2.520	-0.479
Si	-0.720	-2.660	1.449	-0.714	-2.750	1.455
Si	1.464	-1.111	-1.704	1.409	-1.211	-1.809
Si	-0.114	-4.486	-0.065	-0.103	-4.627	-0.037
Si	-1.103	-3.203	-1.790	-1.131	-3.286	-1.752
Si	2.230	-4.997	-0.462	2.279	-5.074	-0.478
Si	1.582	-3.510	1.611	1.637	-3.542	1.638
Si	1.246	-3.489	-2.102	1.240	-3.617	-2.176
Si	1.265	-1.226	0.827	1.310	-1.244	0.815
No.3	PW91			BLYP		
Si	-2.283	0.603	-0.309	-2.293	0.603	-0.325
Si	1.230	1.268	-2.505	1.248	1.310	-2.487
Cs	-0.455	3.702	4.086	-0.227	3.967	4.146
Si	-0.857	2.042	-1.586	-0.901	2.067	-1.647
Si	-2.862	1.638	1.828	-2.983	1.676	1.803
Si	-0.627	1.597	1.149	-0.693	1.647	1.205
Si	-1.621	4.276	-1.497	-1.686	4.341	-1.481
Si	1.463	2.029	-0.235	1.453	2.121	-0.192
Si	1.514	0.996	1.946	1.466	0.993	1.982
Si	0.133	3.965	0.074	0.086	4.062	0.089
Si	-2.116	3.806	0.908	-2.188	3.920	1.000
Si	-0.964	-1.356	-0.222	-0.977	-1.410	-0.260
Si	3.180	-1.783	-0.520	3.230	-1.844	-0.535
Si	-1.787	-3.679	-0.362	-1.793	-3.761	-0.464
Si	1.016	-0.919	-1.563	1.053	-0.958	-1.596
Si	0.468	-4.541	-0.456	0.488	-4.669	-0.463
Si	-0.417	-2.748	-2.311	-0.356	-2.825	-2.401
Si	2.099	-3.476	0.968	2.130	-3.565	0.998
Si	-0.220	-2.961	1.643	-0.237	-3.045	1.661
Si	1.917	-3.346	-1.945	1.988	-3.465	-1.958
Si	1.190	-1.114	0.907	1.191	-1.164	0.924
No.4	PW91			BLYP		
Si	-2.210	0.651	0.736	-2.188	0.657	0.784
Si	1.750	1.243	-2.110	1.669	1.304	-2.086
Si	-0.990	4.010	2.542	-1.046	4.056	2.619
Cs	-1.650	2.205	-2.971	-1.819	2.178	-3.172
Si	-4.020	1.791	-0.017	-3.971	1.807	-0.064
Si	-0.442	1.769	1.791	-0.451	1.810	1.892
Si	-1.371	5.173	-0.201	-1.322	5.237	-0.316
Si	1.571	1.866	0.149	1.608	1.965	0.195
Si	1.739	0.871	2.337	1.787	0.905	2.380
Si	0.338	3.783	0.430	0.363	3.891	0.532
Si	-2.449	3.322	0.743	-2.490	3.471	0.712
Si	-1.014	-1.218	-0.018	-0.997	-1.263	0.079
Si	2.932	-2.159	-0.199	2.976	-2.210	-0.222
Si	-1.042	-3.304	1.147	-1.097	-3.462	1.080
Si	1.135	-0.878	-1.312	1.156	-0.894	-1.330
Si	-0.018	-4.312	-0.723	0.017	-4.418	-0.789
Si	-0.737	-2.439	-2.140	-0.784	-2.452	-2.121
Si	2.379	-4.688	-0.466	2.428	-4.759	-0.435
Si	1.319	-3.519	1.421	1.301	-3.600	1.457
Si	1.626	-3.035	-2.293	1.626	-3.058	-2.389
Si	1.150	-1.132	1.151	1.228	-1.167	1.191
No.5	PW91			BLYP		
Si	-2.496	0.611	-0.289	-2.447	0.630	-0.272
Si	1.446	1.402	-2.001	1.479	1.427	-2.001
Si	-0.903	3.751	1.607	-0.992	3.843	1.656
Si	-0.775	1.836	-1.377	-0.783	1.910	-1.447
Cs	-4.656	2.176	2.262	-4.734	2.217	2.213
Si	-1.011	1.353	1.450	-1.027	1.412	1.540
Si	-0.628	4.174	-0.859	-0.703	4.264	-0.857
Si	1.215	2.105	0.329	1.320	2.155	0.342
Si	1.069	0.728	2.350	1.107	0.748	2.353
Si	1.213	4.508	0.710	1.160	4.579	0.724
Si	-2.652	4.393	0.202	-2.717	4.588	0.243
Si	-1.101	-1.283	-0.412	-1.071	-1.313	-0.423
Si	2.946	-2.045	-0.144	2.999	-2.103	-0.161
Si	-0.926	-3.213	1.038	-0.947	-3.290	1.018
Si	1.142	-0.872	-1.372	1.199	-0.906	-1.405
Si	0.106	-4.448	-0.759	0.115	-4.589	-0.759
Si	-0.631	-2.735	-2.282	-0.693	-2.861	-2.266
Si	2.534	-4.621	-0.581	2.572	-4.697	-0.615
Si	1.429	-3.567	1.389	1.447	-3.650	1.441
Si	1.752	-3.008	-2.293	1.739	-3.073	-2.377
Si	0.923	-1.244	1.033	0.975	-1.291	1.052
No.6	PW91			BLYP		
Si	-2.250	0.773	-0.290	-2.242	0.771	-0.276
Si	1.562	1.384	-2.094	1.573	1.406	-2.132
Si	-1.261	4.993	1.575	-1.217	5.048	1.677
Si	-0.547	2.119	-1.180	-0.586	2.156	-1.245
Si	-3.980	1.705	0.850	-3.915	1.704	0.971
Cs	-1.354	1.452	3.608	-1.403	1.568	3.844
Si	-1.128	4.468	-1.348	-1.217	4.504	-1.420
Si	1.600	1.843	0.268	1.627	1.950	0.241
Si	1.977	0.705	2.297	1.912	0.769	2.291
Si	0.366	3.756	0.539	0.369	3.881	0.456
Si	-2.439	3.372	0.366	-2.490	3.505	0.436
Si	-1.009	-1.199	-0.039	-0.996	-1.231	-0.046
Si	2.907	-2.175	-0.418	2.942	-2.244	-0.405
Si	-1.028	-3.311	1.081	-1.148	-3.446	0.912
Si	1.041	-0.854	-1.425	1.082	-0.901	-1.485
Si	-0.047	-4.286	-0.823	0.020	-4.408	-0.916
Si	-0.853	-2.408	-2.190	-0.839	-2.464	-2.245
Si	2.348	-4.685	-0.629	2.414	-4.768	-0.496
Si	1.340	-3.520	1.280	1.243	-3.579	1.343
Si	1.513	-2.998	-2.465	1.593	-3.061	-2.554
Si	1.241	-1.135	1.038	1.275	-1.161	1.049
No.7	PW91			BLYP		
Si	-2.890	-0.029	0.648	-2.860	-0.006	0.636
Si	0.365	1.412	-1.912	0.424	1.443	-1.881
Si	-1.427	3.347	2.268	-1.483	3.427	2.312
Si	-1.667	1.473	-0.743	-1.688	1.541	-0.798
Si	-3.534	3.788	1.387	-3.594	3.970	1.426
Si	-1.168	0.972	1.972	-1.193	1.025	2.054

Part III: xyz Coordinates for Stationary Points

Cs	1.297	4.877	-2.404	1.165	5.056	-2.533
Si	0.614	2.074	0.429	0.737	2.121	0.462
Si	1.144	0.702	2.374	1.145	0.695	2.417
Si	0.267	4.419	0.968	0.247	4.472	0.986
Si	-1.816	3.794	-0.176	-1.887	3.872	-0.177
Si	-1.205	-1.582	0.070	-1.186	-1.627	0.057
Si	2.886	-1.672	-0.628	2.939	-1.728	-0.606
Si	-0.391	-3.509	1.273	-0.444	-3.638	1.229
Si	0.680	-0.855	-1.372	0.733	-0.879	-1.388
Si	0.423	-4.532	-0.747	0.444	-4.672	-0.792
Si	-0.918	-2.919	-1.936	-0.934	-3.023	-1.947
Si	2.830	-4.259	-1.072	2.873	-4.329	-1.087
Si	2.010	-3.449	1.128	2.013	-3.559	1.187
Si	1.420	-2.812	-2.535	1.433	-2.860	-2.602
Si	1.075	-1.242	1.009	1.111	-1.305	1.046
No.8	PW91			BLYP		
Si	-2.397	0.796	-0.129	-2.379	0.789	-0.114
Si	1.054	1.636	-2.078	1.052	1.682	-2.074
Si	-0.289	3.890	1.898	-0.341	3.978	1.944
Si	-1.318	1.961	-1.870	-1.326	2.002	-1.860
Si	-3.439	1.955	1.647	-3.506	1.973	1.621
Si	-1.026	1.598	1.770	-1.088	1.659	1.919
Si	-1.426	4.294	-1.653	-1.516	4.364	-1.691
Cs	3.332	1.953	1.325	3.436	2.094	1.314
Si	0.475	0.285	3.038	0.538	0.321	3.038
Si	0.297	3.202	-0.351	0.300	3.410	-0.391
Si	-2.179	3.745	0.512	-2.231	3.867	0.535
Si	-1.315	-1.282	-0.265	-1.272	-1.303	-0.236
Si	2.728	-1.792	0.052	2.785	-1.896	0.053
Si	-1.060	-3.378	0.895	-1.136	-3.499	0.805
Si	0.901	-0.555	-1.104	0.977	-0.604	-1.139
Si	0.133	-4.264	-0.997	0.131	-4.389	-1.059
Si	-0.672	-2.406	-2.295	-0.690	-2.457	-2.316
Si	2.536	-4.340	-0.712	2.549	-4.456	-0.660
Si	1.315	-3.548	1.305	1.254	-3.657	1.351
Si	1.730	-2.512	-2.236	1.773	-2.595	-2.310
Si	0.620	-1.237	1.249	0.689	-1.282	1.273
No.9	PW91			BLYP		
Si	-2.218	0.952	-0.617	-2.271	0.890	-0.543
Si	1.442	1.382	-1.908	1.441	1.374	-1.905
Si	-0.716	3.366	2.190	-0.756	3.638	2.207
Si	-0.865	2.335	-1.992	-0.918	2.276	-1.982
Si	-3.553	1.279	1.253	-3.557	1.348	1.367
Si	-1.172	1.001	1.727	-1.130	1.183	1.836
Si	-0.963	4.109	-0.332	-1.012	4.176	-0.449
Si	0.390	2.021	0.119	0.426	2.125	0.135
Cs	4.054	1.840	0.593	4.154	1.883	0.671
Si	1.101	4.255	0.898	1.054	4.468	0.787
Si	-2.798	3.621	1.175	-2.837	3.727	1.156
Si	-1.390	-1.277	-0.787	-1.326	-1.317	-0.578
Si	2.387	-1.788	0.516	2.392	-1.897	0.546
Si	-1.495	-3.281	0.521	-1.568	-3.567	0.269
Si	0.967	-0.849	-1.237	1.008	-0.910	-1.243
Si	0.111	-4.489	-0.806	0.205	-4.615	-1.011
Si	-0.367	-2.755	-2.430	-0.400	-2.692	-2.471
Si	2.352	-4.348	0.187	2.368	-4.432	0.266
Si	0.617	-3.368	1.663	0.492	-3.529	1.588
Si	1.994	-2.928	-1.883	2.051	-3.000	-1.993
Si	0.116	-1.079	1.145	0.181	-1.128	1.343
No.10	PW91			BLYP		
Si	-2.172	0.798	-0.305	-2.168	0.779	-0.221
Si	1.234	1.183	-2.443	1.213	1.179	-2.473
Si	-2.217	3.143	2.753	-2.218	3.245	2.820
Si	-0.925	1.996	-1.964	-0.961	1.987	-1.945
Si	-3.679	2.211	0.880	-3.746	2.213	0.930
Si	-1.069	1.373	1.722	-1.048	1.472	1.787
Si	-0.255	4.216	-1.216	-0.353	4.252	-1.246
Si	1.036	2.327	-0.351	1.130	2.427	-0.406
Si	1.304	1.177	1.780	1.351	1.261	1.774
Cs	1.065	4.781	2.468	1.139	5.025	2.437
Si	-1.811	3.603	0.468	-1.947	3.742	0.506
Si	-1.203	-1.344	-0.375	-1.141	-1.371	-0.284
Si	2.885	-1.977	-0.389	2.923	-2.074	-0.356
Si	-0.873	-3.002	1.332	-1.051	-3.302	1.169
Si	0.929	-1.042	-1.635	0.983	-1.096	-1.660
Si	0.037	-4.423	-0.367	0.087	-4.547	-0.515
Si	-0.814	-2.976	-2.117	-0.805	-2.935	-2.193
Si	2.466	-4.609	-0.294	2.516	-4.667	-0.162
Si	1.499	-3.185	1.496	1.343	-3.271	1.546
Si	1.585	-3.290	-2.224	1.673	-3.360	-2.330
Si	0.975	-0.957	0.782	1.075	-0.958	0.824
No.11	PW91			BLYP		
Si	-2.124	0.960	-0.077	-2.089	0.970	-0.093
Si	1.655	1.432	-1.958	1.718	1.483	-1.925
Si	-1.598	3.921	1.505	-1.590	4.056	1.598
Si	-0.413	2.340	-1.058	-0.423	2.396	-1.155
Si	-2.792	1.865	2.164	-2.857	1.950	2.164
Si	-0.556	1.499	1.720	-0.623	1.481	1.807
Si	-0.853	4.635	-0.805	-0.885	4.712	-0.843
Si	1.702	1.831	0.391	1.702	1.946	0.447
Si	1.516	0.600	2.454	1.507	0.609	2.487
Si	0.682	3.908	0.855	0.666	4.044	0.827
Cs	-4.325	3.660	-1.039	-4.405	3.735	-0.999
Si	-1.058	-1.105	-0.210	-1.025	-1.132	-0.276
Si	2.903	-2.199	-0.286	2.954	-2.268	-0.291
Si	-0.918	-3.057	1.233	-0.944	-3.104	1.211
Si	1.116	-0.800	-1.316	1.201	-0.823	-1.344
Si	-0.168	-4.323	-0.702	-0.150	-4.460	-0.690
Si	-0.915	-2.557	-2.124	-0.990	-2.721	-2.113
Si	2.240	-4.707	-0.808	2.282	-4.773	-0.876
Si	1.431	-3.656	1.321	1.453	-3.746	1.385
Si	1.427	-2.949	-2.349	1.405	-3.001	-2.425
Si	1.048	-1.300	1.091	1.090	-1.356	1.106
No.12	PW91			BLYP		
Si	-1.854	0.709	0.779	-1.762	0.754	0.798
Si	0.560	1.035	-2.723	0.588	1.050	-2.731
Si	-0.277	4.055	1.727	-0.264	4.152	1.773
Si	-0.877	1.925	-0.998	-0.949	1.996	-1.066
Si	-1.670	2.129	2.777	-1.781	2.195	2.801
Si	0.312	1.526	1.570	0.345	1.628	1.803
Si	-1.661	4.195	-0.629	-1.676	4.302	-0.718
Si	1.663	1.863	-0.785	1.644	1.955	-0.768
Si	2.634	1.106	1.271	2.645	1.104	1.274
Si	0.650	3.999	-0.418	0.649	4.102	-0.416
Si	-2.565	4.284	1.740	-2.574	4.415	1.737
Cs	-3.101	-2.208	-1.850	-3.268	-2.338	-1.903
Si	1.885	-1.016	0.497	1.858	-1.058	0.537
Si	-0.600	-4.938	-1.026	-0.636	-4.961	-1.029
Si	0.431	-1.067	-1.596	0.404	-1.122	-1.651
Si	1.399	-4.199	-0.087	1.438	-4.364	-0.139
Si	0.661	-3.253	-2.420	0.735	-3.312	-2.524
Si	1.217	-2.898	1.928	1.367	-3.080	1.912
Si	-0.897	-3.505	1.003	-0.849	-3.575	1.089
Si	2.648	-2.501	-1.313	2.693	-2.554	-1.293
Si	-0.561	-1.243	0.555	-0.610	-1.291	0.514
No.13	PW91			BLYP		
Si	-2.103	0.873	-0.360	-2.071	0.882	-0.388
Si	1.582	1.298	-1.964	1.650	1.368	-1.943
Si	-1.060	4.058	2.508	-1.113	4.143	2.536
Si	-0.593	2.216	-1.531	-0.593	2.277	-1.584
Si	-3.480	1.819	1.234	-3.523	1.804	1.179
Si	-1.084	1.698	1.882	-1.169	1.726	2.021
Si	-1.062	4.549	-1.399	-1.129	4.635	-1.405
Si	1.178	1.808	0.345	1.181	1.924	0.365

Part III: xyz Coordinates for Stationary Points

Si	0.988	0.622	2.427	0.987	0.654	2.419
Si	0.245	3.960	0.526	0.212	4.081	0.536
Si	-2.313	3.841	0.536	-2.401	3.924	0.563
Si	-1.225	-1.308	-0.374	-1.158	-1.310	-0.413
Cs	4.345	-1.709	-0.165	4.558	-1.937	-0.204
Si	-1.040	-3.091	1.288	-1.050	-3.135	1.271
Si	1.011	-0.917	-1.333	1.117	-0.913	-1.350
Si	-0.145	-4.323	-0.652	-0.179	-4.473	-0.642
Si	-0.960	-2.815	-2.311	-1.066	-2.945	-2.283
Si	2.148	-4.739	-0.744	2.142	-4.716	-0.781
Si	1.333	-3.556	1.369	1.331	-3.634	1.482
Si	1.414	-2.998	-2.312	1.337	-3.028	-2.410
Si	0.820	-1.289	1.028	0.936	-1.328	1.029
No.14	PW91			BLYP		
Si	-1.712	0.606	-0.641	-1.701	0.621	-0.630
Si	2.052	1.456	-1.766	2.069	1.490	-1.819
Si	-1.333	3.822	2.443	-1.287	3.946	2.485
Si	-0.244	2.164	-1.570	-0.272	2.200	-1.636
Si	-3.302	1.340	0.865	-3.286	1.345	0.913
Si	-0.972	1.519	1.714	-0.995	1.570	1.912
Si	-1.032	4.412	-1.446	-1.113	4.473	-1.453
Si	1.369	1.891	0.468	1.384	1.990	0.434
Si	1.151	0.680	2.519	1.235	0.720	2.478
Si	0.150	3.913	0.585	0.157	4.031	0.563
Si	-2.361	3.524	0.351	-2.412	3.600	0.429
Si	-0.633	-1.460	-0.453	-0.607	-1.459	-0.492
Si	2.916	-2.590	0.108	2.996	-2.629	0.120
Cs	-2.454	-2.080	2.652	-2.770	-2.272	2.544
Si	1.603	-0.850	-1.315	1.671	-0.875	-1.363
Si	1.351	-4.418	-1.039	1.380	-4.520	-0.999
Si	-1.082	-3.793	-0.747	-1.090	-3.822	-0.736
Si	2.614	-2.734	-2.396	2.647	-2.816	-2.435
Si	0.652	-3.590	1.155	0.687	-3.644	1.226
Si	0.098	-2.575	-2.580	0.101	-2.686	-2.628
Si	1.167	-1.235	1.095	1.205	-1.262	1.088
No.15	PW91			BLYP		
Si	-1.925	0.519	0.556	-1.846	0.530	0.556
Si	1.643	1.216	-1.701	1.685	1.247	-1.695
Si	-1.374	3.917	2.521	-1.431	3.957	2.549
Si	-0.560	1.917	-1.050	-0.593	2.012	-1.227
Si	-3.052	1.781	-1.044	-3.100	1.733	-0.996
Si	-0.653	1.679	2.127	-0.657	1.685	2.219
Si	-0.838	4.346	-1.380	-0.837	4.481	-1.348
Si	1.477	1.921	0.591	1.458	2.002	0.600
Si	1.522	0.814	2.693	1.589	0.849	2.708
Si	0.218	3.931	0.709	0.211	4.035	0.760
Si	-2.307	3.652	0.326	-2.359	3.705	0.307
Si	-0.605	-1.346	0.117	-0.611	-1.428	0.154
Si	1.741	-1.022	-0.856	1.781	-1.033	-0.858
Si	-0.427	-3.379	1.324	-0.461	-3.468	1.397
Cs	-1.107	-0.168	-4.046	-1.083	-0.157	-4.235
Si	-0.660	-4.933	-0.514	-0.684	-5.006	-0.501
Si	-0.151	-2.854	-1.698	-0.199	-2.904	-1.738
Si	1.567	-4.257	-0.165	1.580	-4.382	-0.163
Si	1.786	-3.519	2.126	1.805	-3.573	2.138
Si	2.208	-2.972	-2.111	2.193	-3.031	-2.118
Si	1.494	-1.244	1.475	1.556	-1.254	1.492
No.16	PW91			BLYP		
Si	-1.772	0.575	-0.126	-1.644	0.644	0.061
Si	1.635	1.583	-2.140	1.673	1.575	-2.133
Si	-1.271	3.588	1.832	-1.310	3.721	1.918
Si	-0.524	2.197	-1.278	-0.553	2.209	-1.359
Si	-2.935	1.587	1.690	-3.016	1.619	1.727
Si	-0.566	1.203	1.857	-0.589	1.394	2.143
Si	-1.500	4.333	-0.913	-1.588	4.364	-1.122
Si	1.566	1.959	0.187	1.575	2.132	0.185
Si	1.745	0.791	2.271	1.813	0.956	2.300
Si	0.472	4.056	0.334	0.339	4.171	0.241
Si	-3.331	3.932	0.856	-3.378	3.929	0.832
Si	-0.785	-1.559	-0.374	-0.817	-1.555	-0.337
Si	3.379	-1.759	-0.625	3.387	-1.893	-0.537
Si	-1.916	-3.046	1.209	-1.797	-3.252	1.152
Si	1.259	-0.700	-1.701	1.400	-0.761	-1.709
Cs	-0.928	-5.624	-1.170	-1.177	-5.778	-1.486
Si	-0.338	-2.119	-2.694	-0.324	-2.080	-2.684
Si	2.325	-3.755	0.374	2.382	-4.037	0.274
Si	0.302	-2.933	1.456	0.429	-2.949	1.463
Si	1.605	-3.258	-1.796	1.543	-3.419	-1.793
Si	1.572	-1.050	0.752	1.647	-0.991	0.865
No.17	PW91			BLYP		
Si	-1.889	0.577	0.154	-1.881	0.593	0.163
Si	1.404	1.293	-2.179	1.353	1.324	-2.261
Si	-0.845	4.274	2.358	-0.782	4.390	2.394
Si	-0.823	1.930	-1.428	-0.904	1.982	-1.469
Si	-3.041	1.540	1.905	-3.021	1.541	1.960
Si	-0.597	1.877	2.060	-0.586	1.951	2.261
Si	-1.650	4.169	-1.489	-1.764	4.253	-1.442
Si	1.300	2.036	0.068	1.281	2.132	-0.002
Si	1.680	1.174	2.259	1.720	1.195	2.172
Si	0.076	4.050	0.175	0.056	4.169	0.147
Si	-2.377	3.574	0.723	-2.417	3.675	0.842
Si	-0.724	-1.430	0.021	-0.753	-1.456	-0.075
Si	3.110	-2.327	0.098	3.159	-2.523	0.286
Si	-1.062	-3.745	0.106	-1.143	-3.798	0.099
Si	1.157	-0.916	-1.327	1.172	-0.931	-1.391
Si	0.500	-4.852	-1.579	0.556	-4.844	-1.625
Cs	-1.412	-2.294	-3.528	-1.360	-2.467	-3.737
Si	1.539	-4.127	0.368	1.523	-4.294	0.423
Si	0.178	-2.907	1.988	0.140	-2.931	1.987
Si	2.073	-2.971	-1.947	2.223	-3.002	-1.884
Si	1.402	-0.928	1.197	1.425	-0.961	1.155
No.18	PW91			BLYP		
Si	-2.147	1.014	-0.321	-2.133	1.001	-0.321
Si	1.515	1.381	-2.016	1.536	1.415	-2.044
Si	-0.967	4.182	2.507	-0.965	4.280	2.534
Si	-0.657	2.326	-1.538	-0.687	2.359	-1.588
Si	-3.428	1.917	1.374	-3.454	1.911	1.369
Si	-1.021	1.817	1.916	-1.071	1.863	2.087
Si	-1.137	4.652	-1.397	-1.210	4.719	-1.401
Si	1.166	1.893	0.276	1.181	1.985	0.266
Si	1.078	0.752	2.377	1.104	0.792	2.366
Si	0.257	4.061	0.472	0.247	4.168	0.461
Si	-2.288	3.936	0.586	-2.352	4.014	0.639
Si	-1.265	-1.161	-0.337	-1.230	-1.190	-0.368
Si	2.490	-2.330	-0.225	2.558	-2.371	-0.216
Si	-1.144	-3.202	0.910	-1.178	-3.237	0.932
Si	0.881	-0.844	-1.430	0.946	-0.876	-1.482
Si	0.466	-4.327	-0.663	0.400	-4.428	-0.687
Si	-0.915	-2.772	-2.071	-0.910	-2.798	-2.157
Cs	3.660	-5.671	-0.643	3.683	-5.797	-0.621
Si	1.231	-3.497	1.608	1.230	-3.569	1.609
Si	1.539	-2.909	-2.472	1.582	-2.988	-2.490
Si	0.687	-1.216	1.087	0.721	-1.252	1.113
No.19	PW91			BLYP		
Si	-2.094	0.913	-0.453	-2.074	0.918	-0.456
Si	1.617	1.481	-2.068	1.651	1.506	-2.075
Si	-1.038	4.027	2.503	-1.049	4.158	2.517
Si	-0.608	2.321	-1.577	-0.624	2.358	-1.632
Si	-3.443	1.784	1.207	-3.472	1.789	1.189
Si	-1.039	1.686	1.813	-1.105	1.746	1.994
Si	-1.109	4.636	-1.391	-1.179	4.700	-1.414
Si	1.218	1.884	0.246	1.213	1.990	0.246
Si	1.086	0.675	2.287	1.100	0.736	2.289
Si	0.240	4.012	0.495	0.226	4.135	0.476

Part III: xyz Coordinates for Stationary Points

Si	-2.312	3.836	0.544	-2.380	3.921	0.580
Si	-1.136	-1.229	-0.543	-1.103	-1.246	-0.561
Si	2.738	-2.154	-0.249	2.802	-2.208	-0.223
Si	-1.011	-2.866	1.207	-0.964	-2.905	1.204
Si	1.097	-0.702	-1.350	1.159	-0.737	-1.382
Si	0.150	-4.099	-0.594	0.071	-4.261	-0.663
Si	-0.990	-2.913	-2.298	-1.001	-2.962	-2.352
Si	2.444	-4.496	-1.064	2.428	-4.575	-1.072
Cs	1.946	-4.568	2.622	1.975	-4.757	2.667
Si	1.425	-2.839	-2.432	1.447	-2.908	-2.476
Si	0.815	-1.388	1.096	0.875	-1.397	1.144
No.20	PW91			BLYP		
Si	-1.991	0.755	-0.043	-2.017	0.766	-0.065
Si	1.494	1.297	-1.974	1.502	1.321	-2.006
Si	-1.007	4.217	2.454	-0.982	4.307	2.487
Si	-0.709	2.095	-1.471	-0.744	2.127	-1.521
Si	-3.267	1.631	1.666	-3.310	1.669	1.648
Si	-0.842	1.827	2.051	-0.896	1.866	2.202
Si	-1.448	4.353	-1.461	-1.482	4.431	-1.457
Si	1.246	1.986	0.267	1.242	2.048	0.252
Si	1.386	0.997	2.430	1.386	1.012	2.420
Si	0.105	4.050	0.348	0.115	4.147	0.342
Si	-2.406	3.676	0.639	-2.446	3.794	0.693
Si	-0.964	-1.382	-0.132	-1.004	-1.407	-0.162
Si	2.762	-2.169	-0.140	2.821	-2.176	-0.129
Si	-1.524	-3.541	0.776	-1.523	-3.594	0.792
Si	1.168	-1.046	-1.547	1.208	-1.062	-1.583
Si	0.078	-4.003	-0.866	0.043	-4.135	-0.891
Si	-0.695	-2.244	-2.368	-0.671	-2.301	-2.394
Si	2.153	-4.515	0.180	2.177	-4.559	0.158
Si	0.702	-3.244	1.584	0.732	-3.338	1.632
Cs	2.559	-3.786	-3.512	2.640	-3.893	-3.582
Si	1.194	-0.958	1.120	1.204	-1.025	1.165
No.21	PW91			BLYP		
Si	-1.301	0.678	0.348	-1.315	0.655	0.346
Si	2.169	1.290	-1.543	2.198	1.328	-1.537
Si	-1.752	4.755	1.531	-1.801	4.815	1.552
Si	-0.265	1.400	-1.701	-0.273	1.379	-1.740
Si	-3.466	1.336	1.042	-3.501	1.363	1.050
Si	-1.714	2.431	2.208	-1.768	2.460	2.273
Si	-1.429	3.517	-2.171	-1.465	3.550	-2.195
Si	1.067	2.112	0.367	1.072	2.216	0.361
Si	0.308	1.065	2.340	0.329	1.159	2.361
Si	-0.240	4.036	-0.150	-0.262	4.149	-0.171
Si	-2.691	3.324	-0.115	-2.773	3.409	-0.121
Si	0.086	-1.068	1.104	0.131	-1.029	1.197
Si	3.246	-2.803	-0.633	3.268	-2.851	-0.632
Si	-0.587	-3.317	1.488	-0.609	-3.330	1.478
Si	1.942	-0.831	-0.385	1.968	-0.841	-0.371
Si	-1.040	-3.108	-0.820	-1.082	-3.139	-0.851
Si	-0.166	-1.040	-1.722	-0.122	-1.096	-1.820
Si	0.271	-4.743	-2.004	0.252	-4.804	-2.018
Si	1.223	-4.028	0.034	1.220	-4.129	0.045
Si	1.551	-2.652	-2.294	1.613	-2.721	-2.364
Cs	2.786	-2.352	3.075	2.917	-2.541	3.156
LaSi ₂₀						
Cage	PW91			BLYP		
Si	2.729	-1.121	-1.606	2.766	-1.133	-1.621
Si	2.991	1.081	-0.811	3.037	1.100	-0.818
Si	0.833	-1.114	-3.052	0.840	-1.127	-3.089
Si	0.006	1.090	-3.089	0.001	1.107	-3.138
Si	1.348	2.491	-1.749	1.364	2.522	-1.774
Si	-0.819	-2.449	-2.033	-0.836	-2.485	-2.064
Si	-2.638	-1.084	-1.497	-2.672	-1.096	-1.518
Si	-2.134	1.089	-2.158	-2.160	1.102	-2.181
Si	-0.008	-3.331	0.002	-0.010	-3.373	0.002
Si	-1.347	-2.491	1.749	-1.363	-2.522	1.774
Si	-2.990	-1.081	0.811	-3.037	-1.100	0.818
Si	2.165	-2.448	0.258	2.198	-2.485	0.265
Si	2.135	-1.089	2.158	2.161	-1.102	2.181
Si	-0.006	-1.090	3.089	-0.001	-1.107	3.138
Si	2.638	1.084	1.498	2.672	1.096	1.519
Si	0.820	2.449	2.033	0.836	2.485	2.064
Si	-0.833	1.114	3.053	-0.840	1.127	3.090
Si	-2.728	1.121	1.607	-2.765	1.133	1.622
Si	-2.165	2.448	-0.258	-2.198	2.485	-0.265
Si	0.008	3.331	-0.002	0.010	3.373	-0.002
La	0.000	-0.000	0.000	0.000	-0.000	0.000
No.1	PW91			BLYP		
La	-2.124	0.695	0.067	-2.163	0.685	0.034
Si	1.262	1.149	-2.303	1.246	1.220	-2.353
Si	-0.335	4.753	2.524	-0.353	4.803	2.586
Si	-0.981	2.034	-2.224	-1.033	2.133	-2.242
Si	-3.315	2.387	2.253	-3.383	2.431	2.235
Si	-1.060	2.470	2.675	-1.115	2.486	2.705
Si	-0.898	3.955	-0.967	-0.904	4.054	-0.953
Si	0.801	2.169	-0.198	0.855	2.226	-0.201
Si	0.603	1.006	1.850	0.586	1.018	1.848
Si	0.905	4.501	0.381	0.928	4.588	0.391
Si	-2.121	4.092	1.104	-2.168	4.197	1.138
Si	-1.435	-2.234	-0.487	-1.464	-2.292	-0.495
Si	2.620	-1.724	0.125	2.677	-1.797	0.146
Si	-0.557	-4.400	-0.087	-0.577	-4.470	-0.021
Si	0.698	-1.073	-1.431	0.778	-1.092	-1.477
Si	1.040	-5.142	-1.792	0.959	-5.258	-1.796
Si	-0.318	-3.090	-2.439	-0.315	-3.139	-2.449
Si	2.073	-4.109	0.175	2.124	-4.229	0.153
Si	0.513	-3.415	1.816	0.614	-3.453	1.853
Si	2.276	-2.837	-2.038	2.351	-2.901	-2.084
Si	0.347	-1.188	0.996	0.352	-1.212	0.981
No.2	PW91			BLYP		
Si	-1.833	0.872	0.019	-1.819	0.877	0.065
La	0.615	2.021	-1.989	0.683	2.059	-1.975
Si	-1.081	3.822	2.502	-1.172	3.907	2.524
Si	-2.250	2.459	-1.766	-2.221	2.460	-1.782
Si	-3.924	2.103	-0.117	-3.961	2.091	-0.185
Si	-0.445	1.630	1.735	-0.451	1.697	1.806
Si	-0.959	4.613	-1.258	-0.990	4.686	-1.253
Si	1.861	1.862	0.596	1.927	2.060	0.654
Si	1.525	0.573	2.609	1.580	0.634	2.618
Si	0.377	3.789	0.642	0.369	3.922	0.707
Si	-2.341	3.828	0.456	-2.454	3.917	0.439
Si	-0.929	-1.268	-0.294	-0.893	-1.282	-0.261
Si	3.026	-2.214	-0.268	3.069	-2.288	-0.331
Si	-0.782	-3.034	1.364	-0.820	-3.131	1.343
Si	1.264	-0.959	-1.473	1.286	-1.033	-1.546
Si	-0.029	-4.459	-0.439	-0.045	-4.586	-0.452
Si	-0.784	-2.845	-2.075	-0.848	-2.908	-2.054
Si	2.392	-4.826	-0.507	2.400	-4.918	-0.518
Si	1.555	-3.540	1.452	1.559	-3.610	1.490
Si	1.558	-3.235	-2.194	1.530	-3.334	-2.296
Si	1.182	-1.192	1.007	1.270	-1.219	1.008
No.3	PW91			BLYP		
Si	-2.418	0.580	-0.306	-2.447	0.572	-0.295
Si	1.133	1.267	-2.532	1.138	1.303	-2.522
La	-0.455	3.321	3.225	-0.444	3.416	3.283
Si	-0.914	2.069	-1.497	-0.986	2.082	-1.574
Si	-2.837	1.672	1.939	-2.896	1.793	1.977
Si	-0.637	1.494	1.012	-0.686	1.577	1.019
Si	-1.476	4.409	-1.279	-1.482	4.482	-1.278
Si	1.457	2.085	-0.314	1.445	2.190	-0.293
Si	1.495	1.057	1.880	1.455	1.069	1.879
Si	0.266	4.040	0.401	0.306	4.207	0.449
Si	-2.170	3.765	0.924	-2.217	3.904	0.963

Part III: xyz Coordinates for Stationary Points

Si	-0.962	-1.336	-0.197	-0.975	-1.394	-0.213
Si	3.188	-1.740	-0.449	3.244	-1.815	-0.462
Si	-1.775	-3.670	-0.360	-1.767	-3.775	-0.374
Si	1.026	-0.892	-1.505	1.047	-0.941	-1.542
Si	0.482	-4.540	-0.429	0.510	-4.670	-0.444
Si	-0.390	-2.725	-2.276	-0.375	-2.808	-2.344
Si	2.101	-3.466	1.007	2.149	-3.572	1.017
Si	-0.241	-2.963	1.670	-0.222	-3.048	1.702
Si	1.949	-3.306	-1.884	1.998	-3.404	-1.927
Si	1.178	-1.120	0.970	1.203	-1.167	0.979
No.4	PW91			BLYP		
Si	-2.557	0.266	1.664	-2.577	0.294	1.762
Si	2.276	1.504	-2.100	2.329	1.505	-2.101
Si	-0.990	3.793	1.691	-0.998	3.890	1.719
La	-0.750	1.258	-0.782	-0.774	1.251	-0.813
Si	-3.792	1.564	0.076	-3.853	1.580	0.150
Si	-0.785	1.585	2.352	-0.785	1.662	2.397
Si	-1.301	4.154	-1.179	-1.356	4.213	-1.217
Si	2.018	2.444	0.002	2.043	2.499	-0.000
Si	1.355	1.070	1.795	1.351	1.097	1.800
Si	0.654	4.399	0.142	0.644	4.476	0.110
Si	-2.938	3.763	0.415	-2.969	3.815	0.428
Si	-1.285	-1.454	0.619	-1.320	-1.450	0.702
Si	2.935	-2.331	-0.094	2.983	-2.356	-0.023
Si	-1.329	-3.799	1.024	-1.368	-3.833	0.962
Si	1.653	-0.672	-1.353	1.697	-0.714	-1.367
Si	-0.234	-3.887	-1.035	-0.232	-3.995	-1.113
Si	-0.657	-1.664	-2.056	-0.621	-1.711	-2.156
Si	2.090	-4.575	-0.893	2.127	-4.647	-0.914
Si	1.115	-3.570	1.226	1.106	-3.670	1.241
Si	1.462	-2.772	-2.509	1.509	-2.818	-2.582
Si	1.056	-1.075	0.991	1.062	-1.089	1.012
No.5	PW91			BLYP		
Si	-2.459	0.566	-0.397	-2.394	0.573	-0.419
Si	1.473	1.428	-1.896	1.514	1.487	-1.879
Si	-1.110	3.783	1.687	-1.171	3.908	1.760
Si	-0.760	1.865	-1.340	-0.758	1.960	-1.402
La	-3.672	2.332	1.739	-3.748	2.375	1.633
Si	-1.058	1.198	1.538	-1.110	1.231	1.645
Si	-0.853	4.188	-0.760	-0.916	4.290	-0.741
Si	1.221	2.090	0.420	1.294	2.160	0.452
Si	1.086	0.681	2.368	1.086	0.682	2.376
Si	0.991	4.485	0.770	0.959	4.576	0.792
Si	-2.878	4.636	0.242	-2.933	4.829	0.279
Si	-1.117	-1.341	-0.443	-1.075	-1.381	-0.524
Si	2.929	-2.062	-0.166	2.973	-2.138	-0.188
Si	-0.907	-3.207	1.096	-0.916	-3.245	1.117
Si	1.127	-0.862	-1.367	1.210	-0.865	-1.389
Si	0.106	-4.483	-0.710	0.144	-4.627	-0.659
Si	-0.712	-2.857	-2.255	-0.826	-3.095	-2.216
Si	2.556	-4.592	-0.638	2.621	-4.649	-0.757
Si	1.463	-3.580	1.396	1.516	-3.678	1.462
Si	1.670	-3.000	-2.306	1.603	-3.054	-2.385
Si	0.901	-1.271	1.025	0.925	-1.341	1.045
No.6	PW91			BLYP		
Si	-2.409	0.731	-0.452	-2.407	0.746	-0.473
Si	1.514	1.377	-2.131	1.525	1.413	-2.141
Si	-1.178	4.349	2.250	-1.157	4.422	2.306
Si	-0.609	2.047	-1.196	-0.654	2.123	-1.299
Si	-3.778	1.735	1.110	-3.794	1.743	1.120
La	-0.925	1.304	2.317	-0.940	1.332	2.373
Si	-1.125	4.399	-1.409	-1.184	4.483	-1.392
Si	1.597	1.949	0.227	1.619	2.041	0.231
Si	2.048	0.852	2.239	2.053	0.873	2.239
Si	0.280	3.831	0.505	0.281	3.935	0.508
Si	-2.451	3.533	0.434	-2.527	3.651	0.518
Si	-1.056	-1.114	0.020	-1.066	-1.141	0.001
Si	2.823	-2.183	-0.328	2.874	-2.259	-0.345
Si	-1.259	-3.355	0.863	-1.287	-3.422	0.822
Si	0.990	-0.837	-1.405	1.019	-0.871	-1.456
Si	0.103	-4.247	-0.803	0.129	-4.361	-0.824
Si	-0.840	-2.387	-2.153	-0.843	-2.468	-2.189
Si	2.393	-4.629	-0.187	2.420	-4.731	-0.081
Si	1.080	-3.372	1.439	1.059	-3.430	1.492
Si	1.575	-2.973	-2.437	1.607	-3.028	-2.505
Si	1.225	-1.007	1.094	1.271	-1.048	1.094
No.7	PW91			BLYP		
Si	-2.122	0.869	-0.326	-1.996	0.909	-0.363
Si	1.639	1.349	-2.002	1.711	1.402	-2.020
Si	-1.094	3.879	2.488	-1.016	4.023	2.524
Si	-0.575	2.235	-1.473	-0.561	2.319	-1.604
Si	-3.343	1.801	1.465	-3.372	1.721	1.355
Si	-0.867	1.590	1.747	-0.966	1.643	2.013
La	-1.411	5.002	-1.754	-1.549	5.109	-1.715
Si	1.383	1.908	0.298	1.317	2.007	0.288
Si	1.230	0.688	2.387	1.218	0.714	2.378
Si	0.160	3.917	0.421	0.173	4.084	0.403
Si	-2.566	3.906	0.612	-2.609	3.961	0.732
Si	-1.067	-1.228	-0.280	-1.016	-1.256	-0.400
Si	2.922	-2.161	-0.197	2.964	-2.231	-0.179
Si	-0.943	-3.141	1.193	-0.988	-3.150	1.184
Si	1.133	-0.885	-1.350	1.238	-0.900	-1.388
Si	-0.044	-4.406	-0.661	-0.045	-4.542	-0.622
Si	-0.793	-2.697	-2.166	-0.868	-2.899	-2.177
Si	2.378	-4.708	-0.608	2.406	-4.788	-0.657
Si	1.414	-3.599	1.421	1.413	-3.684	1.500
Si	1.577	-3.051	-2.284	1.554	-3.122	-2.335
Si	0.989	-1.267	1.067	0.991	-1.321	1.082
No.8	PW91			BLYP		
Si	-2.291	0.859	0.040	-2.293	0.865	0.080
Si	0.991	1.569	-2.190	0.896	1.617	-2.338
Si	0.058	3.736	1.742	0.110	3.842	1.761
Si	-1.350	1.972	-1.808	-1.437	2.016	-1.820
Si	-3.254	2.180	1.739	-3.279	2.215	1.775
Si	-0.921	1.506	1.984	-0.935	1.618	2.099
Si	-1.492	4.355	-1.810	-1.565	4.422	-1.773
La	2.069	1.512	1.066	2.072	1.484	0.993
Si	0.501	0.122	3.213	0.550	0.213	3.266
Si	0.411	3.395	-0.658	0.407	3.472	-0.710
Si	-1.927	3.798	0.454	-1.940	3.959	0.549
Si	-1.353	-1.296	-0.134	-1.229	-1.267	-0.007
Si	2.654	-1.641	0.150	2.650	-1.621	0.149
Si	-1.059	-3.559	0.667	-1.207	-3.718	0.331
Si	0.811	-0.530	-1.022	0.851	-0.581	-1.221
Si	0.364	-4.235	-1.131	0.518	-4.394	-1.246
Si	-0.625	-2.322	-2.233	-0.657	-2.407	-2.223
Si	2.724	-4.153	-0.620	2.840	-4.127	-0.345
Si	1.281	-3.597	1.322	1.068	-3.747	1.360
Si	1.866	-2.331	-2.203	1.985	-2.434	-2.277
Si	0.538	-1.339	1.434	0.590	-1.427	1.597
No.9	PW91			BLYP		
Si	-1.299	1.049	-0.080	-1.319	1.053	-0.090
Si	2.576	1.214	-1.353	2.627	1.233	-1.331
Si	-0.985	3.584	1.951	-1.040	3.701	1.995
Si	-1.764	2.414	-2.041	-1.731	2.509	-2.062
Si	-3.147	2.117	1.140	-3.230	2.103	1.159
Si	-1.398	1.239	2.418	-1.439	1.325	2.463
Si	-1.719	4.202	-0.398	-1.739	4.348	-0.422
Si	0.497	2.276	-1.267	0.536	2.327	-1.250
La	1.436	1.571	1.525	1.424	1.612	1.580
Si	0.543	4.265	0.184	0.531	4.356	0.208
Si	-3.129	4.560	1.454	-3.216	4.630	1.421
Si	-0.715	-1.201	-0.410	-0.673	-1.212	-0.425
Si	2.989	-2.636	0.103	3.045	-2.713	0.064

Part III: xyz Coordinates for Stationary Points

Si	-1.018	-3.091	1.095	-1.013	-3.130	1.099
Si	1.636	-0.928	-1.009	1.704	-0.968	-1.046
Si	-0.121	-4.387	-0.807	-0.111	-4.524	-0.791
Si	-0.647	-2.654	-2.300	-0.743	-2.780	-2.262
Si	2.260	-4.969	-0.764	2.304	-5.042	-0.856
Si	1.232	-3.996	1.390	1.278	-4.082	1.445
Si	1.692	-3.067	-2.183	1.654	-3.126	-2.275
Si	1.075	-1.563	1.351	1.147	-1.620	1.375
No.10	PW91			BLYP		
Si	-2.216	0.909	-0.302	-2.209	0.905	-0.377
Si	1.339	1.197	-2.635	1.387	1.264	-2.635
Si	-2.205	3.171	2.847	-2.180	3.190	2.927
Si	-0.776	2.018	-1.842	-0.762	2.089	-1.879
Si	-3.870	2.338	0.901	-3.898	2.352	0.804
Si	-1.111	1.376	1.748	-1.181	1.401	1.749
Si	-0.123	4.194	-1.009	-0.193	4.265	-0.998
Si	1.297	2.232	-0.476	1.363	2.338	-0.467
Si	1.344	1.141	1.729	1.284	1.140	1.768
La	0.591	3.907	2.004	0.625	3.971	2.007
Si	-1.887	3.574	0.515	-2.032	3.847	0.613
Si	-1.186	-1.198	-0.413	-1.154	-1.222	-0.468
Si	2.916	-1.946	-0.394	2.970	-2.013	-0.427
Si	-0.804	-2.783	1.406	-0.809	-2.821	1.414
Si	0.995	-0.952	-1.626	1.060	-0.959	-1.660
Si	0.040	-4.343	-0.245	0.070	-4.474	-0.186
Si	-0.882	-2.981	-1.981	-0.978	-3.162	-1.903
Si	2.469	-4.534	-0.367	2.513	-4.606	-0.445
Si	1.587	-3.143	1.551	1.638	-3.220	1.624
Si	1.497	-3.220	-2.214	1.439	-3.279	-2.280
Si	0.983	-0.957	0.803	1.045	-1.007	0.818
No.11	PW91			BLYP		
Si	-2.580	0.460	-0.317	-2.371	0.613	-0.366
Si	1.358	1.506	-1.836	1.512	1.526	-1.881
Si	-0.789	3.879	1.478	-1.011	4.022	1.617
Si	-0.887	1.924	-1.220	-0.743	2.165	-1.330
Si	-2.447	3.026	2.801	-2.703	2.981	2.775
Si	-1.325	1.282	1.588	-1.336	1.309	1.735
Si	-0.845	4.393	-0.893	-0.959	4.597	-0.904
Si	1.110	2.106	0.504	1.403	2.052	0.466
Si	0.848	0.682	2.409	0.937	0.700	2.418
Si	1.249	4.520	0.497	1.042	4.432	0.592
La	-3.362	3.279	-0.116	-3.470	3.341	-0.154
Si	-1.137	-1.360	-0.486	-1.063	-1.327	-0.594
Si	2.872	-2.025	-0.103	2.919	-2.115	-0.152
Si	-1.050	-3.315	0.906	-1.034	-3.223	0.995
Si	1.094	-0.841	-1.369	1.199	-0.841	-1.414
Si	0.081	-4.446	-0.896	0.062	-4.576	-0.777
Si	-0.599	-2.688	-2.416	-0.796	-2.973	-2.348
Si	2.521	-4.578	-0.582	2.543	-4.650	-0.733
Si	1.289	-3.593	1.331	1.365	-3.686	1.410
Si	1.781	-2.948	-2.311	1.637	-3.027	-2.402
Si	0.816	-1.260	1.028	0.866	-1.318	1.046
No.12	PW91			BLYP		
Si	-1.929	0.669	0.321	-1.899	0.696	0.325
Si	1.103	1.233	-2.524	1.188	1.264	-2.498
Si	-0.834	4.058	1.754	-0.884	4.158	1.783
Si	-0.715	2.015	-1.165	-0.765	2.071	-1.251
Si	-2.440	1.988	2.282	-2.655	2.074	2.177
Si	-0.159	1.523	1.830	-0.347	1.623	2.185
Si	-1.513	4.281	-0.864	-1.527	4.363	-0.935
Si	1.673	1.876	-0.307	1.587	1.957	-0.230
Si	2.046	0.609	1.746	1.855	0.670	1.887
Si	0.657	4.019	-0.052	0.635	4.130	-0.041
Si	-3.030	4.209	1.136	-3.079	4.416	1.079
La	-2.015	-2.015	-1.063	-2.002	-2.039	-0.977
Si	2.757	-1.345	0.094	3.269	-1.772	-0.152
Si	-1.654	-4.548	0.503	-1.635	-4.560	0.659
Si	0.791	-0.941	-1.576	0.882	-0.952	-1.542
Si	0.376	-4.237	-0.654	0.316	-4.401	-0.695
Si	0.261	-2.989	-2.768	0.192	-3.035	-2.813
Si	2.194	-3.638	0.843	2.247	-3.888	0.710
Si	-0.085	-3.066	1.449	0.066	-3.107	1.478
Si	2.413	-2.874	-1.738	2.390	-2.867	-1.959
Si	0.101	-0.831	0.751	0.164	-0.804	0.809
No.13	PW91			BLYP		
Si	-2.042	0.777	-0.002	-2.134	0.806	-0.027
Si	1.329	0.959	-2.130	1.280	0.942	-2.195
Si	-0.518	4.279	2.488	-0.480	4.331	2.517
Si	-0.733	2.060	-1.483	-0.765	2.083	-1.495
Si	-3.185	1.946	1.626	-3.221	2.017	1.639
Si	-0.833	1.918	2.160	-0.881	1.946	2.283
Si	-1.092	4.424	-1.388	-1.104	4.487	-1.379
Si	1.082	1.710	0.200	1.119	1.761	0.165
Si	1.043	0.390	2.297	1.017	0.411	2.282
Si	0.472	3.944	0.357	0.506	4.020	0.353
Si	-2.108	3.939	0.746	-2.120	4.051	0.798
Si	-1.786	-1.515	-0.491	-1.808	-1.489	-0.468
La	2.945	-0.592	0.080	2.980	-0.585	0.080
Si	-1.066	-3.386	1.134	-1.125	-3.477	1.097
Si	0.331	-1.147	-1.645	0.278	-1.194	-1.720
Si	0.006	-4.230	-0.865	0.015	-4.326	-0.901
Si	0.173	-3.108	-2.992	0.275	-3.200	-3.038
Si	2.146	-5.025	-0.350	2.165	-5.084	-0.339
Si	1.557	-3.173	1.033	1.640	-3.210	1.076
Si	2.147	-2.915	-1.669	2.237	-2.950	-1.674
Si	0.130	-1.256	0.894	0.127	-1.340	0.946
No.14	PW91			BLYP		
Si	-1.638	0.672	-0.722	-1.728	0.668	-0.798
Si	1.885	1.867	-2.083	1.872	1.861	-2.127
Si	-1.254	3.514	2.720	-1.242	3.588	2.764
Si	-0.426	2.426	-1.647	-0.462	2.442	-1.671
Si	-3.237	1.054	0.899	-3.254	1.088	0.907
Si	-0.924	1.316	1.825	-0.935	1.327	1.998
Si	-1.344	4.540	-1.074	-1.363	4.590	-1.057
Si	1.229	1.794	0.265	1.304	1.890	0.266
Si	1.321	0.507	2.290	1.371	0.544	2.252
Si	0.043	3.778	0.734	0.068	3.857	0.755
Si	-2.481	3.353	0.688	-2.509	3.414	0.747
Si	-0.108	-1.140	-0.776	-0.220	-1.162	-0.854
Si	2.735	-2.069	-0.693	2.842	-2.117	-0.656
La	-1.723	-1.879	1.401	-1.796	-1.913	1.371
Si	1.686	-0.549	-2.204	1.705	-0.591	-2.128
Si	0.531	-3.913	0.148	0.564	-4.038	0.193
Si	-1.278	-3.187	-1.377	-1.216	-3.318	-1.429
Si	2.258	-4.243	-1.482	2.267	-4.277	-1.480
Si	0.572	-3.490	2.443	0.528	-3.461	2.468
Si	0.766	-2.708	-2.610	0.809	-2.751	-2.752
Si	1.383	-1.646	1.255	1.392	-1.643	1.233
No.15	PW91			BLYP		
Si	-1.744	0.353	0.532	-1.832	0.326	0.596
Si	1.881	1.437	-1.657	1.927	1.488	-1.598
Si	-1.627	3.869	2.382	-1.642	3.913	2.377
Si	-0.332	2.356	-1.416	-0.306	2.466	-1.625
Si	-2.752	1.531	-1.210	-2.773	1.533	-1.193
Si	-0.627	1.736	2.030	-0.663	1.731	2.069
Si	-0.761	4.673	-1.369	-0.754	4.774	-1.369
Si	1.464	2.120	0.586	1.484	2.186	0.636
Si	1.612	1.046	2.718	1.604	1.002	2.730
Si	0.148	4.067	0.752	0.171	4.145	0.773
Si	-2.284	3.526	0.080	-2.308	3.583	0.038
Si	-0.553	-1.603	0.465	-0.645	-1.655	0.533
Si	1.766	-0.789	-0.821	1.835	-0.783	-0.873
Si	-0.638	-3.882	1.139	-0.607	-3.950	1.199
La	-0.710	-0.509	-2.500	-0.737	-0.509	-2.483

Part III: xyz Coordinates for Stationary Points

Si	-0.539	-5.491	-0.669	-0.536	-5.548	-0.660
Si	-0.650	-3.221	-1.469	-0.676	-3.260	-1.488
Si	1.515	-4.226	-0.509	1.562	-4.310	-0.529
Si	1.650	-3.371	1.712	1.716	-3.430	1.712
Si	1.653	-2.616	-2.297	1.651	-2.653	-2.323
Si	1.528	-1.006	1.518	1.529	-1.051	1.476
No.16	PW91			BLYP		
Si	-1.996	0.523	-0.210	-1.864	0.598	-0.058
Si	1.597	1.498	-2.152	1.614	1.486	-2.148
Si	-1.313	3.639	1.817	-1.304	3.715	1.875
Si	-0.547	2.071	-1.222	-0.589	2.123	-1.346
Si	-2.917	1.595	1.787	-3.037	1.650	1.760
Si	-0.567	1.241	1.632	-0.637	1.322	1.937
Si	-1.520	4.237	-0.930	-1.535	4.314	-1.064
Si	1.628	1.951	0.164	1.577	2.044	0.166
Si	1.683	0.829	2.269	1.715	0.874	2.275
Si	0.444	4.004	0.318	0.396	4.107	0.271
Si	-3.376	3.881	0.802	-3.376	3.975	0.829
Si	-0.744	-1.505	-0.208	-0.811	-1.538	-0.221
Si	3.346	-1.972	-0.546	3.379	-2.053	-0.491
Si	-1.929	-3.116	1.239	-1.884	-3.257	1.229
Si	1.309	-0.779	-1.589	1.335	-0.828	-1.612
La	-0.587	-4.618	-0.973	-0.582	-4.732	-1.053
Si	-0.354	-2.139	-2.568	-0.359	-2.176	-2.604
Si	2.095	-4.012	0.113	2.115	-4.152	0.056
Si	0.367	-2.984	1.505	0.415	-3.057	1.487
Si	1.803	-3.262	-2.120	1.843	-3.317	-2.188
Si	1.571	-1.085	0.874	1.582	-1.099	0.902
No.17	PW91			BLYP		
Si	-1.943	0.709	0.155	-1.955	0.724	0.156
Si	1.126	1.429	-2.395	1.139	1.426	-2.401
Si	-0.673	4.279	2.397	-0.661	4.378	2.411
Si	-1.022	2.098	-1.473	-1.046	2.118	-1.505
Si	-2.932	1.589	2.043	-2.966	1.632	2.041
Si	-0.484	1.880	1.994	-0.501	1.934	2.149
Si	-1.822	4.333	-1.360	-1.852	4.387	-1.359
Si	1.219	2.100	-0.116	1.236	2.179	-0.119
Si	1.796	1.146	2.007	1.791	1.159	1.999
Si	0.041	4.121	0.141	0.044	4.216	0.130
Si	-2.365	3.665	0.885	-2.402	3.768	0.931
Si	-0.801	-1.332	-0.021	-0.839	-1.355	-0.045
Si	2.744	-2.975	0.866	2.828	-2.979	0.810
Si	-1.411	-3.605	0.249	-1.407	-3.673	0.199
Si	0.991	-0.800	-1.530	1.004	-0.843	-1.546
Si	1.436	-4.868	-2.341	1.443	-4.946	-2.347
La	-0.816	-2.942	-2.588	-0.816	-3.007	-2.642
Si	0.907	-4.244	-0.158	0.990	-4.360	-0.106
Si	0.228	-2.853	1.926	0.157	-2.922	1.947
Si	2.328	-2.809	-1.548	2.372	-2.876	-1.599
Si	1.450	-0.923	0.871	1.439	-0.962	0.898
No.18	PW91			BLYP		
Si	-2.068	0.811	-0.215	-2.046	0.806	-0.198
Si	1.512	1.366	-2.075	1.523	1.388	-2.085
Si	-0.949	4.214	2.410	-0.934	4.322	2.417
Si	-0.702	2.170	-1.524	-0.736	2.189	-1.570
Si	-3.323	1.750	1.490	-3.330	1.754	1.498
Si	-0.913	1.823	1.949	-0.946	1.887	2.127
Si	-1.308	4.471	-1.497	-1.377	4.511	-1.507
Si	1.241	1.941	0.218	1.248	2.031	0.212
Si	1.277	0.933	2.386	1.297	0.970	2.371
Si	0.190	4.044	0.336	0.185	4.148	0.306
Si	-2.337	3.790	0.567	-2.387	3.867	0.619
Si	-1.045	-1.282	-0.121	-1.019	-1.308	-0.136
Si	2.758	-2.138	-0.004	2.801	-2.181	0.020
Si	-1.257	-3.480	0.806	-1.291	-3.549	0.743
Si	1.086	-0.839	-1.304	1.152	-0.872	-1.336
Si	0.043	-4.396	-0.963	0.029	-4.500	-1.027
Si	-0.739	-2.462	-2.259	-0.735	-2.523	-2.307
La	2.823	-5.026	-0.526	2.827	-5.100	-0.493
Si	1.080	-3.586	1.350	1.047	-3.650	1.391
Si	1.676	-2.952	-2.269	1.717	-3.006	-2.322
Si	0.954	-1.157	1.247	0.974	-1.188	1.279
No.19	PW91			BLYP		
Si	-2.054	0.824	-0.384	-2.033	0.835	-0.389
Si	1.635	1.442	-2.035	1.678	1.467	-2.033
Si	-1.090	4.023	2.464	-1.086	4.137	2.488
Si	-0.616	2.223	-1.569	-0.623	2.260	-1.622
Si	-3.412	1.688	1.271	-3.450	1.704	1.239
Si	-0.986	1.668	1.830	-1.063	1.715	1.997
Si	-1.181	4.531	-1.443	-1.222	4.598	-1.453
Si	1.254	1.920	0.254	1.256	2.001	0.264
Si	1.173	0.741	2.325	1.165	0.772	2.335
Si	0.185	4.001	0.464	0.191	4.111	0.457
Si	-2.356	3.750	0.502	-2.411	3.846	0.549
Si	-1.043	-1.290	-0.427	-1.038	-1.316	-0.460
Si	2.907	-2.126	-0.145	2.962	-2.171	-0.133
Si	-0.946	-2.800	1.382	-0.955	-2.841	1.378
Si	1.234	-0.767	-1.279	1.303	-0.802	-1.309
Si	-0.134	-4.137	-0.599	-0.145	-4.268	-0.610
Si	-0.908	-2.746	-2.331	-0.949	-2.858	-2.344
Si	2.324	-4.506	-0.855	2.361	-4.580	-0.890
La	1.506	-4.212	1.848	1.531	-4.291	1.855
Si	1.520	-2.899	-2.416	1.522	-2.968	-2.483
Si	0.980	-1.331	1.145	1.000	-1.352	1.165
No.20	PW91			BLYP		
Si	-2.077	0.783	-0.254	-2.067	0.783	-0.242
Si	1.569	1.368	-1.964	1.572	1.400	-1.997
Si	-1.074	4.069	2.485	-1.040	4.182	2.507
Si	-0.663	2.164	-1.506	-0.706	2.195	-1.559
Si	-3.412	1.695	1.393	-3.433	1.707	1.399
Si	-0.978	1.701	1.907	-1.023	1.742	2.074
Si	-1.245	4.470	-1.428	-1.321	4.529	-1.438
Si	1.238	1.915	0.306	1.240	2.006	0.288
Si	1.204	0.799	2.421	1.243	0.840	2.402
Si	0.164	3.997	0.465	0.166	4.113	0.437
Si	-2.382	3.740	0.558	-2.436	3.837	0.626
Si	-1.058	-1.328	-0.233	-1.055	-1.359	-0.246
Si	2.917	-2.093	-0.195	2.976	-2.140	-0.188
Si	-1.155	-3.280	1.168	-1.224	-3.386	1.103
Si	1.169	-0.942	-1.483	1.221	-0.957	-1.512
Si	-0.080	-4.128	-0.745	-0.091	-4.248	-0.793
Si	-0.661	-2.284	-2.359	-0.636	-2.312	-2.401
Si	2.328	-4.568	-0.249	2.351	-4.654	-0.215
Si	1.244	-3.453	1.561	1.205	-3.535	1.599
La	1.872	-3.531	-2.857	1.936	-3.614	-2.874
Si	1.071	-1.093	1.009	1.115	-1.131	1.028
No.21	PW91			BLYP		
Si	-1.163	0.708	0.849	-1.258	0.712	0.784
Si	1.665	1.237	-1.866	1.679	1.270	-1.867
Si	-1.258	5.073	1.722	-1.264	5.148	1.815
Si	-0.632	1.752	-1.276	-0.638	1.864	-1.292
Si	-3.051	1.709	1.929	-3.131	1.790	1.888
Si	-1.111	2.889	2.570	-1.190	2.938	2.679
Si	-1.795	3.757	-1.822	-1.777	3.929	-1.812
Si	1.240	2.150	0.305	1.252	2.225	0.330
Si	0.696	1.361	2.471	0.608	1.374	2.479
Si	-0.066	4.098	-0.135	-0.027	4.231	-0.097
Si	-2.555	3.545	0.452	-2.628	3.718	0.475
Si	-0.954	-1.542	-0.196	-0.946	-1.574	-0.201
Si	3.082	-2.259	0.026	3.146	-2.330	-0.049
Si	-0.831	-3.722	0.885	-0.785	-3.784	0.923
Si	1.296	-0.862	-0.779	1.322	-0.931	-0.861
Si	-0.340	-4.065	-1.404	-0.338	-4.246	-1.377
Si	-0.345	-1.910	-2.533	-0.419	-2.092	-2.561

Part III: xyz Coordinates for Stationary Points

Si	1.673	-5.306	-1.683	1.730	-5.437	-1.652
Si	1.526	-4.093	0.369	1.604	-4.197	0.405
Si	1.994	-2.895	-2.042	2.051	-2.976	-2.149
La	0.924	-1.624	2.157	1.007	-1.630	2.138
EuSi ₂₀						
Cage	PW91			BLYP		
Si	13.145	10.158	15.835	13.046	10.188	16.002
Si	11.622	11.944	15.817	11.634	12.034	15.705
Si	9.445	11.276	15.369	9.442	11.275	15.392
Si	9.579	8.971	15.579	9.493	8.926	15.446
Si	11.782	8.188	15.693	11.709	8.267	15.813
Si	13.759	10.272	18.097	14.135	10.263	18.130
Si	11.684	13.301	17.692	11.678	13.295	17.697
Si	8.129	12.017	17.147	8.058	12.036	17.146
Si	8.193	8.208	17.267	8.202	8.260	17.291
Si	11.733	7.300	17.859	11.793	7.175	17.890
Si	13.106	12.198	19.197	13.097	12.147	19.173
Si	9.566	13.106	18.605	9.506	13.232	18.575
Si	7.540	10.135	18.367	7.164	10.144	18.334
Si	9.615	7.106	18.772	9.621	7.112	18.767
Si	13.170	8.390	19.316	13.241	8.371	19.318
Si	11.721	11.436	20.886	11.806	11.481	21.018
Si	9.518	12.219	20.771	9.590	12.140	20.652
Si	8.154	10.249	20.629	8.253	10.219	20.461
Si	9.677	8.462	20.648	9.666	8.373	20.759
Si	11.853	9.131	21.094	11.857	9.132	21.072
Eu	10.650	10.203	18.232	10.650	10.203	18.232
No.1	PW91			BLYP		
Eu	-2.375	0.758	0.362	-2.456	0.698	0.286
Si	1.505	1.193	-2.322	1.440	1.221	-2.362
Si	-0.378	4.985	2.383	-0.369	4.983	2.477
Si	-0.845	1.413	-1.985	-0.896	1.694	-1.985
Si	-2.990	2.432	2.717	-3.135	2.489	2.611
Si	-0.730	2.613	2.721	-0.859	2.581	2.736
Si	-1.268	3.639	-1.186	-1.220	3.924	-1.192
Si	0.728	2.087	-0.163	0.860	2.182	-0.162
Si	0.769	0.982	1.900	0.730	1.004	1.889
Si	0.429	4.393	0.210	0.517	4.489	0.278
Si	-2.125	3.960	1.052	-2.148	4.115	1.057
Si	-1.351	-1.889	-0.789	-1.394	-2.056	-0.703
Si	2.638	-1.852	0.340	2.691	-1.905	0.302
Si	-0.719	-4.156	-0.351	-0.701	-4.319	-0.251
Si	1.007	-1.003	-1.400	0.988	-1.057	-1.464
Si	0.944	-5.074	-1.871	0.933	-5.204	-1.864
Si	-0.090	-2.863	-2.590	-0.162	-2.976	-2.583
Si	1.874	-4.179	0.207	1.989	-4.289	0.191
Si	0.221	-3.403	1.711	0.368	-3.455	1.763
Si	2.463	-2.882	-1.905	2.491	-2.935	-1.975
Si	0.291	-1.153	0.959	0.328	-1.184	0.950
No.2	PW91			BLYP		
Si	-1.405	1.016	-0.129	-1.641	0.938	-0.001
Eu	0.718	1.546	-2.618	0.941	1.820	-2.481
Si	-1.428	3.487	2.837	-1.433	3.702	2.787
Si	-1.731	2.972	-1.619	-1.801	2.784	-1.666
Si	-3.557	2.028	-0.526	-3.713	2.146	-0.475
Si	-0.498	1.445	2.000	-0.565	1.585	1.995
Si	-1.205	5.168	-0.644	-1.028	5.075	-0.887
Si	1.184	2.046	0.232	1.416	2.101	0.425
Si	1.785	0.745	2.182	1.683	0.702	2.370
Si	0.001	3.952	1.046	0.108	4.031	1.037
Si	-2.562	3.830	0.735	-2.536	4.011	0.593
Si	-0.550	-1.118	-0.719	-0.779	-1.239	-0.437
Si	3.058	-2.624	-0.265	3.088	-2.449	-0.432
Si	-0.760	-2.524	1.324	-0.743	-2.889	1.397
Si	1.741	-1.185	-1.679	1.382	-1.192	-1.723
Si	-0.163	-4.405	-0.142	-0.115	-4.610	-0.242
Si	-0.982	-3.112	-1.944	-0.942	-3.100	-1.969
Si	2.173	-5.056	-0.411	2.301	-5.062	-0.440
Si	1.474	-3.500	1.615	1.600	-3.572	1.533
Si	1.360	-3.521	-2.108	1.424	-3.562	-2.247
Si	1.343	-1.189	0.831	1.348	-1.219	0.863
No.3	PW91			BLYP		
Si	-2.380	0.605	-0.328	-2.350	0.616	-0.284
Si	1.166	1.270	-2.515	1.168	1.306	-2.504
Eu	-0.443	3.350	3.292	-0.493	3.583	3.342
Si	-0.871	2.127	-1.480	-0.934	2.136	-1.552
Si	-2.860	1.726	1.842	-2.928	1.808	1.862
Si	-0.659	1.490	1.065	-0.670	1.560	1.152
Si	-1.527	4.415	-1.293	-1.519	4.479	-1.294
Si	1.430	2.035	-0.274	1.407	2.136	-0.240
Si	1.476	1.021	1.921	1.493	1.017	1.941
Si	0.212	3.981	0.301	0.244	4.145	0.367
Si	-2.197	3.870	0.992	-2.288	3.978	0.986
Si	-0.957	-1.347	-0.182	-0.963	-1.410	-0.191
Si	3.188	-1.749	-0.491	3.236	-1.832	-0.547
Si	-1.770	-3.677	-0.344	-1.778	-3.764	-0.387
Si	1.016	-0.907	-1.523	1.031	-0.951	-1.560
Si	0.489	-4.546	-0.423	0.503	-4.683	-0.443
Si	-0.393	-2.747	-2.271	-0.382	-2.823	-2.347
Si	2.135	-3.473	0.989	2.184	-3.582	0.984
Si	-0.203	-2.978	1.673	-0.176	-3.071	1.710
Si	1.947	-3.335	-1.900	1.977	-3.456	-1.953
Si	1.199	-1.135	0.951	1.236	-1.195	0.959
No.4	PW91			BLYP		
Si	-2.496	0.283	1.615	-2.516	0.305	1.646
Si	2.243	1.529	-2.115	2.299	1.523	-2.122
Si	-0.967	3.786	1.732	-0.978	3.862	1.786
Eu	-0.737	1.237	-0.795	-0.776	1.256	-0.891
Si	-3.773	1.497	0.082	-3.840	1.539	0.125
Si	-0.783	1.608	2.488	-0.793	1.662	2.548
Si	-1.269	4.095	-1.251	-1.304	4.217	-1.260
Si	2.053	2.441	-0.011	2.065	2.506	-0.021
Si	1.307	1.087	1.797	1.287	1.121	1.784
Si	0.634	4.312	0.113	0.628	4.396	0.118
Si	-2.871	3.695	0.395	-2.891	3.768	0.417
Si	-1.259	-1.471	0.590	-1.275	-1.480	0.627
Si	2.917	-2.283	-0.093	2.976	-2.287	-0.026
Si	-1.362	-3.807	1.012	-1.373	-3.848	0.991
Si	1.616	-0.636	-1.339	1.653	-0.690	-1.359
Si	-0.252	-3.867	-1.052	-0.248	-4.011	-1.114
Si	-0.674	-1.602	-2.030	-0.680	-1.674	-2.071
Si	2.090	-4.529	-0.873	2.142	-4.594	-0.873
Si	1.075	-3.567	1.226	1.095	-3.686	1.238
Si	1.448	-2.742	-2.504	1.455	-2.800	-2.576
Si	1.055	-1.065	1.015	1.070	-1.084	1.034
No.5	PW91			BLYP		
Si	-2.397	0.647	-0.293	-2.353	0.657	-0.275
Si	1.502	1.396	-1.925	1.512	1.426	-1.926
Si	-1.169	3.807	1.643	-1.203	3.910	1.692
Si	-0.746	1.876	-1.427	-0.774	1.946	-1.503
Eu	-3.760	2.242	1.791	-3.849	2.288	1.725
Si	-0.998	1.283	1.638	-1.050	1.322	1.774
Si	-0.861	4.198	-0.752	-0.931	4.273	-0.755
Si	1.253	2.035	0.368	1.312	2.104	0.379
Si	1.185	0.712	2.355	1.199	0.743	2.365
Si	0.952	4.413	0.756	0.921	4.499	0.737
Si	-2.916	4.525	0.209	-2.958	4.706	0.270
Si	-1.109	-1.306	-0.388	-1.070	-1.336	-0.392
Si	2.930	-2.060	-0.154	2.991	-2.124	-0.166
Si	-0.945	-3.228	1.064	-0.976	-3.320	1.029
Si	1.120	-0.884	-1.369	1.183	-0.917	-1.395
Si	0.069	-4.439	-0.760	0.083	-4.576	-0.778
Si	-0.657	-2.722	-2.292	-0.703	-2.829	-2.289
Si	2.494	-4.649	-0.591	2.533	-4.733	-0.610

Part III: xyz Coordinates for Stationary Points

Si	1.410	-3.577	1.381	1.419	-3.663	1.431
Si	1.722	-3.017	-2.294	1.730	-3.080	-2.376
Si	0.919	-1.253	1.041	0.982	-1.296	1.064
No.6	PW91			BLYP		
Si	-2.381	0.723	-0.457	-2.393	0.736	-0.450
Si	1.521	1.398	-2.088	1.537	1.434	-2.095
Si	-1.255	4.719	1.816	-1.240	4.825	1.866
Si	-0.573	2.088	-1.081	-0.606	2.145	-1.127
Si	-3.875	1.596	1.090	-3.884	1.634	1.129
Eu	-0.946	1.338	2.314	-0.963	1.401	2.384
Si	-1.164	4.495	-1.214	-1.229	4.551	-1.254
Si	1.685	1.835	0.295	1.727	1.934	0.313
Si	2.017	0.790	2.354	2.020	0.800	2.366
Si	0.392	3.721	0.586	0.378	3.807	0.574
Si	-2.536	3.334	0.402	-2.614	3.473	0.468
Si	-1.013	-1.122	0.013	-1.025	-1.151	0.003
Si	2.867	-2.180	-0.364	2.911	-2.243	-0.383
Si	-1.191	-3.294	1.009	-1.233	-3.387	0.926
Si	1.017	-0.835	-1.391	1.039	-0.867	-1.438
Si	-0.024	-4.209	-0.793	0.026	-4.338	-0.836
Si	-0.853	-2.339	-2.179	-0.868	-2.425	-2.209
Si	2.317	-4.646	-0.378	2.369	-4.744	-0.289
Si	1.169	-3.405	1.384	1.142	-3.479	1.438
Si	1.540	-2.986	-2.418	1.579	-3.033	-2.502
Si	1.281	-1.022	1.102	1.324	-1.076	1.117
No.7	PW91			BLYP		
Si	-2.317	0.750	-0.254	-2.021	0.869	-0.340
Si	1.539	1.402	-1.920	1.694	1.413	-1.988
Si	-1.161	3.805	2.411	-0.937	4.004	2.494
Si	-0.682	2.147	-1.203	-0.616	2.311	-1.574
Si	-3.294	2.016	1.577	-3.346	1.741	1.388
Si	-0.933	1.416	1.714	-1.040	1.578	2.136
Eu	-1.115	4.971	-1.998	-1.531	5.157	-1.826
Si	1.300	1.965	0.387	1.184	2.060	0.277
Si	1.147	0.654	2.444	1.158	0.723	2.354
Si	0.213	4.056	0.419	0.218	4.225	0.362
Si	-2.421	3.968	0.418	-2.529	3.989	0.772
Si	-1.101	-1.265	-0.188	-1.016	-1.288	-0.389
Si	2.929	-2.096	-0.265	2.973	-2.239	-0.157
Si	-0.867	-3.223	1.201	-0.997	-3.213	1.148
Si	1.058	-0.873	-1.353	1.248	-0.907	-1.371
Si	0.010	-4.431	-0.691	-0.029	-4.560	-0.667
Si	-0.816	-2.689	-2.127	-0.823	-2.881	-2.211
Si	2.436	-4.668	-0.687	2.422	-4.803	-0.648
Si	1.507	-3.607	1.369	1.405	-3.714	1.483
Si	1.562	-3.011	-2.325	1.601	-3.120	-2.330
Si	1.003	-1.287	1.069	0.979	-1.346	1.086
No.8	PW91			BLYP		
Si	-2.328	0.817	-0.061	-2.325	0.807	-0.065
Si	1.073	1.615	-2.094	1.070	1.678	-2.089
Si	-0.081	3.770	1.871	-0.180	3.898	1.924
Si	-1.285	1.978	-1.824	-1.300	2.032	-1.824
Si	-3.348	2.056	1.657	-3.382	2.056	1.636
Si	-0.993	1.501	1.933	-1.008	1.584	2.059
Si	-1.437	4.347	-1.723	-1.514	4.431	-1.754
Eu	2.280	1.574	1.017	2.315	1.711	1.005
Si	0.572	0.268	3.097	0.648	0.313	3.090
Si	0.373	3.357	-0.484	0.357	3.533	-0.478
Si	-1.988	3.771	0.512	-2.081	3.908	0.525
Si	-1.343	-1.309	-0.231	-1.261	-1.310	-0.204
Si	2.698	-1.699	0.103	2.785	-1.828	0.098
Si	-1.028	-3.431	0.859	-1.101	-3.529	0.778
Si	0.859	-0.553	-1.064	0.975	-0.604	-1.104
Si	0.240	-4.229	-1.025	0.218	-4.365	-1.080
Si	-0.618	-2.362	-2.293	-0.641	-2.428	-2.307
Si	2.625	-4.284	-0.671	2.626	-4.415	-0.627
Si	1.353	-3.514	1.310	1.291	-3.642	1.365
Si	1.815	-2.436	-2.210	1.847	-2.540	-2.292
Si	0.559	-1.238	1.320	0.659	-1.291	1.344
No.9	PW91			BLYP		
Si	-2.003	0.855	-0.141	-2.000	0.852	-0.072
Si	1.501	1.344	-1.753	1.557	1.378	-1.750
Si	-0.512	4.184	1.814	-0.678	4.439	1.814
Si	-0.941	1.986	-1.936	-0.907	1.996	-1.865
Si	-3.266	1.432	1.736	-3.320	1.559	1.748
Si	-0.838	1.686	2.015	-0.886	1.944	2.124
Si	-1.253	4.211	-0.946	-1.311	4.274	-1.042
Si	0.425	2.564	-0.009	0.547	2.727	0.018
Eu	2.066	0.848	1.723	1.929	0.817	1.876
Si	0.877	4.965	0.027	0.777	5.172	-0.019
Si	-2.583	3.579	0.991	-2.694	3.733	0.898
Si	-1.340	-1.421	-0.355	-1.191	-1.400	-0.234
Si	2.562	-2.078	0.408	2.680	-2.258	0.383
Si	-1.246	-3.619	0.654	-1.270	-3.721	0.593
Si	0.950	-0.814	-0.919	1.108	-0.873	-0.928
Si	0.180	-4.462	-1.118	0.156	-4.617	-1.202
Si	-0.462	-2.497	-2.360	-0.563	-2.563	-2.315
Si	2.545	-4.576	-0.553	2.589	-4.689	-0.698
Si	1.066	-3.895	1.324	1.091	-4.147	1.305
Si	1.911	-2.700	-2.071	1.876	-2.792	-2.204
Si	0.357	-1.591	1.470	0.506	-1.831	1.570
No.10	PW91			BLYP		
Si	-2.309	0.840	-0.250	-2.313	0.824	-0.243
Si	1.218	1.223	-2.481	1.222	1.249	-2.499
Si	-2.123	3.137	2.728	-2.139	3.216	2.782
Si	-0.901	2.036	-1.790	-0.923	2.062	-1.807
Si	-3.871	2.443	0.912	-3.915	2.484	0.925
Si	-1.011	1.362	1.652	-1.035	1.430	1.664
Si	-0.159	4.246	-1.115	-0.244	4.310	-1.167
Si	1.242	2.303	-0.386	1.313	2.403	-0.409
Si	1.377	1.148	1.766	1.370	1.180	1.775
Eu	0.637	3.987	2.067	0.667	4.067	2.105
Si	-1.852	3.590	0.429	-1.936	3.778	0.479
Si	-1.163	-1.207	-0.373	-1.141	-1.246	-0.361
Si	2.931	-1.977	-0.381	2.993	-2.033	-0.378
Si	-0.827	-2.876	1.348	-0.885	-3.013	1.307
Si	0.996	-0.996	-1.609	1.048	-1.021	-1.628
Si	0.045	-4.381	-0.308	0.057	-4.509	-0.343
Si	-0.839	-2.936	-2.017	-0.858	-3.000	-2.033
Si	2.475	-4.558	-0.330	2.508	-4.635	-0.320
Si	1.553	-3.172	1.547	1.532	-3.249	1.606
Si	1.550	-3.253	-2.225	1.580	-3.308	-2.295
Si	1.030	-0.959	0.814	1.097	-0.990	0.839
No.11	PW91			BLYP		
Si	-2.175	0.868	-0.099	-2.230	0.772	-0.291
Si	1.570	1.406	-2.058	1.657	1.481	-1.981
Si	-1.575	4.120	1.707	-1.313	4.150	1.675
Si	-0.475	2.292	-1.094	-0.548	2.337	-1.188
Si	-2.898	2.060	2.120	-2.840	2.769	2.711
Si	-0.691	1.575	1.689	-1.167	1.389	1.777
Si	-0.924	4.636	-0.861	-0.982	4.725	-0.949
Si	1.619	1.828	0.299	1.603	1.881	0.364
Si	1.382	0.668	2.414	1.090	0.685	2.433
Si	0.595	3.879	0.734	0.736	4.058	0.570
Eu	-3.561	3.395	-0.526	-3.650	3.370	-0.243
Si	-1.089	-1.183	-0.295	-1.014	-1.224	-0.605
Si	2.885	-2.136	-0.233	2.929	-2.171	-0.154
Si	-0.981	-3.111	1.158	-1.032	-3.113	1.024
Si	1.092	-0.830	-1.361	1.261	-0.847	-1.422
Si	-0.118	-4.342	-0.737	0.026	-4.541	-0.728
Si	-0.827	-2.595	-2.231	-0.857	-2.959	-2.292
Si	2.304	-4.695	-0.704	2.496	-4.687	-0.789
Si	1.371	-3.596	1.341	1.363	-3.698	1.436
Si	1.530	-2.989	-2.323	1.573	-3.049	-2.407

Part III: xyz Coordinates for Stationary Points

Si	0.964	-1.252	1.060	0.897	-1.329	1.059
No.12	PW91			BLYP		
Si	-1.941	0.640	0.445	-1.892	0.654	0.431
Si	1.033	1.164	-2.503	1.138	1.177	-2.474
Si	-0.861	4.122	1.742	-0.904	4.207	1.760
Si	-0.771	1.950	-1.118	-0.803	1.990	-1.209
Si	-2.438	2.072	2.342	-2.624	2.096	2.251
Si	-0.160	1.598	1.888	-0.312	1.679	2.192
Si	-1.503	4.248	-0.923	-1.556	4.298	-0.973
Si	1.640	1.800	-0.287	1.574	1.921	-0.211
Si	2.016	0.597	1.780	1.883	0.716	1.930
Si	0.629	3.921	-0.059	0.597	4.073	-0.075
Si	-3.043	4.226	1.054	-3.100	4.398	1.033
Eu	-2.117	-1.860	-1.188	-2.131	-1.891	-1.126
Si	2.784	-1.439	0.108	3.273	-1.828	-0.163
Si	-1.581	-4.332	0.390	-1.603	-4.362	0.542
Si	0.786	-1.011	-1.526	0.918	-1.033	-1.467
Si	0.463	-4.237	-0.663	0.366	-4.362	-0.693
Si	0.251	-2.996	-2.804	0.193	-3.018	-2.840
Si	2.254	-3.729	0.850	2.263	-3.939	0.748
Si	0.037	-3.059	1.479	0.127	-3.080	1.475
Si	2.417	-2.873	-1.807	2.402	-2.925	-1.998
Si	0.102	-0.804	0.799	0.188	-0.773	0.866
No.13	PW91			BLYP		
Si	-2.065	0.842	-0.339	-2.022	0.855	-0.380
Si	1.596	1.371	-1.985	1.659	1.465	-1.985
Si	-1.078	4.044	2.500	-1.132	4.124	2.539
Si	-0.612	2.230	-1.527	-0.614	2.308	-1.582
Si	-3.442	1.751	1.275	-3.483	1.720	1.213
Si	-1.021	1.684	1.863	-1.107	1.708	2.012
Si	-1.158	4.546	-1.404	-1.227	4.647	-1.394
Si	1.219	1.888	0.316	1.219	2.006	0.330
Si	1.096	0.693	2.408	1.100	0.737	2.401
Si	0.197	3.993	0.501	0.162	4.119	0.521
Si	-2.354	3.806	0.545	-2.441	3.878	0.585
Si	-1.140	-1.317	-0.351	-1.033	-1.303	-0.426
Eu	3.567	-2.074	-0.183	3.669	-2.285	-0.230
Si	-0.962	-3.134	1.301	-0.976	-3.132	1.317
Si	1.036	-0.852	-1.349	1.189	-0.832	-1.358
Si	-0.128	-4.313	-0.691	-0.151	-4.420	-0.655
Si	-0.792	-2.666	-2.351	-0.898	-2.848	-2.345
Si	2.212	-4.739	-0.652	2.183	-4.836	-0.705
Si	1.373	-3.536	1.360	1.383	-3.612	1.441
Si	1.549	-2.988	-2.255	1.489	-3.044	-2.321
Si	0.904	-1.231	1.018	1.028	-1.256	1.022
No.14	PW91			BLYP		
Si	-1.503	0.661	-0.629	-1.573	0.659	-0.693
Si	1.892	1.875	-2.125	1.909	1.884	-2.142
Si	-1.175	3.619	2.694	-1.192	3.721	2.718
Si	-0.439	2.409	-1.708	-0.459	2.437	-1.728
Si	-3.071	0.953	1.054	-3.077	0.986	1.075
Si	-0.825	1.367	1.948	-0.834	1.422	2.066
Si	-1.446	4.479	-1.118	-1.460	4.549	-1.143
Si	1.226	1.777	0.202	1.311	1.891	0.235
Si	1.429	0.608	2.278	1.441	0.623	2.282
Si	0.055	3.809	0.640	0.072	3.912	0.644
Si	-2.413	3.270	0.717	-2.458	3.352	0.740
Si	-0.113	-1.194	-0.740	-0.191	-1.228	-0.760
Si	2.664	-1.981	-0.568	2.749	-2.040	-0.552
Eu	-2.006	-2.095	1.326	-2.086	-2.199	1.357
Si	1.709	-0.537	-2.195	1.750	-0.570	-2.151
Si	0.491	-3.879	0.033	0.532	-4.030	0.033
Si	-1.291	-3.171	-1.484	-1.270	-3.294	-1.499
Si	2.338	-4.145	-1.443	2.364	-4.184	-1.492
Si	0.508	-3.547	2.387	0.538	-3.593	2.402
Si	0.802	-2.694	-2.587	0.802	-2.709	-2.690
Si	1.163	-1.584	1.318	1.128	-1.589	1.298
No.15	PW91			BLYP		
Si	-1.863	0.529	0.332	-1.956	0.440	0.367
Si	1.892	1.468	-1.606	1.939	1.483	-1.540
Si	-1.664	3.781	2.456	-1.737	3.817	2.446
Si	-0.384	2.207	-1.238	-0.271	2.466	-1.548
Si	-2.854	1.752	-1.372	-2.763	1.759	-1.417
Si	-0.782	1.606	2.071	-0.852	1.590	2.088
Si	-0.698	4.593	-1.279	-0.615	4.804	-1.230
Si	1.410	1.961	0.673	1.395	2.006	0.724
Si	1.374	0.677	2.683	1.355	0.668	2.739
Si	0.128	3.947	0.855	0.155	4.014	0.920
Si	-2.312	3.603	0.132	-2.282	3.655	0.055
Si	-0.525	-1.321	0.009	-0.655	-1.449	0.077
Si	1.667	-0.820	-1.015	1.563	-0.840	-1.035
Si	-0.366	-3.258	1.439	-0.288	-3.375	1.605
Eu	-0.679	-0.462	-2.841	-0.851	-0.456	-2.804
Si	-0.612	-5.197	-0.123	-0.534	-5.265	-0.099
Si	-0.565	-3.203	-1.447	-0.607	-3.298	-1.488
Si	1.547	-4.181	-0.477	1.618	-4.275	-0.530
Si	2.007	-3.583	1.846	2.135	-3.607	1.810
Si	1.653	-2.773	-2.400	1.617	-2.801	-2.443
Si	1.623	-1.326	1.302	1.631	-1.337	1.303
No.16	PW91			BLYP		
Si	-1.998	0.523	-0.205	-1.830	0.599	-0.031
Si	1.591	1.505	-2.137	1.622	1.492	-2.142
Si	-1.310	3.642	1.810	-1.305	3.726	1.878
Si	-0.549	2.081	-1.199	-0.586	2.143	-1.337
Si	-2.932	1.630	1.776	-3.037	1.665	1.760
Si	-0.592	1.235	1.646	-0.635	1.340	1.979
Si	-1.480	4.261	-0.935	-1.530	4.339	-1.074
Si	1.616	1.911	0.184	1.566	2.034	0.182
Si	1.645	0.787	2.293	1.724	0.860	2.303
Si	0.472	3.996	0.335	0.410	4.127	0.272
Si	-3.352	3.928	0.760	-3.375	4.006	0.816
Si	-0.762	-1.526	-0.223	-0.835	-1.573	-0.258
Si	3.369	-1.900	-0.552	3.398	-1.991	-0.479
Si	-1.840	-3.153	1.211	-1.828	-3.300	1.155
Si	1.249	-0.766	-1.632	1.294	-0.827	-1.653
Eu	-0.609	-4.697	-1.031	-0.608	-4.841	-1.125
Si	-0.398	-2.153	-2.578	-0.384	-2.198	-2.635
Si	2.194	-3.941	0.151	2.204	-4.088	0.092
Si	0.394	-3.009	1.523	0.396	-3.049	1.530
Si	1.693	-3.273	-2.023	1.729	-3.370	-2.106
Si	1.595	-1.084	0.824	1.608	-1.097	0.872
No.17	PW91			BLYP		
Si	-1.933	0.620	0.073	-1.928	0.648	0.069
Si	1.372	1.346	-2.223	1.336	1.422	-2.302
Si	-0.839	4.232	2.378	-0.784	4.319	2.443
Si	-0.856	2.006	-1.463	-0.922	2.081	-1.503
Si	-3.048	1.543	1.876	-3.036	1.534	1.918
Si	-0.593	1.834	2.012	-0.577	1.878	2.181
Si	-1.658	4.248	-1.463	-1.765	4.353	-1.394
Si	1.277	2.047	0.041	1.280	2.165	-0.012
Si	1.681	1.128	2.209	1.731	1.137	2.120
Si	0.073	4.062	0.195	0.054	4.190	0.198
Si	-2.385	3.597	0.730	-2.426	3.693	0.861
Si	-0.737	-1.371	0.012	-0.787	-1.402	-0.144
Si	3.084	-2.348	-0.001	3.144	-2.553	0.187
Si	-1.073	-3.713	-0.008	-1.156	-3.779	-0.019
Si	1.157	-0.845	-1.308	1.143	-0.847	-1.440
Si	0.412	-4.856	-1.663	0.508	-4.947	-1.653
Eu	-0.930	-2.423	-2.818	-0.837	-2.639	-2.958
Si	1.520	-4.171	0.327	1.474	-4.277	0.401
Si	0.107	-2.964	1.932	0.029	-2.949	1.935
Si	1.963	-2.972	-1.991	2.103	-3.026	-1.923
Si	1.406	-1.002	1.157	1.414	-1.003	1.037
No.18	PW91			BLYP		

Part III: xyz Coordinates for Stationary Points

Si	-2.032	0.884	-0.305	-2.018	0.882	-0.306
Si	1.579	1.417	-2.026	1.605	1.452	-2.045
Si	-1.012	4.128	2.485	-1.011	4.230	2.508
Si	-0.642	2.267	-1.553	-0.667	2.300	-1.600
Si	-3.388	1.752	1.346	-3.411	1.755	1.341
Si	-0.992	1.760	1.930	-1.045	1.802	2.082
Si	-1.200	4.576	-1.410	-1.265	4.637	-1.424
Si	1.188	1.898	0.269	1.202	1.993	0.266
Si	1.158	0.784	2.392	1.178	0.826	2.389
Si	0.213	4.032	0.456	0.206	4.144	0.440
Si	-2.328	3.820	0.569	-2.389	3.907	0.618
Si	-1.077	-1.255	-0.336	-1.038	-1.275	-0.352
Si	2.763	-2.071	-0.167	2.824	-2.136	-0.157
Si	-1.107	-3.203	1.067	-1.160	-3.278	1.027
Si	1.074	-0.840	-1.423	1.154	-0.867	-1.453
Si	0.023	-4.406	-0.711	0.006	-4.511	-0.738
Si	-0.851	-2.723	-2.223	-0.874	-2.794	-2.249
Eu	2.880	-5.058	-0.583	2.892	-5.153	-0.581
Si	1.288	-3.539	1.379	1.271	-3.608	1.431
Si	1.571	-3.018	-2.258	1.596	-3.070	-2.326
Si	0.886	-1.206	1.102	0.939	-1.239	1.127
No.19	PW91			BLYP		
Si	-2.002	0.845	-0.453	-1.996	0.863	-0.450
Si	1.718	1.541	-2.005	1.745	1.543	-2.007
Si	-1.136	4.002	2.481	-1.119	4.123	2.501
Si	-0.556	2.286	-1.575	-0.572	2.315	-1.631
Si	-3.423	1.676	1.164	-3.458	1.705	1.152
Si	-1.028	1.660	1.823	-1.105	1.710	1.988
Si	-1.130	4.591	-1.415	-1.173	4.651	-1.434
Si	1.259	1.943	0.285	1.254	2.010	0.294
Si	1.112	0.706	2.319	1.104	0.739	2.335
Si	0.189	4.021	0.511	0.201	4.127	0.494
Si	-2.352	3.762	0.484	-2.404	3.864	0.533
Si	-0.962	-1.258	-0.517	-0.970	-1.275	-0.530
Si	2.875	-2.130	-0.171	2.931	-2.158	-0.158
Si	-0.959	-2.816	1.303	-0.974	-2.878	1.282
Si	1.340	-0.678	-1.273	1.375	-0.731	-1.304
Si	-0.056	-4.211	-0.526	-0.059	-4.342	-0.553
Si	-1.124	-3.014	-2.200	-1.126	-3.080	-2.216
Si	2.326	-4.496	-0.979	2.369	-4.573	-1.017
Eu	1.695	-4.174	1.877	1.716	-4.251	1.884
Si	1.262	-2.879	-2.287	1.295	-2.959	-2.354
Si	0.953	-1.379	1.154	0.963	-1.404	1.191
No.20	PW91			BLYP		
Si	-2.051	0.760	-0.174	-2.053	0.778	-0.172
Si	1.508	1.334	-1.982	1.512	1.367	-2.017
Si	-1.029	4.132	2.470	-1.000	4.236	2.497
Si	-0.707	2.143	-1.499	-0.745	2.180	-1.554
Si	-3.364	1.691	1.480	-3.395	1.714	1.482
Si	-0.925	1.753	1.944	-0.973	1.794	2.101
Si	-1.311	4.442	-1.441	-1.367	4.510	-1.442
Si	1.241	1.951	0.279	1.241	2.026	0.263
Si	1.287	0.900	2.427	1.307	0.914	2.406
Si	0.154	4.026	0.423	0.163	4.132	0.406
Si	-2.387	3.735	0.588	-2.434	3.837	0.652
Si	-0.987	-1.332	-0.141	-1.004	-1.348	-0.171
Si	2.895	-2.109	-0.176	2.949	-2.134	-0.164
Si	-1.342	-3.479	0.958	-1.367	-3.547	0.913
Si	1.160	-0.986	-1.502	1.199	-1.001	-1.549
Si	-0.009	-4.161	-0.816	-0.008	-4.291	-0.848
Si	-0.668	-2.308	-2.310	-0.655	-2.365	-2.341
Si	2.288	-4.599	-0.130	2.320	-4.686	-0.097
Si	1.009	-3.394	1.409	1.004	-3.487	1.446
Eu	2.063	-3.496	-2.846	2.125	-3.568	-2.861
Si	1.172	-1.006	1.037	1.178	-1.062	1.048
No.21	PW91			BLYP		
Si	-1.002	0.774	0.908	-1.181	0.813	0.842
Si	1.703	1.230	-1.864	1.713	1.267	-1.830
Si	-1.420	5.004	1.660	-1.377	5.109	1.752
Si	-0.603	1.687	-1.307	-0.611	1.839	-1.305
Si	-2.914	1.583	2.056	-3.095	1.745	1.948
Si	-0.981	2.872	2.562	-1.128	2.912	2.660
Si	-1.910	3.601	-1.843	-1.820	3.850	-1.862
Si	1.253	2.199	0.285	1.252	2.248	0.349
Si	0.863	1.391	2.474	0.679	1.367	2.505
Si	-0.182	4.067	-0.158	-0.101	4.211	-0.105
Si	-2.607	3.334	0.441	-2.667	3.599	0.417
Si	-0.846	-1.510	-0.330	-0.817	-1.641	-0.291
Si	3.127	-2.346	0.059	3.225	-2.408	-0.100
Si	-1.025	-3.615	0.812	-0.881	-3.760	0.923
Si	1.431	-0.847	-0.696	1.445	-0.911	-0.761
Si	-0.477	-3.914	-1.481	-0.497	-4.125	-1.406
Si	-0.203	-1.800	-2.644	-0.354	-2.033	-2.663
Si	1.530	-5.211	-1.586	1.607	-5.320	-1.606
Si	1.371	-3.998	0.430	1.551	-4.140	0.449
Si	2.016	-2.891	-2.014	2.014	-2.970	-2.141
Eu	0.874	-1.611	2.236	1.040	-1.653	2.224
GdSi ₂₀						
Cage	PW91			BLYP		
Si	2.707	-1.128	-1.595	2.743	-1.132	-1.612
Si	2.924	1.040	-0.776	2.987	1.072	-0.802
Si	0.820	-1.110	-3.018	0.836	-1.131	-3.057
Si	-0.012	1.063	-3.055	0.001	1.070	-3.066
Si	1.286	2.410	-1.682	1.325	2.461	-1.715
Si	-0.835	-2.468	-2.044	-0.842	-2.504	-2.071
Si	-2.629	-1.085	-1.521	-2.642	-1.097	-1.515
Si	-2.140	1.089	-2.145	-2.147	1.097	-2.145
Si	0.008	-3.340	-0.017	0.001	-3.378	-0.011
Si	-1.286	-2.410	1.682	-1.324	-2.461	1.715
Si	-2.924	-1.041	0.776	-2.987	-1.073	0.802
Si	2.173	-2.460	0.271	2.200	-2.499	0.264
Si	2.140	-1.089	2.145	2.147	-1.098	2.145
Si	0.012	-1.064	3.056	-0.000	-1.070	3.066
Si	2.630	1.085	1.521	2.642	1.097	1.515
Si	0.836	2.468	2.045	0.842	2.504	2.072
Si	-0.820	1.110	3.018	-0.836	1.130	3.057
Si	-2.707	1.128	1.596	-2.743	1.132	1.612
Si	-2.173	2.460	-0.270	-2.200	2.499	-0.263
Si	-0.008	3.339	0.018	-0.001	3.378	0.011
Gd	0.000	-0.000	0.000	0.000	-0.000	0.000
No.1	PW91			BLYP		
Gd	-2.053	0.790	0.336	-2.050	0.746	0.226
Si	1.520	1.203	-2.369	1.439	1.246	-2.400
Si	-0.422	4.860	2.318	-0.435	4.842	2.463
Si	-0.844	1.503	-2.064	-0.929	1.808	-2.129
Si	-3.107	2.138	2.616	-3.250	2.184	2.433
Si	-0.848	2.549	2.774	-0.980	2.497	2.764
Si	-1.205	3.585	-1.029	-1.109	3.854	-1.019
Si	0.757	2.150	-0.234	0.823	2.250	-0.242
Si	0.732	1.057	1.852	0.706	1.071	1.835
Si	0.623	4.536	0.086	0.728	4.649	0.212
Si	-2.236	3.832	1.172	-2.256	3.987	1.157
Si	-1.347	-1.834	-0.762	-1.400	-2.006	-0.657
Si	2.672	-1.843	0.288	2.726	-1.880	0.233
Si	-0.767	-4.098	-0.271	-0.747	-4.259	-0.126
Si	0.998	-0.982	-1.414	0.971	-1.035	-1.468
Si	0.862	-5.076	-1.797	0.823	-5.214	-1.773
Si	-0.142	-2.857	-2.570	-0.224	-2.983	-2.534
Si	1.830	-4.153	0.249	1.948	-4.254	0.221
Si	0.208	-3.337	1.764	0.397	-3.393	1.836
Si	2.392	-2.920	-1.919	2.409	-2.971	-2.005
Si	0.370	-1.104	0.975	0.406	-1.141	0.972
No.2	PW91			BLYP		
Si	-1.852	0.881	-0.030	-1.820	0.895	0.025

Part III: xyz Coordinates for Stationary Points

Gd	0.505	1.872	-1.726	0.572	1.894	-1.706
Si	-1.106	3.809	2.500	-1.204	3.904	2.507
Si	-2.198	2.481	-1.811	-2.163	2.476	-1.822
Si	-3.981	2.074	-0.253	-4.009	2.051	-0.317
Si	-0.388	1.678	1.629	-0.378	1.751	1.709
Si	-0.923	4.570	-1.160	-0.957	4.635	-1.158
Si	1.925	2.001	0.628	1.987	2.205	0.679
Si	1.554	0.605	2.596	1.628	0.668	2.600
Si	0.487	3.859	0.718	0.473	3.993	0.785
Si	-2.387	3.702	0.465	-2.523	3.812	0.431
Si	-0.935	-1.266	-0.291	-0.895	-1.275	-0.248
Si	3.023	-2.205	-0.321	3.058	-2.286	-0.377
Si	-0.766	-3.008	1.387	-0.820	-3.126	1.359
Si	1.239	-0.996	-1.537	1.258	-1.060	-1.595
Si	-0.049	-4.456	-0.414	-0.059	-4.581	-0.439
Si	-0.813	-2.852	-2.065	-0.880	-2.901	-2.042
Si	2.372	-4.825	-0.491	2.384	-4.915	-0.510
Si	1.568	-3.497	1.429	1.565	-3.584	1.466
Si	1.525	-3.277	-2.216	1.493	-3.365	-2.321
Si	1.202	-1.150	0.961	1.291	-1.192	0.973
No.3	PW91			BLYP		
Si	-2.429	0.581	-0.306	-2.434	0.579	-0.282
Si	1.119	1.267	-2.535	1.135	1.304	-2.517
Gd	-0.474	3.244	3.098	-0.478	3.396	3.161
Si	-0.923	2.082	-1.491	-0.981	2.101	-1.559
Si	-2.802	1.669	1.972	-2.876	1.814	1.974
Si	-0.638	1.481	0.986	-0.686	1.545	1.039
Si	-1.464	4.427	-1.247	-1.475	4.493	-1.262
Si	1.459	2.089	-0.325	1.438	2.177	-0.282
Si	1.478	1.073	1.876	1.445	1.064	1.904
Si	0.284	4.034	0.430	0.304	4.185	0.455
Si	-2.153	3.764	0.946	-2.228	3.939	0.979
Si	-0.968	-1.333	-0.204	-0.975	-1.399	-0.205
Si	3.184	-1.725	-0.438	3.242	-1.804	-0.476
Si	-1.774	-3.670	-0.358	-1.770	-3.769	-0.374
Si	1.024	-0.893	-1.505	1.041	-0.941	-1.539
Si	0.483	-4.535	-0.417	0.508	-4.669	-0.444
Si	-0.382	-2.734	-2.277	-0.375	-2.809	-2.346
Si	2.100	-3.455	1.017	2.163	-3.573	1.006
Si	-0.248	-2.955	1.670	-0.208	-3.055	1.709
Si	1.957	-3.303	-1.870	1.997	-3.406	-1.929
Si	1.169	-1.110	0.975	1.211	-1.172	0.986
No.4	PW91			BLYP		
Si	-2.489	0.316	1.681	-2.522	0.332	1.744
Si	2.292	1.595	-2.061	2.370	1.567	-2.070
Si	-1.044	3.765	1.645	-1.052	3.863	1.680
Gd	-0.586	1.172	-0.501	-0.610	1.186	-0.548
Si	-3.738	1.331	-0.065	-3.808	1.389	0.008
Si	-0.753	1.632	2.468	-0.766	1.696	2.478
Si	-1.202	3.858	-1.353	-1.268	3.940	-1.374
Si	2.048	2.402	0.095	2.064	2.456	0.069
Si	1.428	1.074	1.943	1.423	1.108	1.947
Si	0.611	4.276	0.094	0.600	4.347	0.064
Si	-2.874	3.498	0.198	-2.914	3.590	0.233
Si	-1.254	-1.429	0.674	-1.281	-1.432	0.736
Si	2.908	-2.292	-0.168	2.965	-2.303	-0.061
Si	-1.373	-3.766	1.066	-1.397	-3.805	1.014
Si	1.636	-0.577	-1.368	1.684	-0.633	-1.369
Si	-0.346	-3.769	-1.043	-0.323	-3.908	-1.111
Si	-0.739	-1.459	-1.956	-0.727	-1.504	-2.008
Si	1.978	-4.478	-0.993	2.047	-4.534	-1.025
Si	1.066	-3.500	1.188	1.082	-3.642	1.183
Si	1.316	-2.643	-2.555	1.316	-2.678	-2.643
Si	1.113	-1.009	1.008	1.115	-1.036	1.051
No.5	PW91			BLYP		
Si	-2.469	0.552	-0.369	-2.386	0.589	-0.334
Si	1.441	1.417	-1.899	1.473	1.438	-1.902
Si	-1.105	3.789	1.708	-1.166	3.912	1.742
Si	-0.791	1.851	-1.355	-0.793	1.936	-1.447
Gd	-3.530	2.327	1.627	-3.610	2.343	1.593
Si	-1.044	1.208	1.559	-1.077	1.260	1.747
Si	-0.896	4.165	-0.738	-0.974	4.262	-0.749
Si	1.214	2.097	0.407	1.275	2.161	0.411
Si	1.103	0.698	2.362	1.154	0.730	2.367
Si	0.977	4.491	0.750	0.929	4.571	0.729
Si	-2.895	4.651	0.295	-2.972	4.770	0.326
Si	-1.122	-1.346	-0.416	-1.090	-1.377	-0.420
Si	2.928	-2.063	-0.154	2.988	-2.137	-0.161
Si	-0.931	-3.240	1.070	-0.975	-3.336	1.041
Si	1.115	-0.874	-1.363	1.176	-0.910	-1.386
Si	0.103	-4.477	-0.737	0.097	-4.595	-0.766
Si	-0.685	-2.810	-2.273	-0.717	-2.889	-2.294
Si	2.548	-4.600	-0.601	2.563	-4.699	-0.614
Si	1.430	-3.577	1.399	1.423	-3.662	1.442
Si	1.702	-3.003	-2.302	1.718	-3.069	-2.378
Si	0.905	-1.264	1.031	0.962	-1.302	1.054
No.6	PW91			BLYP		
Si	-2.411	0.724	-0.468	-2.413	0.736	-0.480
Si	1.514	1.378	-2.143	1.519	1.414	-2.153
Si	-1.156	4.242	2.299	-1.122	4.340	2.350
Si	-0.616	2.058	-1.194	-0.666	2.129	-1.287
Si	-3.691	1.705	1.180	-3.703	1.717	1.195
Gd	-0.877	1.330	2.119	-0.895	1.380	2.175
Si	-1.138	4.418	-1.397	-1.205	4.501	-1.382
Si	1.592	1.947	0.214	1.609	2.042	0.221
Si	1.949	0.881	2.261	1.948	0.894	2.257
Si	0.273	3.830	0.503	0.276	3.942	0.502
Si	-2.442	3.533	0.451	-2.504	3.651	0.550
Si	-1.051	-1.115	0.009	-1.067	-1.149	-0.021
Si	2.824	-2.175	-0.311	2.874	-2.243	-0.326
Si	-1.272	-3.344	0.873	-1.301	-3.421	0.820
Si	0.996	-0.839	-1.406	1.024	-0.877	-1.457
Si	0.093	-4.235	-0.791	0.128	-4.359	-0.816
Si	-0.831	-2.386	-2.167	-0.827	-2.475	-2.213
Si	2.380	-4.623	-0.163	2.414	-4.722	-0.056
Si	1.064	-3.357	1.451	1.038	-3.422	1.503
Si	1.586	-2.978	-2.423	1.629	-3.037	-2.489
Si	1.213	-0.994	1.099	1.243	-1.041	1.103
No.7	PW91			BLYP		
Si	-2.070	0.869	-0.322	-2.023	0.879	-0.333
Si	1.619	1.369	-2.000	1.654	1.398	-2.038
Si	-0.981	3.939	2.485	-0.938	4.058	2.523
Si	-0.619	2.273	-1.516	-0.632	2.307	-1.594
Si	-3.349	1.748	1.413	-3.366	1.729	1.386
Si	-0.945	1.592	1.901	-1.012	1.651	2.097
Gd	-1.397	4.960	-1.706	-1.503	5.024	-1.693
Si	1.239	1.910	0.283	1.236	2.010	0.254
Si	1.190	0.689	2.374	1.194	0.745	2.353
Si	0.180	4.007	0.379	0.190	4.140	0.366
Si	-2.434	3.850	0.622	-2.491	3.934	0.728
Si	-1.066	-1.257	-0.333	-1.030	-1.282	-0.382
Si	2.914	-2.140	-0.181	2.965	-2.202	-0.157
Si	-0.948	-3.137	1.195	-1.014	-3.205	1.143
Si	1.137	-0.874	-1.355	1.218	-0.909	-1.390
Si	-0.033	-4.416	-0.650	-0.037	-4.537	-0.672
Si	-0.791	-2.750	-2.191	-0.808	-2.848	-2.230
Si	2.391	-4.699	-0.623	2.413	-4.784	-0.602
Si	1.418	-3.604	1.430	1.382	-3.675	1.493
Si	1.585	-3.046	-2.273	1.619	-3.118	-2.337
Si	0.953	-1.281	1.065	0.978	-1.313	1.084
No.8	PW91			BLYP		
Si	-2.013	0.922	0.153	-2.015	0.927	0.137
Si	0.989	1.714	-2.406	0.982	1.721	-2.466
Si	0.106	3.786	1.818	0.031	3.841	1.874

Part III: xyz Coordinates for Stationary Points

Si	-1.256	2.079	-1.748	-1.265	2.129	-1.777
Si	-3.262	2.233	1.711	-3.260	2.265	1.718
Si	-1.018	1.624	2.339	-1.022	1.602	2.394
Si	-1.518	4.476	-1.758	-1.535	4.562	-1.795
Gd	1.272	1.118	0.662	1.291	1.155	0.658
Si	0.505	0.204	3.376	0.536	0.182	3.425
Si	0.457	3.576	-0.667	0.465	3.677	-0.659
Si	-1.816	3.821	0.484	-1.869	3.983	0.492
Si	-0.893	-1.102	-0.042	-0.918	-1.139	-0.050
Si	2.372	-1.549	0.156	2.449	-1.550	0.178
Si	-1.174	-3.516	0.342	-1.201	-3.594	0.353
Si	0.903	-0.606	-1.630	0.933	-0.643	-1.644
Si	0.573	-4.478	-1.136	0.560	-4.562	-1.158
Si	-0.772	-2.578	-2.060	-0.797	-2.642	-2.094
Si	2.995	-3.769	-0.392	3.030	-3.800	-0.377
Si	1.192	-3.749	1.291	1.208	-3.823	1.342
Si	1.859	-2.636	-2.354	1.878	-2.700	-2.423
Si	0.494	-1.567	1.860	0.515	-1.592	1.872
No.9	PW91			BLYP		
Si	-2.089	0.877	-0.526	-2.187	0.872	-0.469
Si	1.177	1.271	-2.508	1.549	1.389	-1.854
Si	-0.195	3.271	2.704	-0.544	3.836	2.110
Si	-1.126	2.241	-2.210	-1.119	2.303	-2.175
Si	-3.316	1.449	1.415	-3.463	1.376	1.502
Si	-0.994	1.162	1.731	-1.052	1.405	1.920
Si	-0.798	4.163	-0.636	-1.060	4.463	-0.671
Si	0.346	1.930	-0.378	0.088	2.293	-0.163
Gd	1.842	1.325	1.901	2.065	1.163	1.262
Si	1.214	3.868	0.733	1.234	4.368	0.578
Si	-2.121	3.531	1.333	-2.663	3.712	1.191
Si	-1.405	-1.479	-0.595	-1.283	-1.377	-0.544
Si	2.593	-1.329	0.378	2.708	-1.854	0.351
Si	-0.977	-3.149	1.293	-1.156	-3.301	1.042
Si	0.849	-0.730	-1.248	1.036	-0.820	-1.162
Si	0.021	-4.161	-0.707	0.105	-4.449	-0.779
Si	-0.291	-2.598	-2.489	-0.476	-2.759	-2.407
Si	2.188	-5.053	-0.532	2.478	-4.749	-0.496
Si	1.567	3.377	1.146	1.323	-3.648	1.499
Si	2.082	-2.861	-1.638	1.934	-2.893	-2.082
Si	0.274	-1.097	1.248	0.481	-1.330	1.347
No.10	PW91			BLYP		
Si	-2.282	0.871	-0.339	-2.267	0.880	-0.377
Si	1.305	1.202	-2.607	1.346	1.263	-2.629
Si	-2.106	3.207	2.847	-2.114	3.238	2.929
Si	-0.774	2.020	-1.784	-0.758	2.079	-1.819
Si	-3.831	2.343	0.992	-3.874	2.374	0.909
Si	-1.136	1.395	1.674	-1.188	1.425	1.700
Si	-0.145	4.214	-1.029	-0.222	4.292	-1.035
Si	1.355	2.295	-0.467	1.425	2.413	-0.473
Si	1.290	1.143	1.725	1.272	1.159	1.732
Gd	0.553	3.778	1.898	0.567	3.825	1.923
Si	-1.893	3.619	0.511	-1.994	3.827	0.603
Si	-1.190	-1.206	-0.391	-1.163	-1.227	-0.433
Si	2.923	-1.941	-0.368	2.972	-1.997	-0.394
Si	-0.821	-2.821	1.394	-0.843	-2.881	1.377
Si	0.990	-0.957	-1.603	1.049	-0.968	-1.642
Si	0.042	-4.344	-0.274	0.067	-4.489	-0.232
Si	-0.846	-2.946	-2.007	-0.928	-3.105	-1.944
Si	2.474	-4.533	-0.342	2.517	-4.605	-0.384
Si	1.571	-3.157	1.563	1.596	-3.222	1.633
Si	1.540	-3.212	-2.210	1.500	-3.277	-2.271
Si	0.981	-0.971	0.820	1.039	-1.006	0.828
No.11	PW91			BLYP		
Si	-2.558	0.487	-0.307	-2.488	0.527	-0.332
Si	1.369	1.507	-1.829	1.412	1.541	-1.857
Si	-0.795	3.871	1.479	-0.865	3.999	1.573
Si	-0.856	1.931	-1.205	-0.859	2.036	-1.364
Si	-2.498	3.016	2.733	-2.589	3.085	2.771
Si	-1.309	1.266	1.606	-1.380	1.282	1.714
Si	-0.900	4.385	-0.906	-0.929	4.494	-0.841
Si	1.144	2.104	0.514	1.231	2.208	0.491
Si	0.873	0.684	2.419	0.878	0.733	2.382
Si	1.204	4.529	0.487	1.192	4.644	0.599
Gd	-3.234	3.203	-0.070	-3.277	3.208	-0.112
Si	-1.147	-1.356	-0.494	-1.112	-1.377	-0.545
Si	2.866	-2.019	-0.112	2.915	-2.092	-0.134
Si	-1.053	-3.293	0.924	-1.069	-3.329	0.934
Si	1.084	-0.835	-1.376	1.157	-0.854	-1.404
Si	0.062	-4.435	-0.887	0.071	-4.573	-0.850
Si	-0.618	-2.688	-2.421	-0.720	-2.888	-2.403
Si	2.506	-4.578	-0.597	2.541	-4.656	-0.654
Si	1.290	-3.582	1.326	1.321	-3.671	1.391
Si	1.760	-2.945	-2.312	1.717	-3.014	-2.394
Si	0.810	-1.249	1.024	0.852	-1.300	1.034
No.12	PW91			BLYP		
Si	-1.901	0.629	0.300	-1.870	0.666	0.308
Si	1.133	1.238	-2.518	1.265	1.252	-2.445
Si	-0.868	4.044	1.744	-0.957	4.163	1.767
Si	-0.705	2.002	-1.181	-0.721	2.051	-1.257
Si	-2.461	1.950	2.247	-2.687	2.031	2.147
Si	-0.162	1.522	1.837	-0.369	1.639	2.183
Si	-1.522	4.261	-0.881	-1.533	4.333	-0.985
Si	1.672	1.872	-0.292	1.619	1.973	-0.166
Si	2.041	0.599	1.757	1.846	0.716	1.970
Si	0.640	4.006	-0.049	0.603	4.114	-0.025
Si	-3.060	4.173	1.106	-3.138	4.338	0.984
Gd	-1.868	-1.973	-0.964	-1.877	-1.989	-0.835
Si	2.790	-1.383	0.068	3.276	-1.831	-0.297
Si	-1.698	-4.447	0.493	-1.650	-4.446	0.673
Si	0.800	-0.924	-1.559	0.946	-0.959	-1.485
Si	0.353	-4.212	-0.651	0.285	-4.355	-0.705
Si	0.186	-2.937	-2.755	0.061	-2.897	-2.809
Si	2.189	-3.669	0.833	2.262	-3.935	0.666
Si	-0.065	-3.052	1.470	0.122	-3.096	1.486
Si	2.363	-2.880	-1.779	2.287	-2.987	-2.032
Si	0.140	-0.822	0.770	0.226	-0.785	0.856
No.13	PW91			BLYP		
Si	-2.041	0.786	-0.001	-2.163	0.920	-0.110
Si	1.327	0.936	-2.121	1.238	0.932	-2.233
Si	-0.494	4.255	2.488	-0.486	4.232	2.552
Si	-0.732	2.067	-1.489	-0.818	2.189	-1.603
Si	-3.178	1.958	1.631	-3.264	2.056	1.599
Si	-0.823	1.898	2.159	-0.897	1.855	2.217
Si	-1.080	4.434	-1.385	-1.028	4.592	-1.329
Si	1.062	1.685	0.190	0.902	1.641	0.145
Si	1.054	0.370	2.275	1.036	0.304	2.252
Si	0.489	3.929	0.351	0.537	3.948	0.399
Si	-2.087	3.945	0.750	-2.129	4.108	0.800
Si	-1.817	-1.515	-0.490	-1.573	-1.352	-0.389
Gd	2.768	-0.595	0.064	2.808	-0.489	-0.030
Si	-1.065	-3.398	1.136	-1.570	-3.323	0.972
Si	0.306	-1.162	-1.645	0.226	-1.226	-1.883
Si	0.036	-4.214	-0.865	0.014	-4.225	-0.730
Si	0.232	-3.114	-2.997	0.299	-3.331	-2.988
Si	2.172	-4.993	-0.345	2.157	-5.097	-0.329
Si	1.592	-3.135	1.029	2.220	-3.121	0.997
Si	2.184	-2.865	-1.628	2.247	-2.865	-1.606
Si	0.096	-1.268	0.894	0.244	-1.745	1.298
No.14	PW91			BLYP		
Si	-1.575	0.662	-0.704	-1.663	0.668	-0.783
Si	1.897	1.865	-2.090	1.898	1.877	-2.136
Si	-1.285	3.496	2.725	-1.283	3.572	2.777
Si	-0.419	2.423	-1.665	-0.451	2.456	-1.690
Si	-3.181	0.950	0.926	-3.201	0.982	0.940

Part III: xyz Coordinates for Stationary Points

Si	-0.881	1.304	1.861	-0.885	1.322	2.011
Si	-1.412	4.501	-1.069	-1.435	4.572	-1.058
Si	1.238	1.805	0.251	1.309	1.914	0.259
Si	1.378	0.539	2.283	1.428	0.572	2.257
Si	0.004	3.761	0.729	0.021	3.857	0.754
Si	-2.510	3.274	0.696	-2.548	3.348	0.755
Si	-0.026	-1.120	-0.764	-0.132	-1.147	-0.835
Si	2.728	-2.087	-0.673	2.835	-2.148	-0.644
Gd	-1.624	-1.764	1.320	-1.691	-1.816	1.294
Si	1.752	-0.568	-2.236	1.774	-0.611	-2.176
Si	0.476	-3.902	0.122	0.502	-4.038	0.159
Si	-1.320	-3.120	-1.331	-1.283	-3.257	-1.381
Si	2.226	-4.248	-1.480	2.255	-4.309	-1.477
Si	0.439	-3.444	2.411	0.410	-3.431	2.432
Si	0.726	-2.701	-2.587	0.769	-2.758	-2.702
Si	1.369	-1.629	1.275	1.369	-1.627	1.245
No.15	PW91			BLYP		
Si	-1.739	0.339	0.582	-1.736	0.354	0.530
Si	1.900	1.426	-1.638	1.877	1.439	-1.657
Si	-1.661	3.873	2.337	-1.628	3.868	2.384
Si	-0.314	2.327	-1.437	-0.338	2.356	-1.411
Si	-2.706	1.448	-1.229	-2.753	1.529	-1.209
Si	-0.625	1.749	2.050	-0.628	1.737	2.032
Si	-0.776	4.632	-1.414	-0.762	4.671	-1.368
Si	1.461	2.122	0.587	1.467	2.120	0.587
Si	1.622	1.058	2.717	1.613	1.045	2.720
Si	0.127	4.060	0.723	0.147	4.064	0.755
Si	-2.293	3.476	0.033	-2.287	3.525	0.081
Si	-0.529	-1.601	0.511	-0.539	-1.597	0.450
Si	1.798	-0.791	-0.797	1.762	-0.788	-0.819
Si	-0.642	-3.879	1.125	-0.644	-3.874	1.137
Gd	-0.637	-0.486	-2.278	-0.702	-0.514	-2.505
Si	-0.587	-5.439	-0.722	-0.544	-5.491	-0.663
Si	-0.697	-3.143	-1.471	-0.655	-3.225	-1.475
Si	1.482	-4.202	-0.565	1.513	-4.230	-0.507
Si	1.653	-3.392	1.675	1.645	-3.369	1.710
Si	1.598	-2.563	-2.325	1.653	-2.618	-2.294
Si	1.563	-1.016	1.535	1.537	-1.005	1.520
No.16	PW91			BLYP		
Si	-2.019	0.534	-0.197	-2.003	0.524	-0.216
Si	1.587	1.480	-2.156	1.593	1.498	-2.154
Si	-1.302	3.670	1.802	-1.311	3.643	1.819
Si	-0.548	2.058	-1.212	-0.548	2.071	-1.220
Si	-2.911	1.632	1.807	-2.915	1.598	1.789
Si	-0.566	1.265	1.622	-0.567	1.241	1.622
Si	-1.510	4.233	-0.944	-1.517	4.240	-0.923
Si	1.639	1.947	0.161	1.630	1.948	0.162
Si	1.676	0.846	2.278	1.680	0.827	2.268
Si	0.458	4.006	0.300	0.448	4.003	0.322
Si	-3.369	3.906	0.786	-3.374	3.887	0.802
Si	-0.770	-1.500	-0.163	-0.744	-1.502	-0.202
Si	3.319	-1.994	-0.509	3.342	-1.965	-0.551
Si	-1.861	-3.239	1.135	-1.927	-3.123	1.230
Si	1.271	-0.786	-1.572	1.309	-0.779	-1.595
Gd	-0.495	-4.531	-0.985	-0.580	-4.624	-0.975
Si	-0.394	-2.150	-2.530	-0.356	-2.143	-2.563
Si	2.083	-4.052	0.086	2.097	-4.004	0.119
Si	0.400	-3.018	1.512	0.371	-2.987	1.513
Si	1.769	-3.237	-2.112	1.803	-3.268	-2.116
Si	1.539	-1.070	0.890	1.565	-1.085	0.868
No.17	PW91			BLYP		
Si	-1.951	0.705	0.134	-1.956	0.721	0.136
Si	1.110	1.433	-2.422	1.133	1.438	-2.432
Si	-0.649	4.241	2.405	-0.642	4.358	2.421
Si	-1.028	2.109	-1.485	-1.056	2.131	-1.524
Si	-2.919	1.567	2.043	-2.960	1.603	2.043
Si	-0.467	1.843	1.962	-0.488	1.905	2.123
Si	-1.828	4.342	-1.345	-1.871	4.401	-1.351
Si	1.226	2.099	-0.146	1.238	2.185	-0.147
Si	1.816	1.122	1.961	1.815	1.145	1.963
Si	0.045	4.113	0.141	0.042	4.220	0.126
Si	-2.354	3.651	0.898	-2.398	3.759	0.948
Si	-0.809	-1.339	-0.035	-0.831	-1.364	-0.059
Si	2.727	-3.004	0.932	2.822	-3.031	0.878
Si	-1.426	-3.601	0.232	-1.433	-3.667	0.187
Si	0.949	-0.800	-1.581	0.977	-0.844	-1.598
Si	1.426	-4.762	-2.349	1.421	-4.857	-2.362
Gd	-0.748	-2.960	-2.466	-0.750	-3.017	-2.518
Si	0.893	-4.219	-0.156	0.966	-4.339	-0.117
Si	0.186	-2.836	1.933	0.120	-2.920	1.958
Si	2.356	-2.756	-1.487	2.409	-2.838	-1.542
Si	1.442	-0.949	0.832	1.441	-0.990	0.868
No.18	PW91			BLYP		
Si	-2.046	0.840	-0.248	-2.030	0.843	-0.244
Si	1.543	1.382	-2.061	1.558	1.410	-2.085
Si	-0.961	4.163	2.451	-0.953	4.275	2.471
Si	-0.674	2.205	-1.537	-0.708	2.239	-1.591
Si	-3.348	1.739	1.438	-3.364	1.743	1.444
Si	-0.945	1.788	1.938	-0.985	1.846	2.111
Si	-1.262	4.507	-1.457	-1.333	4.569	-1.467
Si	1.224	1.912	0.237	1.233	2.005	0.228
Si	1.230	0.866	2.395	1.258	0.911	2.389
Si	0.200	4.026	0.386	0.194	4.138	0.365
Si	-2.343	3.802	0.581	-2.402	3.889	0.635
Si	-1.059	-1.283	-0.224	-1.024	-1.303	-0.241
Si	2.762	-2.108	-0.094	2.811	-2.166	-0.078
Si	-1.200	-3.383	0.922	-1.252	-3.463	0.856
Si	1.080	-0.848	-1.378	1.147	-0.882	-1.415
Si	0.033	-4.400	-0.853	0.025	-4.511	-0.901
Si	-0.759	-2.562	-2.281	-0.770	-2.634	-2.319
Gd	2.762	-4.931	-0.503	2.780	-5.023	-0.476
Si	1.170	-3.546	1.378	1.140	-3.619	1.426
Si	1.652	-3.005	-2.259	1.694	-3.065	-2.315
Si	0.938	-1.165	1.171	0.978	-1.204	1.208
No.19	PW91			BLYP		
Si	-2.060	0.820	-0.374	-2.053	0.823	-0.382
Si	1.631	1.432	-2.035	1.638	1.444	-2.032
Si	-1.079	4.023	2.463	-1.089	4.025	2.463
Si	-0.617	2.211	-1.563	-0.614	2.221	-1.567
Si	-3.408	1.693	1.284	-3.414	1.690	1.269
Si	-0.980	1.667	1.829	-0.987	1.669	1.828
Si	-1.174	4.521	-1.446	-1.180	4.530	-1.444
Si	1.255	1.909	0.256	1.254	1.922	0.255
Si	1.174	0.735	2.332	1.171	0.742	2.326
Si	0.193	3.996	0.460	0.186	4.003	0.463
Si	-2.350	3.752	0.505	-2.356	3.751	0.502
Si	-1.060	-1.302	-0.416	-1.044	-1.291	-0.427
Si	2.898	-2.116	-0.129	2.902	-2.131	-0.140
Si	-0.926	-2.835	1.371	-0.947	-2.805	1.381
Si	1.219	-0.768	-1.277	1.239	-0.767	-1.279
Si	-0.128	-4.142	-0.610	-0.136	-4.138	-0.597
Si	-0.892	-2.733	-2.343	-0.909	-2.748	-2.330
Si	2.322	-4.521	-0.814	2.323	-4.509	-0.859
Gd	1.485	-4.100	1.742	1.520	-4.205	1.846
Si	1.531	-2.917	-2.373	1.517	-2.898	-2.418
Si	0.962	-1.324	1.138	0.974	-1.327	1.142
No.20	PW91			BLYP		
Si	-2.075	0.778	-0.258	-2.065	0.779	-0.236
Si	1.569	1.365	-1.974	1.566	1.391	-2.004
Si	-1.069	4.062	2.482	-1.033	4.187	2.501
Si	-0.663	2.160	-1.509	-0.708	2.188	-1.561
Si	-3.404	1.687	1.397	-3.421	1.702	1.414
Si	-0.969	1.694	1.899	-1.008	1.749	2.072
Si	-1.247	4.464	-1.431	-1.328	4.520	-1.444

Si	1.242	1.912	0.298	1.246	2.008	0.281
Si	1.215	0.802	2.417	1.259	0.853	2.403
Si	0.165	3.994	0.460	0.164	4.115	0.427
Si	-2.380	3.733	0.557	-2.436	3.831	0.623
Si	-1.058	-1.335	-0.244	-1.050	-1.365	-0.240
Si	2.913	-2.090	-0.200	2.974	-2.138	-0.176
Si	-1.162	-3.280	1.171	-1.255	-3.416	1.084
Si	1.161	-0.935	-1.473	1.222	-0.961	-1.507
Si	-0.079	-4.123	-0.738	-0.077	-4.250	-0.796
Si	-0.635	-2.304	-2.363	-0.608	-2.339	-2.391
Si	2.316	-4.588	-0.289	2.339	-4.682	-0.250
Si	1.239	-3.463	1.511	1.182	-3.538	1.522
Gd	1.842	-3.450	-2.724	1.915	-3.528	-2.751
Si	1.074	-1.086	1.009	1.118	-1.107	1.025
No.21	PW91			BLYP		
Si	-1.170	0.702	0.797	-1.150	0.699	0.858
Si	1.643	1.248	-1.913	1.654	1.232	-1.878
Si	-1.212	5.022	1.805	-1.251	5.076	1.719
Si	-0.643	1.786	-1.296	-0.639	1.746	-1.274
Si	-3.051	1.670	1.910	-3.028	1.703	1.954
Si	-1.100	2.811	2.587	-1.087	2.893	2.569
Si	-1.777	3.825	-1.777	-1.818	3.743	-1.814
Si	1.246	2.114	0.284	1.247	2.159	0.289
Si	0.693	1.275	2.431	0.722	1.366	2.458
Si	-0.043	4.086	-0.082	-0.074	4.095	-0.145
Si	-2.533	3.549	0.493	-2.554	3.536	0.468

Si	-0.973	-1.551	-0.277	-0.960	-1.540	-0.219
Si	3.069	-2.178	0.038	3.072	-2.253	0.050
Si	-0.835	-3.661	0.932	-0.855	-3.720	0.860
Si	1.269	-0.854	-0.847	1.297	-0.858	-0.770
Si	-0.346	-4.080	-1.344	-0.337	-4.065	-1.424
Si	-0.330	-1.991	-2.588	-0.318	-1.907	-2.550
Si	1.690	-5.305	-1.546	1.687	-5.300	-1.667
Si	1.535	-4.007	0.445	1.510	-4.086	0.382
Si	2.024	-2.919	-2.013	2.003	-2.890	-2.030
Gd	0.843	-1.539	1.963	0.877	-1.628	2.165

2. For structures in Table 2

Eu@Si ₂₀						
	PW91			BLYP		
Si	13.145	10.158	15.835	13.046	10.188	16.002
Si	11.622	11.945	15.817	11.634	12.034	15.705
Si	9.445	11.276	15.369	9.442	11.275	15.392
Si	9.579	8.971	15.579	9.493	8.926	15.446
Si	11.782	8.188	15.693	11.709	8.267	15.813
Si	13.759	10.272	18.097	14.135	10.263	18.130
Si	11.684	13.301	17.692	11.678	13.295	17.697
Si	8.129	12.017	17.147	8.058	12.036	17.146
Si	8.193	8.208	17.267	8.202	8.260	17.291
Si	11.733	7.300	17.859	11.793	7.175	17.890
Si	13.106	12.198	19.197	13.097	12.147	19.173
Si	9.566	13.106	18.605	9.506	13.232	18.575
Si	7.540	10.135	18.367	7.164	10.144	18.334
Si	9.615	7.106	18.772	9.621	7.112	18.767
Si	13.170	8.390	19.316	13.241	8.371	19.318
Si	11.721	11.436	20.886	11.806	11.481	21.018
Si	9.518	12.219	20.771	9.590	12.140	20.652
Si	8.154	10.249	20.629	8.253	10.219	20.461
Si	9.677	8.462	20.648	9.666	8.373	20.759
Si	11.853	9.131	21.094	11.857	9.132	21.072
Eu	10.650	10.203	18.232	10.650	10.203	18.232

[Eu@Si ₂₀] ₂						
	PW91			BLYP		
Si	1.956	0.000	0.039	1.956	0.000	0.039
Si	0.600	1.843	0.057	0.600	1.843	0.057
Si	-1.577	1.144	0.042	-1.577	1.144	0.042
Si	-1.577	-1.144	0.042	-1.577	-1.144	0.042
Si	0.600	-1.843	0.057	0.600	-1.843	0.057
Si	3.086	0.000	2.075	3.086	0.000	2.075
Si	0.952	2.944	2.079	0.952	2.944	2.079
Si	-2.494	1.815	2.075	-2.494	1.815	2.075
Si	-2.494	-1.815	2.075	-2.494	-1.815	2.075
Si	0.952	-2.944	2.079	0.952	-2.944	2.079
Si	2.802	2.038	3.213	2.802	2.038	3.213
Si	-1.075	3.303	3.217	-1.075	3.303	3.217
Si	-3.462	0.000	3.211	-3.462	0.000	3.211
Si	-1.075	-3.303	3.217	-1.075	-3.303	3.217
Si	2.802	-2.038	3.213	2.802	-2.038	3.213
Si	1.644	1.193	5.100	1.644	1.193	5.100
Si	-0.627	1.931	5.099	-0.627	1.931	5.099
Si	-2.029	0.000	5.099	-2.029	0.000	5.099
Si	-0.627	-1.931	5.099	-0.627	-1.931	5.099
Si	1.644	-1.193	5.100	1.644	-1.193	5.100
Si	1.644	1.193	7.545	1.644	1.193	7.545
Si	-0.627	1.931	7.545	-0.627	1.931	7.545
Si	-2.029	-0.000	7.545	-2.029	-0.000	7.545
Si	-0.627	-1.931	7.545	-0.627	-1.931	7.545
Si	1.644	-1.193	7.545	1.644	-1.193	7.545
Si	2.802	2.038	9.432	2.802	2.038	9.432
Si	-1.075	3.303	9.427	-1.075	3.303	9.427
Si	-3.462	-0.000	9.433	-3.462	-0.000	9.433
Si	-1.075	-3.303	9.427	-1.075	-3.303	9.427
Si	2.802	-2.038	9.432	2.802	-2.038	9.432
Si	3.086	0.000	10.569	3.086	0.000	10.569
Si	0.952	2.944	10.566	0.952	2.944	10.566
Si	-2.494	1.815	10.570	-2.494	1.815	10.570
Si	-2.494	-1.815	10.570	-2.494	-1.815	10.570
Si	0.952	-2.944	10.566	0.952	-2.944	10.566
Si	1.956	0.000	12.605	1.956	0.000	12.605
Si	0.600	1.843	12.587	0.600	1.843	12.587
Si	-1.577	1.144	12.602	-1.577	1.144	12.602
Si	-1.577	-1.144	12.602	-1.577	-1.144	12.602

Si	0.600	-1.843	12.587	0.600	-1.843	12.587
Eu	0.000	0.000	2.638	0.000	0.000	2.638
Eu	0.000	-0.000	10.007	0.000	-0.000	10.007

Unit cell of [Eu@Si ₂₀] _{n→∞}						
	PW91			BLYP		
	21.829	20.626	15.215	21.194	20.617	15.215
	90.19	88.91	88.32	90.22	88.93	90.03
Si	12.469	-10.402	0.243	12.497	-10.379	0.242
Si	11.112	-8.438	0.276	11.078	-8.419	0.277
Si	8.834	-9.180	0.316	8.778	-9.170	0.323
Si	8.760	-11.571	0.312	8.780	-11.589	0.315
Si	11.030	-12.314	0.262	11.079	-12.339	0.264
Si	13.755	-10.408	2.233	13.805	-10.387	2.240
Si	11.571	-7.278	2.290	11.508	-7.224	2.298
Si	7.896	-8.465	2.374	7.793	-8.435	2.368
Si	7.773	-12.305	2.339	7.794	-12.342	2.352
Si	11.419	-13.486	2.285	11.509	-13.551	2.274
Si	13.219	-8.475	3.418	13.192	-8.438	3.404
Si	9.573	-7.294	3.471	9.476	-7.229	3.482
Si	7.236	-10.372	3.524	7.181	-10.393	3.516
Si	9.420	-13.502	3.467	9.477	-13.556	3.459
Si	13.096	-12.315	3.383	13.193	-12.346	3.389
Si	12.232	-9.209	5.445	12.206	-9.192	5.442
Si	9.961	-8.466	5.495	9.907	-8.441	5.493
Si	8.522	-10.379	5.514	8.488	-10.402	5.515
Si	9.880	-12.342	5.480	9.908	-12.361	5.480
Si	12.158	-11.600	5.440	12.207	-11.610	5.433
Si	12.276	-9.221	7.861	12.254	-9.200	7.860
Si	10.005	-8.477	7.905	9.955	-8.450	7.910
Si	8.567	-10.391	7.926	8.537	-10.409	7.932
Si	9.923	-12.354	7.896	9.957	-12.367	7.897
Si	12.201	-11.611	7.851	12.257	-11.620	7.851
Si	13.346	-8.502	9.850	13.312	-8.464	9.870
Si	9.694	-7.322	9.952	9.596	-7.255	9.944
Si	7.360	-10.397	9.965	7.301	-10.418	9.974
Si	9.541	-13.523	9.921	9.598	-13.580	9.920
Si	13.222	-12.339	9.862	13.315	-12.372	9.855
Si	13.922	-10.442	11.004	13.968	-10.421	10.995
Si	11.741	-7.316	11.048	11.671	-7.259	11.049
Si	8.060	-8.500	11.107	7.954	-8.467	11.114
Si	7.936	-12.337	11.119	7.957	-12.375	11.099
Si	11.588	-13.517	11.017	11.674	-13.585	11.025
Si	12.715	-10.448	13.043	12.733	-10.429	13.037
Si	11.360	-8.485	13.072	11.313	-8.471	13.072
Si	9.081	-9.228	13.118	9.012	-9.219	13.118
Si	9.007	-11.618	13.108	9.015	-11.639	13.109
Si	11.277	-12.362	13.064	11.314	-12.389	13.059
Eu	10.496	-10.390	2.878	10.493	-10.390	2.878
Eu	10.641	-10.420	10.485	10.635	-10.419	10.485

3. For structures in Table 3

No. (1,2)			
Eu	0.910	2.390	1.113
Eu	-0.572	0.652	-1.353
Si	1.944	-1.108	0.895
Si	-0.829	-0.024	1.607
Si	-0.417	-2.210	-1.131
Si	-2.203	2.041	0.448
Si	0.060	1.139	3.679
Si	1.696	-1.002	-1.755
Si	-2.427	-1.670	0.119
Si	-0.014	4.279	-1.167
Si	3.424	0.706	1.152
Si	0.385	-4.025	0.259
Si	-3.503	0.149	-0.888
Si	0.821	-2.802	2.188
Si	0.254	1.891	-4.182
Si	2.825	1.116	-1.325
Si	-2.115	3.406	-1.699
Si	2.991	-2.372	3.042
Si	-1.468	-1.455	-3.361
Si	3.427	-2.375	-0.635
Si	0.085	-0.427	5.505
Si	-1.998	2.081	-3.544
Si	-1.761	4.254	1.504
Si	-3.229	1.036	2.505
Si	-1.948	-4.087	-0.549
Si	1.283	-3.469	-2.592
Si	4.473	-1.482	1.343
Si	0.513	-0.400	-3.991
Si	2.551	1.600	3.444
Si	0.278	5.321	0.889
Si	1.388	2.757	-2.303
Si	-3.212	0.087	-3.220
Si	-0.663	-1.564	3.532
Si	-2.775	-1.288	2.468
Si	2.091	-0.534	4.184
Si	4.110	-0.801	-2.430
Si	-1.143	-3.774	-2.896
Si	-4.597	1.683	0.636
Si	-3.767	3.999	0.030
Si	2.483	-4.645	-0.912
Si	-1.749	2.773	3.381
Si	2.393	-1.843	-3.993
No. (1,3)			
Eu	0.508	1.880	-0.370
Si	-1.596	0.018	-0.996
Eu	1.411	-0.909	0.228
Si	-1.087	-1.195	1.951
Si	-0.574	-2.075	-1.401
Si	-1.785	1.185	1.218
Si	0.546	0.623	2.429
Si	1.045	-0.525	-2.593
Si	-2.790	-2.041	0.449
Si	0.883	4.714	-1.076
Si	3.701	1.150	0.837
Si	0.209	-3.587	0.641
Si	-3.935	-0.291	-0.783
Si	0.555	-2.940	2.883
Si	0.649	1.667	-3.511
Si	3.427	1.465	-1.448
Si	-1.422	4.090	-1.712
Si	2.226	-1.183	3.018
Si	-1.317	-1.377	-3.694
Si	3.837	-2.247	-0.380
Si	-0.486	0.323	4.536
Si	-1.487	1.945	-2.644

Si	-1.029	3.446	2.047
Si	-3.549	0.711	2.682
Si	-1.882	-4.118	-0.550
Si	1.289	-3.243	-2.639
Si	4.199	-1.047	1.643
Si	0.542	-0.371	-4.993
Si	2.156	2.347	2.194
Si	1.103	4.393	1.470
Si	2.211	3.206	-2.539
Si	-3.097	0.186	-3.081
Si	-1.357	-2.016	4.200
Si	-3.436	-1.781	2.833
Si	1.949	0.686	4.524
Si	3.484	-0.766	-2.194
Si	-1.093	-3.771	-3.105
Si	-4.266	1.744	0.619
Si	-2.485	3.375	0.252
Si	2.237	-3.930	-0.607
Si	-1.979	2.085	3.836
Si	2.483	-1.822	-4.176
No. (1,4)			
Eu	0.677	1.405	-0.498
Si	-1.663	0.136	-1.416
Si	1.892	-0.906	0.677
Eu	-0.977	-0.919	1.242
Si	-0.118	-1.666	-1.425
Si	-2.009	1.840	0.701
Si	-0.176	1.638	2.308
Si	1.710	-0.520	-2.452
Si	-3.557	-2.392	0.504
Si	0.804	4.396	-0.852
Si	3.590	0.949	0.711
Si	0.588	-3.524	0.655
Si	-3.861	-0.287	-0.691
Si	0.631	-2.950	2.952
Si	0.631	1.568	-3.519
Si	3.458	1.216	-1.638
Si	-1.443	3.546	-1.030
Si	2.225	-1.204	3.019
Si	-1.398	-1.326	-3.547
Si	3.472	-2.234	-0.477
Si	-0.342	0.247	4.233
Si	-1.585	2.031	-2.861
Si	-1.418	3.781	2.504
Si	-3.374	0.646	2.578
Si	-1.546	-3.371	-0.403
Si	1.281	-3.337	-2.590
Si	4.220	-1.257	1.596
Si	0.565	-0.455	-4.789
Si	2.222	2.063	2.303
Si	0.939	3.877	1.503
Si	2.218	3.119	-2.550
Si	-3.338	0.170	-3.192
Si	-1.238	-1.979	4.009
Si	-3.351	-1.692	2.816
Si	2.083	0.749	4.425
Si	4.179	-0.993	-2.473
Si	-1.139	-3.653	-2.856
Si	-4.515	1.706	0.750
Si	-3.192	3.972	0.651
Si	2.371	-4.374	-0.739
Si	-2.032	1.950	4.086
Si	2.512	-1.962	-4.230
No. (1,5)			
Eu	0.277	1.484	-0.177
Si	-2.208	1.519	-2.229

Si	2.037	-0.699	0.840
Si	-1.388	-0.753	1.582
Eu	-0.593	-1.532	-0.964
Si	-3.177	1.993	-0.191
Si	-0.144	0.917	2.714
Si	1.976	-1.005	-1.810
Si	-2.950	-2.616	0.676
Si	1.265	4.238	-0.694
Si	3.826	1.122	0.780
Si	0.403	-4.216	0.761
Si	-3.948	-0.986	-0.602
Si	0.573	-2.364	2.168
Si	0.144	1.955	-3.323
Si	3.317	1.086	-1.500
Si	-0.887	4.249	-1.451
Si	2.547	-1.524	3.174
Si	-1.589	-1.820	-3.955
Si	3.919	-2.250	-0.533
Si	-0.427	0.537	5.088
Si	-1.708	3.456	-3.600
Si	-0.892	3.287	2.129
Si	-3.257	0.627	2.254
Si	-1.637	-4.212	-0.439
Si	1.231	-3.493	-2.934
Si	4.353	-1.124	1.552
Si	0.380	-0.415	-3.672
Si	2.216	1.992	2.212
Si	1.322	4.048	1.666
Si	2.118	2.843	-2.348
Si	-3.074	-0.587	-2.683
Si	-0.947	-1.645	3.863
Si	-3.190	-1.734	3.002
Si	1.919	0.664	4.169
Si	4.241	-0.929	-2.599
Si	-1.076	-3.810	-2.766
Si	-4.992	0.798	0.601
Si	-2.239	4.000	0.414
Si	1.951	-3.495	-0.786
Si	-2.080	2.102	3.895
Si	2.382	-1.708	-4.286
No. (1,6)			
Eu	0.895	1.163	-0.570
Si	-1.509	-0.471	-1.415
Si	2.406	-0.940	0.556
Si	-0.799	-1.621	1.713
Si	0.489	-1.879	-0.542
Eu	-1.662	1.082	1.063
Si	0.811	0.193	2.188
Si	0.841	-0.629	-2.710
Si	-3.107	-1.768	0.374
Si	0.742	4.318	-0.914
Si	3.689	1.159	0.751
Si	0.071	-3.864	0.858
Si	-3.941	0.043	-0.835
Si	0.530	-3.140	3.285
Si	0.532	1.659	-3.619
Si	3.830	1.693	-1.592
Si	-1.472	3.515	-1.072
Si	2.432	-1.389	3.039
Si	-1.359	-1.362	-3.699
Si	4.104	-2.254	-0.576
Si	-0.531	0.557	4.144
Si	-1.570	1.864	-2.648
Si	-1.588	3.845	2.333
Si	-4.127	1.036	2.929
Si	-1.550	-3.073	-0.943

Si	1.099	-3.159	-2.610
Si	4.584	-0.996	1.632
Si	0.509	-0.322	-5.119
Si	2.161	2.199	2.270
Si	0.528	3.587	1.325
Si	2.042	3.006	-2.418
Si	-3.224	0.212	-3.217
Si	-1.381	-1.734	4.124
Si	-3.200	-1.122	2.669
Si	1.951	0.734	4.285
Si	3.249	-0.540	-2.112
Si	-1.198	-3.782	-3.265
Si	-4.611	1.853	0.651
Si	-3.124	3.787	0.526
Si	2.169	-3.884	-0.581
Si	-2.196	2.180	3.848
Si	2.482	-1.751	-4.109
No. (1,7)			
Eu	-0.127	0.769	-1.516
Si	-2.953	-0.433	-1.898
Si	1.683	-0.969	0.639
Si	-1.421	-1.255	1.523
Si	-1.547	-2.319	-1.866
Si	-2.508	0.471	0.287
Eu	0.068	1.284	1.620
Si	1.990	-0.928	-1.928
Si	-3.563	-2.330	1.232
Si	0.740	3.651	-0.436
Si	3.134	1.036	0.894
Si	0.606	-3.182	1.108
Si	-4.692	-0.565	-0.164
Si	0.925	-3.301	3.546
Si	0.894	2.331	-4.069
Si	3.287	1.124	-1.437
Si	-1.377	3.706	-1.368
Si	2.225	-1.345	3.066
Si	-0.904	-0.882	-4.211
Si	3.620	-2.218	-0.439
Si	-0.138	0.630	4.608
Si	-1.324	2.601	-3.392
Si	-1.259	3.916	2.416
Si	-3.178	0.708	2.908
Si	-1.615	-3.418	0.236
Si	1.097	-3.032	-2.713
Si	4.047	-1.075	1.579
Si	1.173	0.011	-4.203
Si	2.827	2.657	2.599
Si	1.067	4.246	1.838
Si	2.107	2.961	-2.185
Si	-2.629	0.701	-3.917
Si	-0.696	-1.504	3.732
Si	-3.151	-1.596	3.489
Si	2.019	0.840	3.892
Si	4.397	-0.900	-2.342
Si	-1.020	-3.293	-3.916
Si	-4.469	1.607	1.116
Si	-2.432	2.930	0.572
Si	2.000	-4.014	-0.726
Si	-1.746	2.169	3.927
Si	2.839	-1.789	-4.106
No. (1,8)			
Eu	0.494	1.684	0.048
Si	-2.991	-0.857	-2.082
Si	2.023	-0.622	0.979
Si	-0.550	-0.976	1.145
Si	-1.933	-2.904	-1.716
Si	-2.110	0.320	-0.148
Si	-0.672	0.975	2.650

Eu	0.614	-0.918	-1.737
Si	-2.909	-1.960	1.265
Si	0.892	4.412	-0.855
Si	3.716	1.156	0.835
Si	-0.085	-3.275	0.336
Si	-4.365	-0.625	-0.132
Si	0.599	-2.663	2.696
Si	0.951	1.734	-3.519
Si	3.311	1.284	-1.455
Si	-1.335	3.833	-1.534
Si	2.583	-1.363	3.193
Si	-0.833	-0.914	-4.451
Si	3.285	-2.017	-0.478
Si	-0.178	0.586	5.033
Si	-1.197	1.870	-2.818
Si	-0.943	3.327	2.256
Si	-3.120	0.791	3.095
Si	-2.332	-4.116	0.292
Si	1.483	-3.427	-3.035
Si	4.409	-1.099	1.533
Si	1.227	-0.031	-5.059
Si	2.460	2.540	2.238
Si	1.134	4.401	1.597
Si	2.280	3.165	-2.257
Si	-2.718	0.472	-4.041
Si	-1.028	-1.344	3.775
Si	-3.391	-1.554	3.592
Si	1.645	0.821	3.564
Si	4.033	-0.771	-2.336
Si	-0.725	-3.140	-3.657
Si	-4.093	1.491	1.056
Si	-2.258	2.867	0.379
Si	1.958	-3.962	-0.775
Si	-1.889	2.412	4.434
Si	2.553	-1.599	-3.908
No. (2,3)			
Si	1.351	1.836	0.664
Eu	-0.535	0.526	-1.338
Eu	1.289	-0.984	0.658
Si	-1.207	-1.089	2.026
Si	-0.311	-2.378	-1.347
Si	-2.312	1.709	0.463
Si	-0.543	1.138	1.913
Si	2.228	-0.338	-1.971
Si	-2.674	-1.888	0.313
Si	0.654	3.691	-0.760
Si	3.629	1.121	0.552
Si	0.246	-3.932	0.734
Si	-3.577	0.029	-0.757
Si	0.480	-2.736	2.808
Si	0.321	1.929	-4.032
Si	4.128	1.543	-1.858
Si	-1.655	3.334	-1.214
Si	2.628	-1.497	3.235
Si	-1.442	-1.446	-3.427
Si	3.662	-2.024	-0.730
Si	-0.534	0.418	4.256
Si	-1.902	2.286	-3.305
Si	-1.342	3.370	2.325
Si	-3.433	0.779	2.688
Si	-1.920	-4.100	-0.487
Si	1.146	-3.668	-3.043
Si	4.167	-1.065	1.405
Si	0.565	-0.399	-4.048
Si	2.873	2.584	2.482
Si	0.986	4.141	1.653
Si	1.856	2.306	-2.263
Si	-3.114	0.205	-3.104
Si	-1.375	-1.976	4.302

Si	-3.436	-1.621	2.748
Si	1.699	0.641	3.443
Si	4.449	-0.927	-2.822
Si	-1.316	-3.874	-3.028
Si	-4.687	1.698	0.837
Si	-3.120	3.965	0.654
Si	1.959	-3.648	-0.856
Si	-2.305	2.162	4.316
Si	2.421	-1.816	-4.086
No. (2,4)			
Si	0.613	1.979	0.954
Eu	-0.220	0.820	-1.525
Si	1.716	-0.684	0.373
Eu	-0.806	-0.705	1.484
Si	-0.381	-1.949	-1.254
Si	-2.055	1.727	0.551
Si	1.034	1.165	3.224
Si	1.801	-1.015	-2.126
Si	-3.276	-2.082	0.370
Si	0.505	3.683	-0.965
Si	3.266	1.274	0.517
Si	0.486	-3.477	0.590
Si	-3.365	0.070	-0.697
Si	0.539	-3.105	2.919
Si	0.261	1.924	-4.308
Si	3.030	1.124	-1.842
Si	-1.756	3.415	-1.438
Si	1.982	-1.194	2.940
Si	-1.430	-1.329	-3.422
Si	3.430	-2.166	-0.543
Si	-0.563	-0.273	4.756
Si	-1.939	2.292	-3.465
Si	-1.292	3.629	2.117
Si	-3.307	0.696	2.539
Si	-1.732	-3.732	-0.396
Si	1.189	-3.423	-2.551
Si	3.966	-0.864	1.441
Si	0.579	-0.405	-4.223
Si	2.576	2.838	2.240
Si	0.871	4.414	1.303
Si	1.798	2.883	-2.781
Si	-3.081	0.273	-3.033
Si	-1.450	-2.268	3.937
Si	-3.406	-1.680	2.672
Si	1.864	0.013	5.082
Si	4.198	-0.970	-2.628
Si	-1.227	-3.674	-2.848
Si	-4.569	1.731	0.742
Si	-3.178	3.852	0.491
Si	2.380	-4.387	-0.639
Si	-1.486	1.631	3.673
Si	2.430	-2.047	-4.234
No. (2,5)			
Si	1.260	1.127	0.379
Eu	-0.348	0.892	-1.765
Si	1.960	-0.951	1.186
Si	-1.213	-1.013	1.943
Eu	-0.137	-1.664	-0.578
Si	-2.104	1.729	0.290
Si	-0.503	1.242	2.005
Si	1.841	-0.826	-2.320
Si	-2.896	-2.087	0.496
Si	0.539	3.492	-0.707
Si	3.636	1.095	0.863
Si	0.201	-4.317	0.691
Si	-3.355	-0.062	-0.767
Si	0.575	-2.688	2.400
Si	0.266	2.104	-4.329

Si	2.967	1.231	-1.593
Si	-1.738	3.506	-1.361
Si	2.625	-1.544	3.376
Si	-1.415	-1.332	-3.520
Si	3.215	-2.134	-0.475
Si	-0.265	0.315	4.233
Si	-2.013	2.453	-3.511
Si	-1.300	3.538	2.139
Si	-3.204	0.703	2.585
Si	-1.889	-4.023	-0.513
Si	1.121	-3.258	-2.820
Si	4.343	-1.284	1.546
Si	0.556	-0.289	-4.362
Si	2.022	2.238	2.350
Si	0.934	4.348	1.547
Si	1.858	3.103	-2.683
Si	-3.041	0.281	-3.093
Si	-1.085	-2.016	4.136
Si	-3.314	-1.666	2.931
Si	2.091	0.717	4.356
Si	4.208	-0.884	-2.432
Si	-1.218	-3.563	-2.854
Si	-4.488	1.573	0.768
Si	-3.264	3.865	0.574
Si	2.000	-4.133	-0.843
Si	-1.955	2.097	4.117
Si	2.526	-1.911	-4.387
No. (2,6)			
Si	1.699	0.996	0.743
Eu	-0.388	0.761	-1.485
Si	0.589	-1.171	0.933
Si	-0.204	-0.670	3.207
Si	-0.399	-2.041	-1.340
Eu	-1.253	1.306	1.208
Si	1.059	2.802	2.504
Si	1.771	-1.005	-2.052
Si	-2.515	-1.763	0.114
Si	0.113	3.691	-0.754
Si	4.182	0.928	0.651
Si	0.489	-3.652	0.347
Si	-3.465	0.032	-0.966
Si	0.362	-3.218	2.706
Si	0.305	2.049	-4.093
Si	2.801	1.139	-1.473
Si	-2.003	3.507	-1.573
Si	2.166	-1.676	3.170
Si	-1.394	-1.310	-3.504
Si	3.416	-2.434	-0.916
Si	-0.168	1.565	4.065
Si	-1.956	2.246	-3.494
Si	-2.148	3.975	2.172
Si	-3.715	0.640	2.822
Si	-1.767	-3.944	-0.605
Si	1.233	-3.411	-2.802
Si	3.111	-1.201	1.015
Si	0.604	-0.284	-4.209
Si	3.060	1.648	2.750
Si	0.032	4.580	1.436
Si	1.698	3.055	-2.424
Si	-3.154	0.217	-3.277
Si	-1.389	-2.499	4.190
Si	-2.582	-1.356	2.443
Si	2.118	0.281	4.575
Si	4.200	-0.850	-2.639
Si	-1.144	-3.672	-3.108
Si	-4.363	1.371	0.683
Si	-3.360	3.409	0.305
Si	2.333	-4.585	-1.000
Si	-2.446	2.367	3.939

Si	2.470	-1.818	-4.261
No. (2,7)			
Si	1.960	1.290	-1.093
Eu	-0.736	0.375	-1.066
Si	1.016	-1.437	0.634
Si	-1.193	-0.817	1.927
Si	-0.531	-2.322	-1.206
Si	-2.256	1.615	0.956
Eu	0.681	1.293	1.572
Si	1.590	-1.009	-1.933
Si	-2.660	-1.918	0.212
Si	0.657	3.540	-0.597
Si	3.611	1.503	0.710
Si	0.403	-3.854	0.537
Si	-3.679	0.007	-0.746
Si	0.368	-2.758	2.673
Si	0.358	1.897	-3.524
Si	4.241	1.827	-1.762
Si	-1.649	3.261	-0.997
Si	2.190	-1.206	3.120
Si	-1.478	-1.414	-3.383
Si	3.265	-2.233	-0.571
Si	-0.371	0.217	4.102
Si	-1.894	2.319	-3.122
Si	-1.315	3.641	2.201
Si	-3.830	0.664	2.757
Si	-1.937	-4.222	-0.489
Si	1.289	-3.413	-2.635
Si	3.429	-0.786	1.221
Si	0.478	-0.345	-4.082
Si	2.913	2.814	2.745
Si	1.012	4.215	1.651
Si	2.157	3.279	-2.562
Si	-3.084	0.231	-2.980
Si	-1.428	-2.046	4.150
Si	-3.355	-1.714	2.596
Si	1.928	0.819	4.328
Si	3.939	-0.727	-2.363
Si	-1.114	-3.823	-3.034
Si	-4.663	1.703	0.745
Si	-3.257	3.966	0.638
Si	2.414	-4.532	-0.779
Si	-1.901	1.871	3.587
Si	2.430	-1.766	-4.134
No. (2,8)			
Si	2.003	0.927	0.195
Eu	-0.610	0.423	-1.122
Si	1.399	-1.352	0.310
Si	-1.247	-0.553	1.668
Si	-0.074	-2.387	-1.459
Si	-2.343	1.687	0.668
Si	0.054	1.787	1.430
Eu	2.781	-1.027	-2.546
Si	-2.822	-1.749	0.328
Si	0.344	3.622	-0.541
Si	4.104	1.740	1.073
Si	0.263	-4.134	0.472
Si	-3.756	0.189	-0.693
Si	0.675	-2.538	2.304
Si	0.320	1.743	-3.820
Si	3.918	1.569	-1.293
Si	-1.870	3.372	-1.145
Si	2.597	-1.105	2.479
Si	-1.771	-1.433	-3.253
Si	3.478	-2.531	0.161
Si	-0.353	0.573	3.693
Si	-1.928	2.258	-3.193
Si	-1.570	3.399	2.354

Si	-3.353	0.708	2.678
Si	-1.856	-3.724	-0.578
Si	0.811	-3.633	-3.331
Si	4.860	-0.501	1.727
Si	0.192	-0.581	-4.184
Si	2.220	2.418	2.366
Si	0.692	4.273	1.725
Si	1.714	2.355	-1.961
Si	-3.263	0.315	-2.978
Si	-1.064	-1.788	3.756
Si	-3.316	-1.696	2.694
Si	2.005	0.690	4.041
Si	5.100	-0.949	-0.596
Si	-1.656	-3.856	-3.054
Si	-4.802	1.725	0.972
Si	-3.360	3.903	0.686
Si	1.980	-4.001	-1.257
Si	-2.152	2.049	4.291
Si	1.649	-2.189	-5.069
No. (3,4)			
Si	-0.108	1.779	-0.830
Si	-2.376	1.843	-1.887
Eu	1.318	-0.516	0.907
Eu	-1.840	0.087	0.773
Si	-0.519	-1.262	-1.512
Si	-3.611	2.541	-0.024
Si	0.113	2.216	1.642
Si	1.917	-1.129	-1.818
Si	-3.283	-2.828	0.704
Si	1.138	3.949	-0.334
Si	4.279	0.799	0.855
Si	1.085	-3.639	0.665
Si	-4.359	-1.156	-0.558
Si	1.062	-3.128	2.941
Si	0.292	1.954	-3.362
Si	3.472	0.666	-1.309
Si	-1.053	4.214	-1.137
Si	2.749	-1.557	3.222
Si	-1.516	-1.657	-3.738
Si	3.472	-2.530	-0.470
Si	-0.307	0.521	3.592
Si	-1.598	3.514	-3.446
Si	-2.112	3.015	1.859
Si	-3.872	0.244	2.904
Si	-1.103	-3.147	-0.119
Si	1.492	-3.524	-2.503
Si	4.264	-1.472	1.452
Si	0.545	-0.397	-3.778
Si	2.688	1.917	2.095
Si	1.620	4.041	2.041
Si	2.041	2.429	-1.908
Si	-2.826	-0.444	-2.145
Si	-0.762	-1.698	3.143
Si	-3.044	-1.907	2.818
Si	2.057	0.551	3.896
Si	4.393	-1.283	-2.492
Si	-0.855	-3.600	-2.468
Si	-4.800	0.720	0.805
Si	-2.820	4.799	0.461
Si	2.660	-4.768	-0.788
Si	-2.374	1.796	3.909
Si	2.476	-1.950	-4.062
No. (3,5)			
Si	0.931	1.644	-0.869
Si	-1.597	2.216	-0.524
Eu	1.586	-0.426	0.915
Si	-1.194	-1.262	1.753
Eu	-1.101	-0.514	-1.165

Si	-0.847	1.114	1.780
Si	1.232	2.597	1.537
Si	1.343	-1.990	-1.642
Si	-2.998	-2.152	0.320
Si	0.129	4.036	-0.888
Si	4.288	0.829	1.117
Si	0.363	-3.432	0.429
Si	-4.218	-0.645	-1.099
Si	0.593	-2.886	2.680
Si	0.269	1.697	-3.394
Si	3.342	1.378	-1.050
Si	-2.195	4.169	-1.907
Si	2.730	-1.988	3.343
Si	-1.626	-1.554	-4.175
Si	3.789	-2.432	-0.430
Si	-0.332	0.270	4.022
Si	-1.994	1.962	-2.958
Si	-1.564	3.472	1.767
Si	-3.241	0.519	2.399
Si	-1.715	-3.891	-0.647
Si	1.501	-3.904	-3.094
Si	4.319	-1.497	1.610
Si	0.454	-0.546	-3.837
Si	3.093	1.974	2.795
Si	0.395	4.822	1.423
Si	1.880	3.289	-2.520
Si	-3.168	-0.079	-3.158
Si	-1.251	-2.065	4.108
Si	-3.389	-1.873	2.750
Si	2.014	0.185	3.800
Si	3.426	-0.783	-2.002
Si	-0.776	-3.102	-2.643
Si	-3.693	1.201	0.219
Si	-3.478	3.623	0.202
Si	2.278	-4.242	-0.795
Si	-2.075	2.050	3.841
Si	2.494	-1.782	-4.015
No. (3,6)			
Si	2.075	2.026	-0.881
Si	-1.726	1.088	-1.982
Eu	1.613	-0.466	0.858
Si	-0.926	-0.971	2.401
Si	-0.360	-1.780	-1.171
Eu	-1.249	1.420	0.676
Si	1.496	2.530	1.515
Si	1.318	-0.159	-1.962
Si	-2.470	-1.726	0.358
Si	-0.287	3.991	-0.989
Si	4.399	0.306	1.371
Si	0.594	-3.652	0.410
Si	-3.575	-0.058	-0.864
Si	0.454	-2.982	2.676
Si	-0.104	1.984	-3.493
Si	4.187	0.867	-0.836
Si	-2.445	3.429	-1.543
Si	2.449	-1.925	3.308
Si	-1.414	-1.185	-3.307
Si	3.269	-2.820	-0.132
Si	0.024	1.060	3.307
Si	-2.560	2.487	-3.825
Si	-2.017	3.737	2.088
Si	-3.351	0.519	2.708
Si	-1.639	-3.812	-0.477
Si	1.288	-3.329	-2.538
Si	4.264	-2.008	1.827
Si	0.578	-0.211	-4.205
Si	3.433	1.896	2.837
Si	0.081	4.414	1.256
Si	1.420	3.606	-2.545

Si	-3.481	0.073	-3.354
Si	-1.396	-2.413	4.218
Si	-3.214	-1.888	2.651
Si	2.128	0.264	3.948
Si	3.479	-1.178	-1.756
Si	-1.053	-3.514	-2.852
Si	-4.354	1.345	0.820
Si	-3.679	3.539	0.457
Si	2.224	-4.811	-0.875
Si	-2.039	2.154	3.846
Si	2.560	-1.847	-3.950
No. (3,7)			
Si	1.635	1.368	-1.095
Si	-1.341	0.479	-0.633
Eu	0.989	-1.385	0.060
Si	-1.168	-0.886	2.117
Si	-0.891	-1.623	-2.011
Si	-2.392	1.666	1.263
Eu	0.434	1.335	1.487
Si	1.182	-0.619	-2.661
Si	-2.868	-2.002	0.599
Si	0.840	3.680	-0.446
Si	3.403	1.269	0.757
Si	0.423	-4.342	0.909
Si	-3.665	-0.155	-0.604
Si	0.437	-2.670	2.667
Si	0.679	1.645	-3.545
Si	4.094	1.649	-1.591
Si	-1.396	3.119	-0.825
Si	2.230	-1.202	3.076
Si	-1.507	-1.751	-4.361
Si	3.772	-2.343	-0.464
Si	-0.429	0.270	4.196
Si	-1.555	1.870	-2.802
Si	-1.344	3.732	2.333
Si	-4.048	0.787	2.932
Si	-1.332	-3.446	-0.494
Si	1.296	-3.285	-2.652
Si	3.714	-0.971	1.356
Si	0.692	-0.400	-5.016
Si	2.794	2.661	2.677
Si	1.064	4.382	1.899
Si	2.310	3.229	-2.502
Si	-2.737	-0.220	-2.854
Si	-1.299	-2.057	4.328
Si	-3.332	-1.611	2.905
Si	1.883	0.856	4.116
Si	3.552	-0.738	-2.169
Si	-1.055	-3.880	-3.065
Si	-4.742	1.745	0.717
Si	-3.177	3.920	0.595
Si	2.260	-4.142	-0.707
Si	-2.023	1.946	3.705
Si	2.614	-1.876	-4.197
No. (3,8)			
Si	0.758	1.665	-0.439
Si	-1.281	0.764	-1.786
Eu	1.354	-0.525	1.280
Si	-1.428	-0.554	1.849
Si	-1.019	-1.621	-0.289
Si	-1.932	1.508	0.508
Si	1.112	2.625	1.750
Eu	1.089	-0.798	-1.863
Si	-3.260	-2.248	0.367
Si	0.333	3.971	-0.840
Si	4.163	0.789	1.177
Si	0.391	-3.476	0.601
Si	-3.434	-0.169	-0.879

Si	0.776	-3.349	2.924
Si	0.336	1.555	-3.602
Si	3.220	1.046	-1.048
Si	-1.836	3.280	-1.459
Si	2.658	-1.969	3.251
Si	-1.311	-1.198	-3.693
Si	3.626	-2.113	-0.492
Si	-0.206	0.342	3.870
Si	-2.012	2.352	-3.608
Si	-1.402	3.334	1.961
Si	-3.398	0.626	2.690
Si	-1.767	-4.062	-0.469
Si	1.366	-3.565	-3.121
Si	4.350	-1.535	1.629
Si	0.639	-0.403	-4.880
Si	2.943	1.761	2.886
Si	0.416	4.859	1.432
Si	1.984	2.866	-2.322
Si	-3.215	0.192	-3.276
Si	-0.977	-1.936	3.841
Si	-3.255	-1.775	2.868
Si	2.091	0.080	4.297
Si	4.067	-0.774	-2.448
Si	-0.864	-3.139	-2.566
Si	-4.456	1.419	0.633
Si	-3.312	3.592	0.377
Si	2.098	-3.743	-0.931
Si	-1.946	2.062	3.981
Si	2.535	-1.731	-4.165
No. (4,5)			
Si	0.856	1.942	0.700
Si	-0.513	1.585	-2.150
Si	1.734	-1.798	-0.135
Eu	-0.296	-0.433	1.981
Eu	-0.752	-1.044	-1.151
Si	-2.055	1.188	0.314
Si	1.336	2.066	3.284
Si	1.847	-0.438	-2.102
Si	-2.966	-2.067	0.453
Si	0.480	3.753	-1.103
Si	3.054	1.196	0.434
Si	0.256	-3.486	0.803
Si	-3.757	-0.138	-0.814
Si	0.523	-3.394	3.185
Si	0.198	1.987	-4.572
Si	3.527	1.302	-1.906
Si	-1.845	3.581	-1.488
Si	2.037	-1.564	3.334
Si	-1.655	-1.558	-3.979
Si	4.053	-2.512	-0.330
Si	-0.893	-0.140	4.849
Si	-2.208	2.602	-3.720
Si	-0.782	2.794	2.510
Si	-3.331	0.539	2.527
Si	-1.737	-3.844	-0.484
Si	1.222	-3.304	-2.470
Si	3.325	-0.975	1.457
Si	0.420	-0.448	-4.068
Si	2.893	3.119	1.867
Si	0.907	4.323	1.173
Si	1.701	2.667	-2.796
Si	-2.649	0.316	-2.860
Si	-1.390	-2.245	4.024
Si	-3.241	-1.764	2.701
Si	1.405	0.205	4.707
Si	4.229	-1.091	-2.598
Si	-1.067	-3.508	-2.736
Si	-4.517	1.591	0.756
Si	-2.797	3.420	0.757

Si	2.242	-4.199	-0.489
Si	-2.177	1.710	4.163
Si	2.382	-1.929	-4.028
No. (4,6)			
Si	1.067	0.977	-0.272
Si	-1.121	-0.066	-1.475
Si	1.988	-1.162	0.283
Eu	-0.704	-1.073	1.225
Si	0.040	-2.142	-1.253
Eu	-1.501	1.655	0.752
Si	0.848	1.080	2.238
Si	1.049	0.147	-2.608
Si	-3.490	-2.262	0.494
Si	0.464	3.548	-0.587
Si	3.398	1.053	0.569
Si	0.484	-3.796	0.799
Si	-3.532	-0.144	-0.587
Si	0.541	-3.051	3.074
Si	0.446	2.109	-4.119
Si	4.214	1.616	-1.663
Si	-1.787	3.895	-1.276
Si	2.036	-1.181	2.763
Si	-1.419	-1.381	-3.554
Si	3.792	-2.386	-0.537
Si	-0.582	0.493	4.043
Si	-1.522	2.027	-2.677
Si	-1.636	4.196	2.540
Si	-3.778	0.882	2.553
Si	-1.627	-3.658	-0.335
Si	1.273	-3.484	-2.679
Si	4.197	-1.046	1.562
Si	0.407	-0.340	-4.917
Si	2.761	2.456	2.606
Si	0.641	3.578	1.785
Si	1.919	2.453	-2.159
Si	-3.126	0.165	-2.999
Si	-1.329	-1.851	4.116
Si	-3.176	-1.386	2.670
Si	1.961	0.712	4.372
Si	3.409	-0.643	-2.107
Si	-1.167	-3.692	-2.813
Si	-4.664	1.757	0.527
Si	-3.205	3.883	0.608
Si	2.400	-4.453	-0.701
Si	-2.226	2.165	3.678
Si	2.255	-1.649	-3.942
No. (4,7)			
Si	1.472	1.161	-0.947
Si	-1.229	0.635	-1.145
Si	1.658	-1.048	0.502
Eu	-1.075	-0.927	1.262
Si	-0.363	-1.695	-1.455
Si	-2.267	1.813	0.863
Eu	0.432	1.383	1.650
Si	1.642	-0.752	-2.339
Si	-3.604	-2.344	0.444
Si	0.727	3.487	-0.465
Si	3.375	1.147	0.746
Si	0.530	-3.478	0.690
Si	-3.558	-0.173	-0.636
Si	0.563	-3.022	3.032
Si	0.527	1.547	-3.376
Si	3.907	1.461	-1.585
Si	-1.582	3.335	-0.989
Si	2.038	-1.139	2.942
Si	-1.444	-1.297	-3.545
Si	3.454	-2.178	-0.542
Si	-0.401	0.269	4.415

Si	-1.756	2.091	-2.996
Si	-1.392	3.729	2.306
Si	-3.627	0.509	2.595
Si	-1.633	-3.477	-0.397
Si	1.227	-3.338	-2.518
Si	3.998	-1.079	1.497
Si	0.560	-0.430	-4.682
Si	2.839	2.642	2.650
Si	1.056	4.313	1.771
Si	2.146	3.077	-2.455
Si	-3.304	0.147	-3.044
Si	-1.269	-1.929	3.947
Si	-3.384	-1.801	2.821
Si	1.943	0.839	4.242
Si	4.078	-0.913	-2.498
Si	-1.145	-3.610	-2.875
Si	-4.702	1.583	0.702
Si	-3.309	4.042	0.679
Si	2.353	-4.351	-0.659
Si	-1.961	1.810	3.646
Si	2.476	-2.036	-4.256
No. (4,8)			
Si	1.195	1.199	0.808
Si	-1.468	0.085	-1.532
Si	1.752	-1.446	0.453
Eu	-0.908	-0.886	1.141
Si	-0.270	-2.028	-1.442
Si	-2.182	1.665	0.347
Si	-0.735	1.691	2.224
Eu	1.288	0.291	-1.818
Si	-3.541	-2.303	0.567
Si	0.801	3.132	-0.679
Si	3.630	0.992	0.520
Si	0.506	-3.634	0.755
Si	-3.685	-0.200	-0.638
Si	0.599	-2.961	3.045
Si	0.547	2.053	-4.349
Si	4.091	1.546	-1.770
Si	-1.509	3.331	-1.191
Si	2.184	-1.198	2.883
Si	-1.408	-1.450	-3.601
Si	3.644	-2.166	-0.692
Si	-0.308	0.469	4.196
Si	-1.486	1.863	-3.085
Si	-1.438	3.931	2.496
Si	-3.311	0.770	2.665
Si	-1.649	-3.624	-0.345
Si	1.254	-3.318	-2.651
Si	4.154	-1.185	1.476
Si	0.494	-0.323	-4.548
Si	2.686	2.153	2.459
Si	0.951	3.653	1.682
Si	2.249	3.034	-2.646
Si	-3.309	0.136	-3.197
Si	-1.193	-1.740	3.866
Si	-3.338	-1.563	2.877
Si	2.123	0.674	4.378
Si	3.908	-0.720	-2.550
Si	-1.165	-3.844	-2.954
Si	-4.550	1.718	0.785
Si	-3.176	3.940	0.538
Si	2.375	-4.242	-0.718
Si	-2.140	2.190	4.288
Si	2.336	-1.683	-4.045
No. (5,6)			
Si	1.103	1.105	-1.080
Si	-1.366	0.710	-1.804
Si	1.688	-0.276	1.386

Si	-1.502	-1.210	1.984
Eu	-0.115	-1.528	-0.487
Eu	-0.871	1.367	1.077
Si	1.801	1.949	2.577
Si	1.567	-0.734	-2.589
Si	-3.048	-2.176	0.370
Si	0.513	3.496	-0.738
Si	3.635	1.427	0.855
Si	0.133	-4.275	0.695
Si	-3.366	-0.084	-0.787
Si	0.290	-2.785	2.481
Si	0.354	1.545	-3.631
Si	3.452	1.262	-1.549
Si	-1.721	3.234	-1.297
Si	2.397	-1.726	3.288
Si	-1.309	-1.145	-3.443
Si	3.064	-1.801	-0.372
Si	-0.937	0.101	4.034
Si	-2.008	2.296	-3.508
Si	-1.440	3.772	2.487
Si	-3.461	0.480	2.635
Si	-1.818	-3.922	-0.642
Si	1.171	-3.192	-2.681
Si	4.104	-0.895	1.594
Si	0.527	-0.455	-4.929
Si	3.442	3.527	2.102
Si	0.884	3.964	1.534
Si	1.985	2.950	-2.577
Si	-3.358	0.165	-3.306
Si	-1.543	-2.293	4.150
Si	-3.705	-1.956	2.790
Si	1.384	0.263	4.129
Si	4.044	-0.972	-2.433
Si	-1.144	-3.406	-2.834
Si	-4.161	1.530	0.724
Si	-2.935	3.561	0.644
Si	2.035	-3.882	-0.622
Si	-2.345	2.005	4.130
Si	2.576	-1.991	-4.358
No. (5,7)			
Si	0.916	1.075	-1.108
Si	-1.384	0.821	-1.845
Si	2.296	-0.409	0.566
Si	-1.351	-0.871	2.051
Eu	-0.133	-1.507	-0.478
Si	-2.019	1.482	0.481
Eu	0.490	1.271	1.772
Si	1.648	-0.787	-2.530
Si	-2.897	-2.104	0.539
Si	0.604	3.467	-0.465
Si	3.840	1.228	1.128
Si	0.208	-4.177	0.777
Si	-3.501	-0.187	-0.819
Si	0.350	-2.616	2.527
Si	0.374	1.756	-3.676
Si	3.506	1.098	-1.310
Si	-1.624	3.295	-1.294
Si	2.262	-1.201	2.852
Si	-1.381	-1.186	-3.408
Si	3.488	-2.113	-0.456
Si	-0.477	0.214	4.266
Si	-2.026	2.499	-3.574
Si	-1.417	3.362	2.095
Si	-3.322	0.651	2.664
Si	-1.806	-3.915	-0.488
Si	1.164	-3.210	-2.687
Si	4.437	-1.241	1.661
Si	0.514	-0.397	-4.707
Si	2.829	2.666	3.008

Si	0.839	4.254	1.773
Si	2.064	2.832	-2.292
Si	-3.370	0.227	-3.298
Si	-1.333	-2.115	4.241
Si	-3.447	-1.735	2.917
Si	1.872	0.619	4.315
Si	4.133	-0.969	-2.555
Si	-1.167	-3.402	-2.726
Si	-4.432	1.486	0.709
Si	-3.256	3.717	0.457
Si	2.014	-3.943	-0.670
Si	-2.003	2.070	4.063
Si	2.495	-2.002	-4.483
No. (5,8)			
Si	1.550	1.293	-0.053
Si	-0.621	1.490	-1.512
Si	2.435	-0.908	0.357
Si	-1.608	-0.824	2.262
Eu	-0.474	-1.117	-0.193
Si	-2.089	1.269	0.571
Si	0.141	0.939	1.972
Eu	1.239	-0.584	-2.270
Si	-3.072	-2.178	0.712
Si	0.568	3.658	-0.669
Si	4.004	1.171	0.860
Si	0.197	-4.010	0.724
Si	-3.656	-0.349	-0.639
Si	0.128	-2.589	2.592
Si	0.313	1.730	-4.052
Si	3.664	1.232	-1.703
Si	-1.699	3.608	-1.380
Si	2.047	-1.291	2.684
Si	-1.359	-1.432	-3.961
Si	4.128	-2.295	-0.651
Si	-0.693	0.397	4.239
Si	-2.037	2.381	-3.453
Si	-1.230	2.969	2.214
Si	-3.472	0.701	2.721
Si	-1.850	-3.931	-0.474
Si	1.398	-3.547	-2.935
Si	4.411	-1.257	1.661
Si	0.542	-0.473	-5.095
Si	2.242	2.236	2.150
Si	0.851	4.263	1.703
Si	1.827	2.522	-2.399
Si	-2.406	0.089	-2.596
Si	-1.405	-2.003	4.384
Si	-3.748	-1.763	3.106
Si	1.766	0.665	3.973
Si	4.245	-0.912	-2.793
Si	-0.845	-3.128	-2.499
Si	-4.547	1.491	0.694
Si	-3.054	3.527	0.608
Si	1.972	-3.310	-0.707
Si	-2.341	2.210	4.278
Si	2.535	-1.939	-4.431
No. (6,7)			
Si	3.071	2.694	-1.203
Si	-2.822	-0.242	-2.330
Si	1.203	-1.023	1.282
Si	-1.615	-0.132	2.506

Si	-1.099	-1.970	-2.015
Eu	-0.867	0.804	-0.255
Eu	1.488	1.566	2.873
Si	0.900	-0.543	-2.279
Si	-2.927	-1.635	0.896
Si	0.028	3.837	-1.059
Si	3.727	1.043	0.836
Si	0.440	-3.298	0.578
Si	-4.374	-0.413	-0.468
Si	0.599	-3.128	2.913
Si	0.523	1.693	-3.278
Si	4.828	1.127	-1.255
Si	-2.198	3.630	-1.546
Si	2.130	-1.495	3.613
Si	-1.115	-1.200	-4.555
Si	2.983	-2.231	-0.076
Si	-0.312	-0.153	4.846
Si	-1.804	1.813	-3.084
Si	-1.129	2.796	2.095
Si	-3.781	0.635	3.496
Si	-1.756	-3.324	-0.194
Si	1.128	-3.193	-2.753
Si	3.727	-1.150	1.881
Si	0.973	-0.103	-4.740
Si	3.089	3.382	1.029
Si	0.690	3.926	1.139
Si	1.654	3.681	-2.748
Si	-3.013	0.302	-4.625
Si	-1.276	-2.071	3.915
Si	-3.542	-1.817	3.232
Si	1.940	0.024	5.382
Si	3.261	-0.569	-1.699
Si	-1.026	-3.499	-3.859
Si	-3.703	1.159	1.139
Si	-2.958	3.258	0.685
Si	2.081	-4.325	-0.802
Si	-1.725	1.731	4.236
Si	2.574	-1.585	-3.752
No. (6,8)			
Si	2.538	1.450	0.301
Si	-1.530	0.830	-2.130
Si	1.946	-0.743	0.946
Si	-1.066	-1.010	2.237
Si	-0.331	-2.111	0.142
Eu	-0.961	1.393	0.588
Si	1.499	2.568	2.138
Eu	1.008	-0.466	-1.737
Si	-2.816	-1.982	0.402
Si	0.072	3.866	-0.952
Si	3.918	0.610	2.044
Si	0.207	-4.492	0.634
Si	-3.429	-0.100	-0.926
Si	0.217	-3.090	2.613
Si	0.002	1.679	-3.935
Si	3.573	1.684	-1.857
Si	-2.038	3.266	-1.622
Si	2.314	-1.925	2.926
Si	-1.442	-1.138	-3.711
Si	3.551	-1.923	-0.459
Si	-0.083	0.926	3.312
Si	-2.369	2.346	-3.836
Si	-1.910	3.714	1.979

Si	-3.250	0.597	2.523
Si	-1.906	-3.993	-0.572
Si	1.294	-3.523	-3.085
Si	4.527	-1.778	1.823
Si	0.426	-0.387	-5.027
Si	3.347	2.166	3.794
Si	0.219	4.375	1.312
Si	1.404	2.516	-2.297
Si	-3.535	0.089	-3.445
Si	-1.432	-2.328	4.214
Si	-3.328	-1.808	2.741
Si	2.048	0.192	3.972
Si	3.887	-0.688	-2.500
Si	-0.870	-2.935	-2.466
Si	-4.271	1.389	0.626
Si	-3.412	3.522	0.235
Si	1.820	-3.408	-0.851
Si	-2.077	2.193	3.864
Si	2.236	-1.542	-3.960
No. (7,8)			
Si	3.226	1.426	-0.226
Si	-1.369	0.838	-1.727
Si	3.451	-0.861	0.473
Si	-1.916	-1.053	1.079
Si	0.123	-2.016	0.241
Si	-2.180	1.339	0.523
Eu	0.468	0.579	1.583
Eu	1.281	-0.371	-1.755
Si	-3.858	-2.278	0.315
Si	0.834	2.769	-0.612
Si	3.670	1.384	2.051
Si	0.520	-4.338	0.890
Si	-3.732	-0.047	-0.833
Si	0.779	-2.575	2.612
Si	0.119	1.641	-3.806
Si	3.957	1.407	-2.488
Si	-1.509	3.264	-1.203
Si	2.439	-1.015	3.308
Si	-1.528	-1.032	-3.410
Si	3.967	-2.382	-1.221
Si	-0.695	0.398	4.328
Si	-2.101	2.525	-3.367
Si	-1.354	3.137	2.041
Si	-3.627	0.684	2.595
Si	-1.727	-3.628	-0.124
Si	1.029	-3.858	-3.195
Si	4.668	-0.768	2.539
Si	0.163	-0.418	-4.922
Si	2.142	2.589	3.214
Si	0.856	3.771	1.576
Si	1.906	2.600	-2.729
Si	-3.479	0.393	-3.219
Si	-1.236	-1.594	3.382
Si	-3.667	-1.705	2.779
Si	1.583	0.740	4.696
Si	3.842	-0.988	-3.197
Si	-0.804	-2.825	-2.142
Si	-4.590	1.668	0.655
Si	-3.142	3.779	0.501
Si	1.872	-3.455	-1.016
Si	-2.271	2.062	3.947
Si	1.887	-1.783	-4.142