Supporting Information File

New Insights into Small Molecule Activation by Acyclic Silylenes: A Computational Investigation

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1. The Figure and the Table discussed in the manuscript.

Fig. S1 A linear transit calculation, showing the drop in energy as two Si-H silylenes approach each other; the reaction coordinate chosen is the Si-Si bond length, the energy values, in kcal/mol, are the ΔE values.

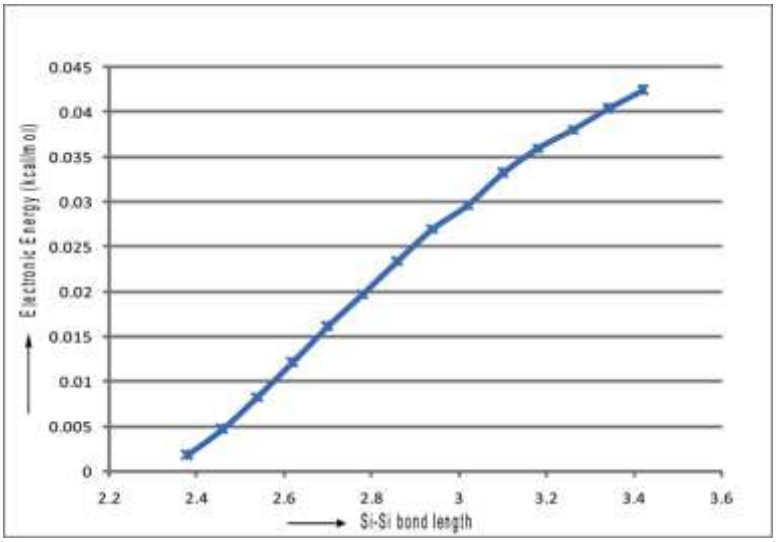
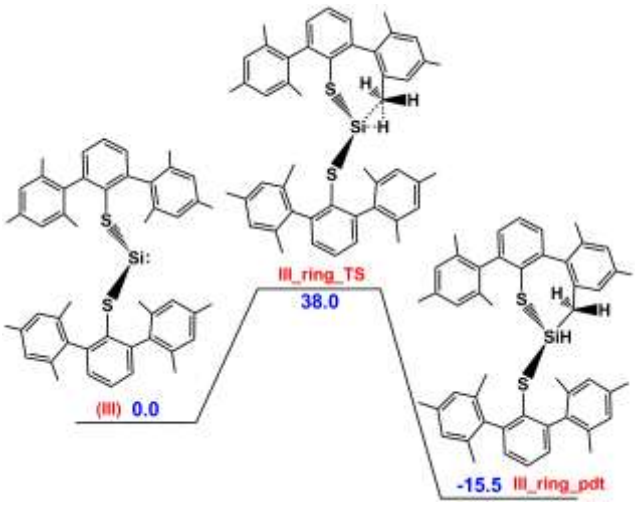


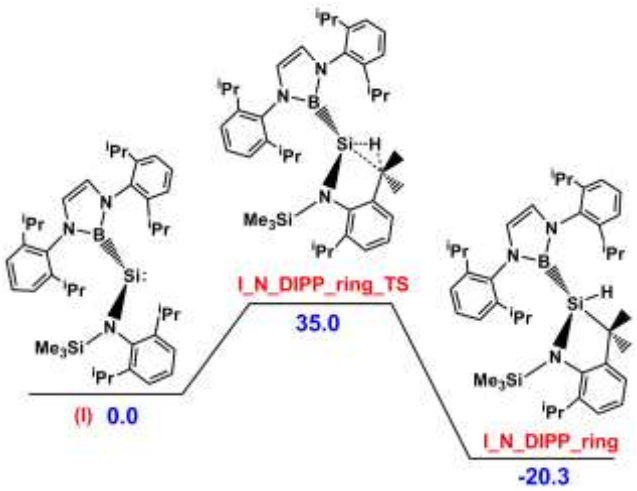
Table S1 A comparison of the energy barriers for the silylene cases **I**, **II**, and **III** in the presence and absence of the dispersion correction; all values are in kcal/mol.

	Transition state	Barrier without dispersion	Barrier with dispersion
Silylene**I**	TS 1	18.5	17.7
	TS 2	20.8	18.7
Silylene**II**	TS_si_1	20.6	20.8
	TS_si_2	20.4	22.3
Silylene**III**	TS A	39.8	38.4
	TS B	33.5	32.0

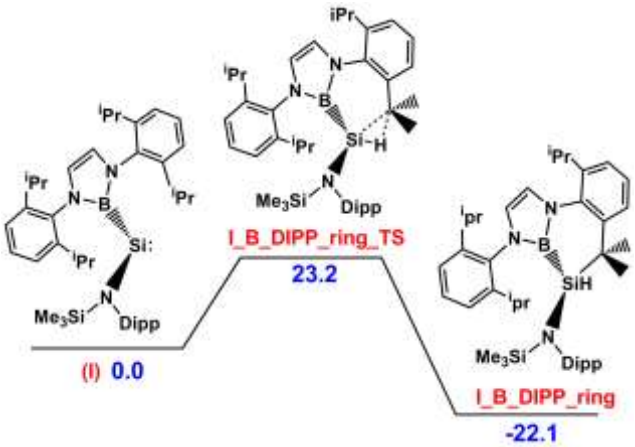
2. The Schemes discussed in the manuscript.



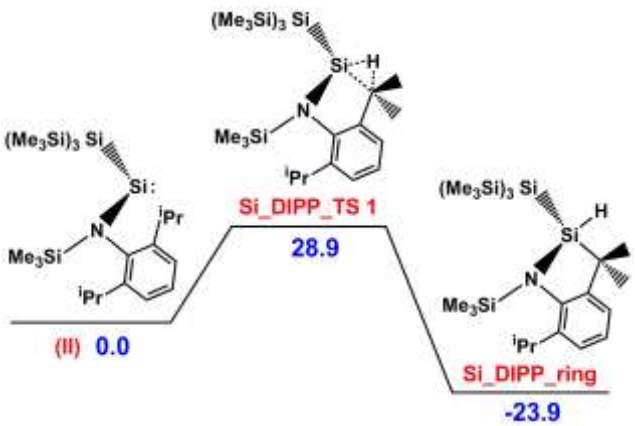
Scheme S1 The free energy profile obtained for the ring formation reaction of **III** with $–CH_3$ group on the ligand; all values are in kcal/mol.



Scheme S2 The free energy profile obtained for the ring formation reaction of **I** by the amido Dipp isopropyl C-H bond activation; all values are in kcal/mol.



Scheme S3 The free energy profile obtained for the ring formation reaction of **I** by the boryl Dipp isopropyl C-H bond activation; all values are in kcal/mol.



Scheme S4 The free energy profile obtained for the ring formation reaction of **II** by the amido Dipp isopropyl C-H bond activation; all values are in kcal/mol.

3. The xyz coordinates of all the structures discussed in the manuscript.

Silylene_rct_tzvp (I)

Si	1.786	9.955	10.612
Si	1.843	7.178	12.316
B	2.404	8.779	9.026
N	3.601	9.228	8.325
N	1.782	7.881	8.054
N	1.721	8.979	12.085
C	3.661	8.636	7.061
C	2.577	7.832	6.899
C	4.530	10.250	8.719
C	4.206	11.603	8.457
C	5.134	12.585	8.830
C	6.347	12.243	9.425
C	6.651	10.905	9.667
C	5.751	9.885	9.328
C	2.922	11.994	7.739
C	2.214	13.195	8.382
C	3.197	12.244	6.245
C	6.110	8.428	9.575
C	7.057	7.906	8.478
C	6.712	8.192	10.967
C	0.555	7.144	8.114
C	0.590	5.731	8.062
C	-0.627	5.034	8.082
C	-1.841	5.705	8.172
C	-1.858	7.099	8.236
C	-0.675	7.847	8.195
C	1.891	4.939	8.000
C	1.979	3.886	9.117
C	2.072	4.269	6.625
C	-0.726	9.370	8.196
C	-2.052	9.953	8.693
C	-0.378	9.942	6.809
C	1.480	9.742	13.296
C	0.162	10.029	13.723
C	-0.014	10.744	14.917
C	1.070	11.174	15.675
C	2.364	10.903	15.234
C	2.595	10.192	14.051
C	-1.068	9.628	12.922
C	-1.785	10.873	12.370
C	-2.031	8.753	13.742
C	4.022	9.978	13.562
C	4.501	11.213	12.780
C	5.012	9.622	14.680
C	2.043	6.820	14.166
C	0.250	6.355	11.713
C	3.352	6.495	11.404
H	4.473	8.840	6.370
H	2.294	7.233	6.040
H	4.904	13.636	8.645
H	7.057	13.024	9.703
H	7.604	10.647	10.134
H	2.234	11.138	7.806
H	1.246	13.366	7.887
H	2.800	14.122	8.282
H	2.024	13.011	9.448
H	3.884	13.094	6.110
H	2.259	12.475	5.716
H	3.648	11.362	5.769
H	5.177	7.850	9.511
H	7.288	6.842	8.640
H	8.005	8.466	8.482
H	6.608	8.008	7.480
H	6.835	7.114	11.150
H	6.068	8.602	11.758
H	7.705	8.656	11.070
H	-0.617	3.943	8.041
H	-2.778	5.145	8.198
H	-2.816	7.614	8.306
H	2.723	5.644	8.142
H	2.973	3.413	9.115
H	1.234	3.088	8.982
H	1.816	4.336	10.104
H	3.036	3.740	6.577
H	1.273	3.535	6.440
H	2.044	5.001	5.806
H	0.051	9.734	8.899
H	-1.954	11.042	8.811
H	-2.343	9.535	9.667
H	-2.871	9.772	7.980
H	0.606	9.606	6.462
H	-0.373	11.042	6.840
H	-1.130	9.624	6.070
H	-1.028	10.972	15.255
H	0.909	11.726	16.603
H	3.214	11.256	15.821
H	-0.729	9.035	12.061
H	-2.116	11.534	13.186
H	-2.673	10.585	11.788
H	-1.114	11.451	11.718
H	-2.472	9.314	14.580
H	-2.859	8.397	13.110
H	-1.520	7.876	14.164
H	4.003	9.133	12.856
H	5.520	11.066	12.391
H	3.840	11.426	11.923
H	4.499	12.104	13.426
H	5.989	9.359	14.246
H	4.662	8.767	15.277
H	5.181	10.465	15.366
H	2.981	7.232	14.562
H	1.216	7.245	14.753
H	2.053	5.731	14.323
H	0.028	6.606	10.668
H	-0.604	6.661	12.331
H	0.338	5.260	11.787
H	3.273	6.632	10.318
H	4.269	6.992	11.750
H	3.451	5.418	11.613

TS 1

Si	0.265	-0.586	0.577
Si	1.061	-1.817	-2.225
B	-1.160	0.684	-0.083
N	-1.035	2.135	-0.081
N	-2.576	0.475	-0.372
N	1.431	-1.344	-0.537
C	-2.285	2.706	-0.340
C	-3.205	1.718	-0.505
C	0.053	2.984	0.315
C	0.293	3.182	1.695
C	1.295	4.090	2.062
C	2.019	4.795	1.103
C	1.768	4.583	-0.250
C	0.792	3.670	-0.672
C	-0.538	2.496	2.769
C	0.327	1.799	3.827
C	-1.519	3.491	3.412
C	0.528	3.465	-2.157
C	-0.257	4.648	-2.750
C	1.822	3.226	-2.950
C	-3.335	-0.737	-0.446
C	-3.591	-1.458	0.747
C	-4.331	-2.644	0.652
C	-4.819	-3.094	-0.574
C	-4.576	-2.359	-1.731
C	-3.832	-1.171	-1.694
C	-3.145	-0.928	2.104
C	-4.174	0.078	2.652
C	-2.853	-2.026	3.135
C	-3.610	-0.380	-2.977
C	-4.904	0.337	-3.406
C	-3.081	-1.249	-4.128
C	2.672	-1.782	0.058
C	3.811	-0.937	0.008
C	5.012	-1.381	0.577
C	5.108	-2.629	1.188
C	3.985	-3.450	1.244
C	2.761	-3.050	0.689
C	3.739	0.462	-0.580
C	3.694	1.505	0.549
C	4.881	0.766	-1.561
C	1.566	-3.987	0.798
C	1.832	-5.339	0.115
C	1.139	-4.186	2.263
C	2.657	-2.448	-3.024
C	-0.256	-3.184	-2.301
C	0.428	-0.307	-3.178
H	-2.423	3.782	-0.365
H	-4.269	1.801	-0.700
H	1.499	4.260	3.121
H	2.787	5.507	1.412

H	2.345	5.133	-0.996
H	-1.137	1.716	2.277
H	-0.311	1.263	4.545
H	0.936	2.515	4.399
H	1.000	1.064	3.362
H	-2.154	2.981	4.153
H	-2.176	3.946	2.656
H	-0.981	4.302	3.926
H	-0.095	2.564	-2.257
H	-0.468	4.476	-3.816
H	-1.216	4.793	-2.233
H	0.317	5.583	-2.663
H	1.588	2.961	-3.991
H	2.414	2.409	-2.514
H	2.457	4.125	-2.974
H	-4.534	-3.223	1.553
H	-5.393	-4.021	-0.625
H	-4.967	-2.716	-2.686
H	-2.206	-0.369	1.956
H	-3.832	0.491	3.614
H	-5.147	-0.410	2.813
H	-4.320	0.916	1.957
H	-2.392	-1.583	4.029
H	-3.771	-2.540	3.461
H	-2.161	-2.784	2.739
H	-2.853	0.389	-2.766
H	-4.727	0.948	-4.304
H	-5.694	-0.392	-3.641
H	-5.286	0.997	-2.615
H	-2.838	-0.618	-4.995
H	-3.828	-1.987	-4.457
H	-2.175	-1.793	-3.835
H	5.890	-0.731	0.547
H	6.054	-2.957	1.625
H	4.056	-4.425	1.731
H	2.789	0.531	-1.132
H	3.602	2.522	0.143
H	2.836	1.333	1.216
H	4.609	1.456	1.160
H	4.735	1.756	-2.020
H	4.933	0.020	-2.367
H	5.859	0.783	-1.057
H	0.728	-3.511	0.271
H	0.928	-5.967	0.138
H	2.133	-5.208	-0.933
H	2.635	-5.894	0.623
H	0.234	-4.811	2.321
H	1.930	-4.685	2.845
H	0.926	-3.221	2.746
H	3.424	-1.662	-3.059
H	2.454	-2.774	-4.055
H	3.078	-3.299	-2.469
H	-1.175	-2.896	-1.769
H	-0.523	-3.385	-3.350
H	0.111	-4.124	-1.866
H	-0.462	0.121	-2.698
H	0.159	-0.588	-4.207
H	1.201	0.471	-3.227
H	-1.002	-1.701	0.337
H	-0.489	-1.743	1.313

Silylene_H2_rct (I-H_2)

C	2.694	10.320	13.946
C	1.548	9.725	13.353
C	0.257	10.014	13.868
C	0.142	10.859	14.981
C	1.264	11.425	15.581
C	2.526	11.158	15.057
N	1.716	8.842	12.223
Si	1.802	7.079	12.493
C	3.321	6.390	11.591
C	-1.012	9.450	13.245
C	-1.788	8.557	14.227
C	4.094	10.101	13.392
C	5.048	9.503	14.439
C	1.977	6.769	14.350
C	0.232	6.217	11.862
Si	1.511	9.628	10.640
B	2.344	8.819	8.984
N	1.780	7.926	7.982
C	0.535	7.211	7.984
C	0.542	5.801	8.096
C	-0.691	5.135	8.108
C	-1.890	5.837	8.015
C	-1.875	7.224	7.874
C	-0.670	7.938	7.835
C	1.834	4.995	8.152
C	2.114	4.331	6.790
C	-0.668	9.433	7.539
C	-0.526	9.668	6.022
N	3.574	9.281	8.363
C	4.514	10.279	8.792
C	4.202	11.642	8.582
C	5.162	12.597	8.944
C	6.391	12.216	9.481
C	6.676	10.868	9.683
C	5.744	9.874	9.350
C	2.897	12.073	7.927
C	3.104	12.320	6.421
C	6.082	8.404	9.557
C	6.671	8.126	10.948
C	3.696	8.704	7.096
C	2.626	7.895	6.869
C	2.255	13.293	8.601
C	7.032	7.898	8.457
C	1.834	3.930	9.260
C	-1.885	10.179	8.097
C	-1.915	10.567	12.694
C	4.671	11.405	12.816
H	4.538	8.926	6.449
H	2.393	7.299	5.993
H	4.947	13.657	8.796
H	7.127	12.976	9.752
H	7.638	10.579	10.110
H	2.189	11.235	8.023
H	1.262	13.484	8.166
H	2.854	14.205	8.458
H	2.129	13.132	9.681
H	3.809	13.149	6.255
H	2.150	12.580	5.938
H	3.505	11.426	5.923
H	5.142	7.838	9.475
H	7.245	6.827	8.593
H	7.988	8.443	8.486
H	6.598	8.032	7.456
H	6.786	7.043	11.100
H	6.021	8.516	11.742
H	7.665	8.582	11.071
H	-0.711	4.048	8.201
H	-2.841	5.301	8.042
H	-2.820	7.762	7.777
H	2.656	5.696	8.361
H	2.825	3.456	9.324
H	1.102	3.134	9.059
H	1.600	4.367	10.238
H	3.075	3.794	6.813
H	1.324	3.606	6.544
H	2.155	5.066	5.975
H	0.223	9.864	8.015
H	-1.748	11.263	7.969
H	-2.022	9.980	9.169
H	-2.814	9.907	7.572
H	0.389	9.205	5.630
H	-0.481	10.747	5.804
H	-1.386	9.244	5.480
H	-0.849	11.080	15.383
H	1.154	12.079	16.449
H	3.406	11.613	15.517
H	-0.709	8.826	12.393
H	-2.283	11.220	13.500
H	-2.790	10.137	12.182
H	-1.370	11.194	11.974
H	-2.150	9.133	15.093
H	-2.665	8.111	13.734
H	-1.161	7.740	14.613
H	4.000	9.382	12.564
H	5.660	11.227	12.369
H	4.020	11.816	12.031
H	4.783	12.169	13.601
H	6.037	9.311	13.996
H	4.666	8.554	14.842
H	5.195	10.189	15.287
H	2.913	7.190	14.743
H	1.149	7.218	14.915
H	1.981	5.686	14.545
H	0.039	6.433	10.801
H	-0.645	6.539	12.439
H	0.317	5.125	11.971
H	3.279	6.602	10.513
H	4.237	6.848	11.991
H	3.397	5.300	11.721
H	2.080	11.010	10.802
H	0.039	9.832	10.368

TS 2

C	3.721	8.973	13.180
C	2.385	9.462	13.202
C	1.980	10.358	14.225
C	2.896	10.712	15.225
C	4.198	10.221	15.220
C	4.603	9.368	14.196
N	1.441	9.066	12.179
Si	0.458	7.594	12.451
C	-1.360	8.023	12.746
C	0.584	10.962	14.257
C	-0.197	10.534	15.510
C	4.245	8.065	12.074
C	4.899	6.782	12.614
Si	1.712	9.981	10.660
B	0.186	10.037	9.173
N	-1.222	9.838	8.808
C	-2.396	9.551	9.585
C	-2.989	8.269	9.499

C	-4.173	8.041	10.214
C	-4.755	9.043	10.988
C	-4.164	10.303	11.049
C	-2.988	10.588	10.342
C	-2.391	7.156	8.650
C	-3.082	7.067	7.274
C	-2.426	12.001	10.355
C	-3.267	12.927	9.459
C	-1.397	10.162	7.457
C	-0.205	10.534	6.917
N	0.776	10.460	7.901
C	2.151	10.715	7.579
C	2.650	12.031	7.669
C	3.990	12.253	7.326
C	4.810	11.203	6.913
C	4.298	9.909	6.836
C	2.963	9.637	7.162
C	1.772	13.187	8.125
C	1.453	14.134	6.955
C	2.430	8.215	7.080
C	3.229	7.259	7.980
C	-2.452	5.785	9.344
C	-2.292	12.566	11.776
C	2.394	7.715	5.626
C	2.393	13.951	9.306
C	0.673	6.480	10.929
C	1.110	6.695	13.984
C	0.641	12.495	14.145
C	5.223	8.821	11.155
H	0.025	10.838	5.901
H	-2.377	10.127	6.993
H	4.401	13.263	7.390
H	5.853	11.395	6.654
H	4.949	9.092	6.517
H	0.818	12.760	8.471
H	1.690	14.710	9.682
H	3.316	14.472	9.011
H	2.639	13.268	10.132
H	2.372	14.590	6.555
H	0.787	14.946	7.284
H	0.958	13.598	6.132
H	1.394	8.227	7.451
H	1.966	6.703	5.576
H	3.406	7.676	5.192
H	1.783	8.377	4.994
H	2.774	6.257	7.977
H	3.252	7.624	9.017
H	4.270	7.156	7.638
H	-4.646	7.059	10.168
H	-5.673	8.841	11.543
H	-4.632	11.088	11.646
H	-1.333	7.409	8.478
H	-1.828	5.060	8.802
H	-3.477	5.386	9.359
H	-2.094	5.840	10.379
H	-2.640	6.255	6.676
H	-4.155	6.856	7.396
H	-2.980	7.999	6.703
H	-1.416	11.960	9.921
H	-1.761	13.528	11.756
H	-1.729	11.878	12.422
H	-3.274	12.740	12.242
H	-3.301	12.553	8.425
H	-2.838	13.940	9.442
H	-4.301	13.000	9.829
H	2.582	11.393	16.020
H	4.900	10.508	16.006
H	5.630	8.998	14.182
H	0.046	10.576	13.377
H	1.185	12.937	14.994
H	-0.372	12.924	14.139
H	1.151	12.806	13.222
H	0.270	10.927	16.426
H	-1.229	10.916	15.471
H	-0.241	9.439	15.604
H	3.381	7.763	11.463
H	5.573	8.168	10.341
H	4.742	9.701	10.703
H	6.104	9.165	11.719
H	5.170	6.114	11.782
H	4.226	6.233	13.288
H	5.822	7.003	13.173
H	2.137	6.331	13.844
H	1.106	7.351	14.867
H	0.465	5.829	14.199
H	-1.752	8.704	11.981
H	-1.484	8.504	13.727
H	-1.982	7.115	12.735
H	0.358	6.987	10.006
H	1.732	6.203	10.818
H	0.090	5.554	11.024
H	0.313	11.117	10.543
H	1.143	11.497	11.078

Silylene_amido_fragment

C	3.147	12.366	7.158
C	1.798	12.743	7.359
C	1.462	14.081	7.687
C	2.493	15.018	7.820
C	3.826	14.660	7.626
C	4.142	13.344	7.299
N	0.745	11.767	7.226
Si	-0.049	11.583	5.591
C	0.503	13.025	4.503
C	0.018	14.487	7.952
C	-0.339	15.877	7.411
C	3.555	10.938	6.827
C	4.338	10.852	5.507
Si	0.239	10.695	8.529
C	0.485	9.940	4.814
C	-1.928	11.587	5.819
C	-0.296	14.387	9.456
C	4.345	10.306	7.986
H	5.188	13.064	7.152
H	4.617	15.406	7.732
H	2.249	16.050	8.079
H	2.634	10.350	6.702
H	5.290	10.842	8.162
H	4.589	9.256	7.762
H	3.766	10.336	8.921
H	5.300	11.383	5.572
H	4.554	9.803	5.254
H	3.771	11.295	4.675
H	-0.625	13.758	7.439
H	-1.353	14.623	9.653
H	-0.088	13.378	9.844
H	0.327	15.091	10.028
H	-1.420	16.056	7.514
H	-0.075	15.979	6.348
H	0.174	16.679	7.962
H	0.157	13.989	4.902
H	1.598	13.069	4.423
H	0.087	12.903	3.491
H	0.253	9.099	5.486
H	1.562	9.922	4.598
H	-0.052	9.777	3.868
H	-2.246	10.771	6.484
H	-2.278	12.536	6.250
H	-2.424	11.450	4.846
H	1.260	11.241	9.561

Silylene_boryl_fragment

C	-0.565	5.692	4.651
C	-1.369	5.981	5.752
C	-0.872	5.869	7.059
C	0.467	5.463	7.223
C	1.297	5.159	6.123
C	0.755	5.284	4.837
N	1.009	5.377	8.546
B	1.611	6.415	9.341
N	1.952	5.767	10.581
C	1.567	4.421	10.506
C	1.001	4.188	9.288
C	-1.749	6.219	8.253
C	-3.104	5.494	8.217
C	2.755	4.770	6.326
C	3.209	3.629	5.404
C	2.561	6.333	11.747
C	1.733	6.849	12.767
C	2.351	7.433	13.882
C	3.740	7.497	13.981
C	4.540	6.972	12.966
C	3.969	6.376	11.833
C	0.217	6.827	12.630
C	-0.286	8.166	12.059
C	4.844	5.837	10.710
C	6.003	4.970	11.223
C	-1.936	7.743	8.360
C	3.663	6.004	6.167
C	5.360	6.991	9.831
C	-0.503	6.482	13.941
H	1.731	3.737	11.333
H	0.590	3.268	8.884
H	5.627	7.027	13.056
H	4.203	7.957	14.857
H	1.736	7.846	14.683
H	4.209	5.200	10.077
H	5.951	6.602	8.987
H	6.001	7.670	10.413
H	4.527	7.580	9.422
H	6.729	5.557	11.805
H	6.547	4.527	10.375
H	5.640	4.153	11.862
H	-0.034	6.044	11.899
H	-1.582	6.369	13.760
H	-0.382	7.272	14.698
H	-0.128	5.542	14.370
H	-1.376	8.138	11.908
H	0.186	8.388	11.091
H	-0.055	8.994	12.747
H	-2.402	6.301	5.596
H	-0.970	5.785	3.641
H	1.375	5.061	3.967

H	-1.221	5.887	9.159
H	-2.532	7.999	9.249
H	-2.456	8.139	7.474
H	-0.966	8.255	8.439
H	-3.673	5.706	9.135
H	-3.721	5.821	7.366
H	-2.971	4.406	8.139
H	2.860	4.417	7.363
H	4.714	5.741	6.366
H	3.373	6.801	6.866
H	3.598	6.407	5.145
H	2.550	2.753	5.495
H	4.231	3.317	5.665
H	3.222	3.934	4.347
H	1.783	7.556	9.041

Silylene_NH3BH3_5m_TS (TS 3)

C	5.075	9.727	8.681
C	3.815	10.247	8.310
C	3.580	11.642	8.232
C	4.649	12.501	8.522
C	5.905	12.006	8.872
C	6.111	10.632	8.956
N	2.765	9.334	7.942
C	2.723	8.809	6.648
C	1.651	7.980	6.541
N	0.974	7.924	7.764
C	-0.189	7.087	7.885
C	-0.044	5.681	7.802
C	-1.199	4.891	7.900
C	-2.454	5.465	8.078
C	-2.579	6.852	8.134
C	-1.463	7.691	8.018
C	1.300	4.994	7.593
C	1.535	3.841	8.583
C	-1.641	9.201	7.946
C	-2.884	9.714	8.679
C	2.218	12.199	7.844
C	1.964	13.611	8.387
C	5.337	8.230	8.760
C	6.094	7.734	7.514
B	1.656	8.793	8.721
Si	1.363	9.649	10.560
N	1.266	8.557	11.959
Si	1.407	6.761	12.016
C	-0.199	5.934	11.457
C	1.246	9.294	13.206
C	2.446	9.878	13.698
C	2.398	10.622	14.885
C	1.209	10.793	15.590
C	0.039	10.213	15.105
C	0.028	9.465	13.918
C	3.790	9.727	12.994
C	4.353	11.079	12.522
C	-1.287	8.849	13.455
C	-2.436	9.868	13.407
C	2.853	6.231	10.917
C	1.840	6.247	13.789
C	-1.692	7.664	14.353
C	4.815	8.997	13.880
C	1.433	4.469	6.151
C	-1.644	9.666	6.476
C	2.003	12.185	6.318
C	6.089	7.834	10.039
H	3.458	9.080	5.898
H	1.299	7.431	5.675
H	4.498	13.579	8.472
H	6.722	12.696	9.088
H	7.094	10.252	9.239
H	1.457	11.537	8.288
H	0.896	13.856	8.296
H	2.528	14.373	7.827
H	2.252	13.698	9.445
H	2.755	12.815	5.817
H	1.006	12.579	6.073
H	2.072	11.170	5.906
H	4.360	7.726	8.778
H	6.254	6.647	7.568
H	7.079	8.220	7.437
H	5.536	7.950	6.593
H	6.133	6.738	10.130
H	5.594	8.232	10.936
H	7.125	8.205	10.036
H	-1.108	3.805	7.845
H	-3.339	4.831	8.168
H	-3.568	7.294	8.255
H	2.090	5.742	7.754
H	2.569	3.476	8.499
H	0.868	2.990	8.378
H	1.367	4.159	9.619
H	2.422	4.012	5.996
H	0.668	3.704	5.947
H	1.308	5.268	5.406
H	-0.771	9.668	8.425
H	-2.863	10.812	8.713
H	-2.919	9.353	9.716
H	-3.815	9.414	8.173
H	-0.718	9.374	5.959
H	-1.728	10.762	6.427
H	-2.495	9.229	5.932
H	-0.892	10.345	15.658
H	1.194	11.374	16.514
H	3.317	11.074	15.266
H	-1.130	8.475	12.433
H	-2.711	10.218	14.414
H	-3.332	9.403	12.967
H	-2.176	10.739	12.794
H	-1.873	8.005	15.384
H	-2.622	7.203	13.984
H	-0.920	6.885	14.394
H	3.625	9.110	12.098
H	5.292	10.933	11.967
H	3.646	11.585	11.851
H	4.561	11.744	13.374
H	5.756	8.840	13.330
H	4.442	8.017	14.209
H	5.052	9.582	14.782
H	2.889	6.483	14.016
H	1.218	6.742	14.545
H	1.708	5.159	13.894
H	-0.521	6.309	10.476
H	-1.011	6.110	12.175
H	-0.060	4.845	11.370
H	2.684	6.478	9.860
H	3.771	6.737	11.245
H	3.019	5.146	10.994
H	1.423	11.355	11.093
H	-0.323	10.353	10.471
N	0.489	12.321	11.338
B	-0.648	11.672	10.520
H	0.342	12.366	12.349
H	0.807	13.230	11.001
H	-0.622	12.005	9.353
H	-1.736	11.642	11.043

Silylene_NH3BH3_6m_TS (TS 4)

C	3.096	10.662	7.301
C	1.771	11.136	7.402
C	1.426	12.459	7.045
C	2.445	13.308	6.593
C	3.763	12.865	6.506
C	4.082	11.555	6.858
N	0.729	10.238	7.822
C	-0.013	9.579	6.850
C	-1.002	8.860	7.445
N	-0.940	9.032	8.829
C	-1.921	8.355	9.625
C	-1.919	6.940	9.661
C	-2.953	6.293	10.355
C	-3.945	7.016	11.007
C	-3.926	8.410	10.970
C	-2.934	9.108	10.271
C	-0.843	6.099	8.981
C	-0.188	5.102	9.952
C	-2.978	10.628	10.158
C	-3.865	11.296	11.214
C	-0.007	12.963	7.133
C	-0.103	14.382	7.719
C	3.448	9.212	7.601
C	3.506	8.394	6.297
B	0.192	9.917	9.164
Si	1.691	9.488	10.715
N	1.287	9.545	12.487
Si	1.096	7.922	13.274
C	1.522	8.045	15.117
C	1.702	10.589	13.392
C	3.091	10.816	13.624
C	3.474	11.750	14.593
C	2.536	12.468	15.329
C	1.183	12.272	15.073
C	0.743	11.353	14.109
C	4.196	10.105	12.851
C	5.068	11.099	12.062
C	-0.757	11.224	13.870
C	-1.432	12.603	13.723
C	-0.680	7.309	13.076
C	2.292	6.659	12.505
C	-1.464	10.455	15.001
C	5.078	9.232	13.759
C	-1.409	5.347	7.763
C	-3.421	11.075	8.750
C	-0.705	12.911	5.762
C	4.746	9.063	8.404
H	0.215	9.680	5.794
H	-1.774	8.253	6.985
H	2.206	14.336	6.317
H	4.546	13.544	6.161
H	5.116	11.214	6.780
H	-0.552	12.277	7.800
H	-1.148	14.627	7.962
H	0.244	15.140	7.002
H	0.510	14.497	8.626
H	-0.186	13.558	5.039

H	-1.747	13.257	5.846
H	-0.719	11.890	5.357
H	2.639	8.796	8.221
H	3.732	7.339	6.515
H	4.291	8.780	5.627
H	2.549	8.434	5.757
H	4.885	8.013	8.700
H	4.715	9.670	9.320
H	5.632	9.363	7.821
H	-2.967	5.202	10.393
H	-4.736	6.495	11.551
H	-4.714	8.964	11.482
H	-0.056	6.781	8.627
H	0.645	4.585	9.455
H	-0.901	4.334	10.287
H	0.206	5.604	10.843
H	-0.615	4.773	7.263
H	-2.194	4.639	8.071
H	-1.849	6.031	7.024
H	-1.950	10.992	10.308
H	-3.730	12.387	11.177
H	-3.621	10.955	12.229
H	-4.933	11.096	11.034
H	-2.758	10.688	7.967
H	-3.422	12.175	8.682
H	-4.443	10.723	8.541
H	0.446	12.847	15.637
H	2.857	13.186	16.086
H	4.538	11.920	14.774
H	-0.890	10.650	12.938
H	-1.471	13.128	14.689
H	-2.467	12.494	13.371
H	-0.898	13.271	13.030
H	-1.354	10.991	15.956
H	-2.541	10.356	14.791
H	-1.053	9.448	15.136
H	3.722	9.433	12.112
H	5.812	10.555	11.459
H	4.464	11.721	11.389
H	5.616	11.772	12.738
H	5.842	8.709	13.163
H	4.491	8.475	14.297
H	5.601	9.843	14.511
H	2.579	8.297	15.274
H	0.926	8.799	15.646
H	1.330	7.065	15.583
H	-0.990	7.308	12.023
H	-1.392	7.944	13.621
H	-0.779	6.281	13.456
H	2.172	6.556	11.419
H	3.334	6.955	12.694
H	2.128	5.672	12.968
H	0.157	11.127	10.076
H	2.242	11.074	10.628
N	0.300	12.364	10.609
H	-0.111	13.065	9.992
B	1.841	12.398	10.696
H	-0.179	12.391	11.511
H	2.299	12.752	11.750
H	2.369	12.795	9.686

I_B_DIPP_ring_TS

Si	1.532	9.778	10.769
C	2.800	12.130	9.946
C	3.598	12.450	11.138
C	4.519	11.536	11.749
N	4.578	10.208	11.246
B	3.466	9.306	10.957
N	4.118	8.080	10.530
C	5.500	8.284	10.526
C	5.775	9.548	10.952
C	5.272	11.898	12.889
C	5.168	13.211	13.374
C	4.281	14.118	12.802
C	3.492	13.735	11.724
C	3.485	11.498	8.751
C	1.804	13.184	9.500
C	6.136	10.911	13.669
C	7.634	11.231	13.525
C	5.738	10.863	15.155
N	0.538	9.833	12.235
C	-0.883	9.653	12.015
C	-1.750	10.770	11.918
C	-1.245	12.204	11.969
C	-1.768	12.949	13.209
C	-1.616	12.969	10.687
C	-3.125	10.547	11.755
C	-3.648	9.261	11.671
C	-2.786	8.168	11.743
C	-1.406	8.336	11.918
C	-0.514	7.101	11.951
C	-0.348	6.521	10.535
C	-1.015	6.023	12.925
Si	1.093	9.993	13.947
C	-0.348	9.510	15.075
C	2.542	8.822	14.279
C	1.651	11.759	14.329
C	3.567	6.824	10.095
C	3.157	6.677	8.751
C	3.289	7.802	7.737
C	1.955	8.118	7.043
C	4.393	7.485	6.713
C	3.505	5.746	11.008
C	3.995	5.878	12.442
C	5.406	5.281	12.598
C	3.032	5.244	13.457
C	3.013	4.517	10.546
C	2.592	4.357	9.227
C	2.663	5.430	8.343
H	1.350	11.011	9.901
H	1.184	12.802	8.675
H	2.326	14.083	9.119
H	1.128	13.500	10.304
H	4.405	10.957	8.992
H	2.807	10.805	8.221
H	3.745	12.292	8.027
H	2.801	14.461	11.299
H	4.194	15.129	13.206
H	5.759	13.508	14.242
H	5.965	9.905	13.262
H	8.245	10.486	14.058
H	7.865	12.221	13.948
H	7.951	11.245	12.472
H	6.286	10.058	15.668
H	4.662	10.674	15.271
H	5.972	11.805	15.672
H	-1.239	12.453	9.793
H	-1.192	13.984	10.704
H	-2.707	13.068	10.583
H	-3.799	11.405	11.687
H	-0.147	12.164	12.033
H	-1.336	13.960	13.266
H	-2.864	13.054	13.174
H	-1.518	12.418	14.138
H	-4.722	9.108	11.543
H	-3.195	7.159	11.662
H	0.064	7.276	9.848
H	0.337	5.661	10.541
H	-1.317	6.192	10.131
H	0.480	7.422	12.293
H	-1.134	6.420	13.943
H	-0.301	5.186	12.964
H	-1.984	5.608	12.612
H	3.597	8.702	8.284
H	1.183	8.382	7.780
H	2.077	8.970	6.357
H	1.590	7.265	6.451
H	4.145	6.590	6.122
H	5.356	7.303	7.212
H	4.523	8.327	6.016
H	2.338	5.299	7.309
H	2.208	3.393	8.889
H	2.956	3.671	11.233
H	4.061	6.952	12.669
H	6.126	5.769	11.926
H	5.402	4.205	12.367
H	5.766	5.408	13.630
H	3.352	5.481	14.482
H	2.006	5.614	13.325
H	3.006	4.148	13.368
H	0.832	12.483	14.229
H	2.466	12.073	13.663
H	2.025	11.812	15.364
H	3.413	9.057	13.652
H	2.252	7.780	14.094
H	2.847	8.908	15.334
H	-1.244	10.118	14.886
H	-0.629	8.456	14.938
H	-0.051	9.652	16.125
H	6.738	10.041	11.028
H	6.187	7.511	10.195

I_B_DIPP_ring

C	5.629	9.997	9.033
C	4.239	10.238	9.125
C	3.730	11.340	9.874
C	4.658	12.271	10.356
C	6.031	12.112	10.163
C	6.508	10.967	9.538
N	3.323	9.355	8.478
C	3.457	8.944	7.148
C	2.401	8.150	6.822
N	1.546	8.030	7.925
C	0.378	7.198	7.873
C	0.538	5.793	7.892
C	-0.613	4.997	7.832
C	-1.881	5.568	7.767
C	-2.018	6.955	7.746
C	-0.899	7.797	7.788
C	1.910	5.134	7.961
C	1.996	4.058	9.055
C	-1.066	9.305	7.666
C	-2.271	9.853	8.442

C	2.238	11.526	10.148
C	1.939	12.564	11.244
C	6.210	8.689	8.505
C	7.103	8.896	7.271
B	2.084	8.819	9.014
Si	1.424	9.814	10.613
N	1.838	9.105	12.192
Si	1.909	7.312	12.325
C	0.351	6.519	11.584
C	1.729	9.868	13.412
C	2.912	10.331	14.053
C	2.798	11.005	15.277
C	1.558	11.255	15.861
C	0.403	10.831	15.212
C	0.461	10.132	13.998
C	4.299	10.140	13.446
C	5.172	11.400	13.578
C	-0.849	9.684	13.362
C	-1.708	10.887	12.937
C	3.450	6.659	11.431
C	1.946	6.832	14.158
C	-1.652	8.748	14.281
C	5.054	8.950	14.066
C	2.301	4.537	6.596
C	-1.127	9.713	6.183
C	1.525	11.994	8.851
C	6.979	7.957	9.621
H	4.278	9.272	6.520
H	2.178	7.664	5.878
H	4.302	13.142	10.903
H	6.726	12.865	10.541
H	7.585	10.806	9.453
H	-0.053	10.115	10.541
H	0.858	12.593	11.443
H	2.233	13.581	10.932
H	2.439	12.335	12.195
H	1.897	12.995	8.577
H	0.437	12.070	9.004
H	1.708	11.328	7.997
H	5.378	8.033	8.212
H	7.471	7.931	6.891
H	7.980	9.515	7.515
H	6.563	9.400	6.456
H	7.325	6.974	9.266
H	6.339	7.799	10.500
H	7.863	8.527	9.945
H	-0.512	3.910	7.847
H	-2.767	4.930	7.732
H	-3.016	7.394	7.687
H	2.644	5.916	8.208
H	3.029	3.688	9.139
H	1.354	3.193	8.828
H	1.695	4.456	10.032
H	3.312	4.104	6.639
H	1.601	3.739	6.306
H	2.289	5.297	5.802
H	-0.168	9.770	8.092
H	-2.259	10.953	8.422
H	-2.246	9.534	9.494
H	-3.228	9.530	8.005
H	-0.228	9.381	5.643
H	-1.196	10.808	6.086
H	-2.005	9.269	5.690
H	-0.570	11.035	15.662
H	1.494	11.786	16.813
H	3.702	11.353	15.780
H	-0.601	9.121	12.453
H	-2.013	11.488	13.808
H	-2.622	10.548	12.425
H	-1.159	11.545	12.250
H	-1.967	9.259	15.204
H	-2.561	8.396	13.770
H	-1.064	7.867	14.575
H	4.158	9.931	12.375
H	6.077	11.293	12.964
H	4.642	12.301	13.241
H	5.492	11.564	14.618
H	6.052	8.854	13.611
H	4.527	7.999	13.921
H	5.187	9.097	15.149
H	2.725	7.348	14.732
H	0.983	7.057	14.637
H	2.118	5.747	14.239
H	0.212	6.752	10.519
H	-0.544	6.854	12.125
H	0.404	5.424	11.681
H	3.412	6.896	10.358
H	4.363	7.112	11.842
H	3.528	5.566	11.536

I_N_DIPP_ring_TS

C	2.435	12.344	14.672
C	3.688	11.758	14.392
C	4.408	12.059	13.213
C	3.843	12.977	12.319
C	2.611	13.574	12.580
C	1.915	13.257	13.745
N	4.266	10.845	15.338
C	5.031	11.293	16.411
C	5.536	10.214	17.071
N	5.113	9.038	16.442
C	5.569	7.764	16.923
C	5.097	7.297	18.171
C	5.564	6.057	18.633
C	6.469	5.309	17.888
C	6.946	5.800	16.672
C	6.526	7.038	16.167
C	4.144	8.108	19.042
C	2.933	7.297	19.529
C	7.120	7.592	14.871
C	7.938	6.570	14.071
C	5.765	11.434	12.921
C	5.895	10.945	11.471
C	1.669	12.015	15.944
C	1.826	13.136	16.987
B	4.278	9.389	15.303
Si	3.351	8.582	13.704
N	2.009	7.444	13.858
Si	1.267	6.695	15.309
C	-0.251	5.703	14.775
C	1.686	7.058	12.501
C	2.705	6.401	11.735
C	2.394	6.024	10.417
C	1.142	6.292	9.861
C	0.201	7.013	10.589
C	0.471	7.446	11.899
C	4.086	6.286	12.252
C	5.195	6.343	11.234
C	-0.472	8.428	12.581
C	-1.959	8.119	12.367
C	4.322	5.310	13.370
C	2.389	5.492	16.262
C	0.803	8.107	16.486
C	-0.140	9.859	12.111
C	4.893	8.704	20.250
C	8.004	8.830	15.132
C	6.902	12.406	13.286
C	0.184	11.725	15.677
H	5.166	12.349	16.619
H	6.191	10.188	17.936
H	4.374	13.224	11.397
H	2.187	14.286	11.868
H	0.946	13.723	13.935
H	5.868	10.552	13.571
H	6.832	10.381	11.347
H	5.920	11.781	10.755
H	5.059	10.285	11.202
H	6.848	13.319	12.673
H	7.882	11.935	13.113
H	6.849	12.702	14.343
H	2.114	11.102	16.367
H	1.296	12.878	17.917
H	1.409	14.082	16.608
H	2.883	13.309	17.235
H	-0.302	11.369	16.597
H	0.062	10.955	14.903
H	-0.354	12.625	15.346
H	5.206	5.674	19.591
H	6.814	4.341	18.256
H	7.668	5.209	16.111
H	3.761	8.943	18.437
H	2.248	7.949	20.093
H	3.233	6.478	20.199
H	2.377	6.864	18.690
H	4.223	9.343	20.844
H	5.269	7.903	20.906
H	5.757	9.309	19.942
H	6.275	7.911	14.235
H	8.227	7.008	13.105
H	7.380	5.646	13.863
H	8.867	6.298	14.596
H	7.453	9.650	15.607
H	8.414	9.206	14.182
H	8.849	8.561	15.783
H	-1.096	6.339	14.481
H	-0.009	5.045	13.928
H	-0.575	5.071	15.616
H	3.390	5.896	16.469
H	2.506	4.537	15.729
H	1.912	5.265	17.228
H	1.694	8.692	16.760
H	0.082	8.792	16.019
H	0.357	7.716	17.412
H	3.145	5.502	9.821
H	0.915	5.963	8.844
H	-0.752	7.272	10.125
H	4.078	8.216	12.433
H	6.165	6.511	11.727
H	5.293	5.387	10.675
H	5.039	7.139	10.491
H	5.296	5.451	13.859
H	3.541	5.372	14.132
H	4.301	4.271	12.976
H	-0.270	8.390	13.661

H	-0.788	10.596	12.612
H	0.906	10.117	12.328
H	-0.293	9.954	11.025
H	-2.579	8.788	12.983
H	-2.261	8.273	11.320
H	-2.204	7.080	12.635

I_N_DIPP_ring

C	3.005	7.310	10.104
C	2.715	7.726	11.405
C	1.558	8.517	11.648
C	0.829	9.055	10.561
C	1.142	8.596	9.271
C	2.191	7.706	9.040
C	3.626	7.440	12.606
C	3.412	6.008	13.123
N	1.286	8.846	13.024
Si	-0.144	8.161	13.855
C	0.076	6.331	14.326
C	-0.099	10.246	10.747
C	0.708	11.538	10.509
C	5.107	7.651	12.255
Si	2.953	8.879	13.722
B	3.190	9.167	15.711
N	3.211	8.368	16.931
C	3.183	6.942	17.116
C	2.074	6.338	17.753
C	2.074	4.942	17.896
C	3.140	4.170	17.446
C	4.252	4.788	16.875
C	4.310	6.178	16.713
C	0.936	7.150	18.358
C	1.106	7.243	19.888
C	5.588	6.842	16.204
C	6.375	7.461	17.378
C	3.437	9.217	18.021
C	3.576	10.496	17.581
N	3.443	10.520	16.193
C	3.815	11.702	15.459
C	5.182	11.891	15.151
C	5.547	13.048	14.451
C	4.592	13.989	14.070
C	3.252	13.786	14.389
C	2.836	12.645	15.090
C	6.250	10.886	15.561
C	7.155	11.458	16.665
C	1.370	12.472	15.450
C	0.469	12.519	14.206
C	-0.456	6.592	18.033
C	6.515	5.910	15.412
C	0.935	13.511	16.498
C	7.076	10.399	14.361
C	-0.464	9.185	15.412
C	-1.697	8.179	12.768
C	-1.352	10.223	9.862
H	3.771	11.401	18.149
H	3.497	8.834	19.034
H	6.596	13.212	14.199
H	4.895	14.884	13.521
H	2.510	14.529	14.089
H	5.738	10.009	15.982
H	7.761	9.594	14.670
H	7.689	11.208	13.934
H	6.428	10.012	13.564
H	7.703	12.345	16.308
H	7.895	10.709	16.984
H	6.569	11.756	17.546
H	1.258	11.477	15.905
H	-0.110	13.345	16.795
H	1.016	14.535	16.101
H	1.561	13.452	17.401
H	-0.586	12.401	14.492
H	0.728	11.715	13.504
H	0.558	13.479	13.675
H	1.221	4.455	18.372
H	3.114	3.084	17.555
H	5.095	4.175	16.557
H	0.994	8.169	17.948
H	-1.230	7.279	18.405
H	-0.626	5.617	18.515
H	-0.599	6.465	16.954
H	0.326	7.886	20.323
H	1.022	6.246	20.346
H	2.084	7.654	20.173
H	5.292	7.665	15.534
H	7.335	6.496	14.972
H	5.995	5.395	14.593
H	6.975	5.149	16.061
H	5.783	8.208	17.922
H	7.286	7.955	17.008
H	6.677	6.676	18.088
H	-2.118	9.183	12.623
H	-1.501	7.739	11.779
H	-2.460	7.560	13.264
H	0.910	6.152	15.020
H	0.235	5.721	13.425
H	-0.847	5.967	14.802
H	0.425	9.238	16.055
H	-0.757	10.210	15.148
H	-1.280	8.735	15.996
H	3.882	6.685	9.916
H	2.409	7.368	8.025
H	0.574	8.979	8.420
H	3.588	10.106	13.111
H	5.741	7.561	13.150
H	5.462	6.892	11.537
H	5.282	8.641	11.810
H	3.941	5.828	14.068
H	2.354	5.785	13.291
H	3.786	5.283	12.379
H	-0.417	10.261	11.797
H	0.088	12.427	10.706
H	1.589	11.579	11.166
H	1.062	11.587	9.468
H	-2.013	11.065	10.118
H	-1.098	10.325	8.796
H	-1.922	9.292	9.985

Silylene_Silicon_rct (II)

C	2.015	11.751	14.622
C	3.137	11.442	15.431
C	3.889	10.300	15.126
C	3.554	9.475	14.054
C	2.439	9.780	13.277
C	1.653	10.910	13.540
C	3.516	12.277	16.647
C	3.194	11.515	17.944
C	0.416	11.171	12.691
C	-0.678	10.136	13.002
N	1.233	12.942	14.898
Si	-0.091	12.656	16.030
Si	-1.462	14.604	16.496
Si	-3.460	13.280	16.532
C	-5.017	14.298	16.963
C	0.729	11.217	11.187
Si	1.767	14.459	14.050
C	0.386	15.011	12.880
C	2.189	15.759	15.356
C	3.313	14.072	13.030
C	4.983	12.734	16.623
Si	-0.911	14.974	18.796
C	-2.460	15.341	19.847
Si	-2.099	16.717	15.561
C	-3.171	17.661	16.830
C	-0.023	13.474	19.572
C	0.263	16.473	18.936
C	-0.654	17.881	15.120
C	-3.161	16.462	13.994
C	-3.716	12.519	14.798
C	-3.341	11.854	17.795
H	2.168	9.123	12.448
H	4.155	8.591	13.832
H	4.754	10.049	15.745
H	0.020	12.155	12.975
H	-0.347	9.119	12.739
H	-1.595	10.354	12.432
H	-0.927	10.138	14.074
H	1.080	10.243	10.814
H	-0.174	11.482	10.617
H	1.506	11.961	10.960
H	2.890	13.180	16.636
H	3.416	12.134	18.827
H	2.132	11.230	17.980
H	3.790	10.592	18.017
H	5.192	13.391	17.481
H	5.218	13.290	15.704
H	5.677	11.882	16.684
H	4.144	13.730	13.661
H	3.120	13.291	12.282
H	3.637	14.982	12.501
H	-0.578	15.038	13.405
H	0.299	14.311	12.037
H	0.586	16.012	12.471
H	1.352	15.904	16.051
H	3.071	15.443	15.934
H	2.417	16.728	14.889
H	-4.642	11.924	14.769
H	-3.786	13.299	14.026
H	-2.880	11.854	14.532
H	-5.895	13.632	16.980
H	-4.929	14.767	17.953
H	-5.209	15.089	16.225
H	-4.247	11.231	17.736
H	-2.468	11.217	17.595
H	-3.257	12.233	18.824
H	0.164	13.669	20.640
H	-0.623	12.557	19.491
H	0.945	13.284	19.088
H	0.510	16.654	19.995
H	1.203	16.300	18.394
H	-0.194	17.389	18.536
H	-2.163	15.560	20.886
H	-3.017	16.207	19.462

H	-3.143	14.479	19.866
H	-3.474	17.442	13.599
H	-2.613	15.937	13.199
H	-4.069	15.884	14.217
H	-1.068	18.844	14.783
H	-0.009	18.073	15.989
H	-0.028	17.478	14.314
H	-3.545	18.591	16.371
H	-4.037	17.071	17.160
H	-2.587	17.937	17.719

Silylene_Silicon(II)_3membered_ts (TS Si_1)

C	3.841	10.856	14.649
C	2.596	11.383	14.281
C	2.253	12.695	14.702
C	3.148	13.433	15.520
C	4.382	12.862	15.860
C	4.738	11.588	15.424
C	1.641	10.521	13.467
C	1.168	9.303	14.281
N	1.001	13.284	14.286
Si	-0.350	12.973	15.414
Si	-2.458	14.109	15.412
Si	-2.285	16.202	16.556
C	-0.733	16.232	17.655
C	2.795	14.807	16.073
C	2.694	14.765	17.608
Si	0.941	14.126	12.707
C	0.278	15.878	12.985
C	2.690	14.218	11.993
C	-0.172	13.179	11.495
C	3.781	15.896	15.618
C	2.247	10.078	12.125
Si	-3.914	14.352	13.537
C	-3.222	15.410	12.111
Si	-3.459	12.576	16.966
C	-3.317	10.760	16.394
C	-4.358	12.626	12.860
C	-5.509	15.223	14.124
C	-2.615	12.730	18.668
C	-5.322	12.941	17.168
C	-2.205	17.680	15.352
C	-3.830	16.472	17.645
H	4.112	9.848	14.324
H	5.706	11.163	15.696
H	5.078	13.428	16.484
H	0.756	11.135	13.246
H	2.009	8.632	14.517
H	0.423	8.723	13.714
H	0.713	9.616	15.232
H	3.122	9.427	12.274
H	1.508	9.513	11.537
H	2.573	10.940	11.525
H	1.804	15.070	15.676
H	2.397	15.746	18.007
H	1.951	14.022	17.934
H	3.660	14.495	18.062
H	3.468	16.880	15.998
H	3.838	15.957	14.522
H	4.797	15.702	15.994
H	3.366	14.781	12.651
H	3.124	13.219	11.850
H	2.661	14.725	11.017
H	-1.130	12.904	11.958
H	0.317	12.254	11.158
H	-0.389	13.791	10.606
H	-0.699	15.853	13.483
H	0.973	16.448	13.619
H	0.156	16.416	12.033
H	-3.914	10.126	17.069
H	-3.698	10.622	15.372
H	-2.280	10.400	16.427
H	-5.730	12.302	17.967
H	-5.515	13.988	17.438
H	-5.874	12.716	16.244
H	-3.048	11.999	19.369
H	-1.537	12.531	18.583
H	-2.745	13.732	19.101
H	-0.712	17.150	18.263
H	-0.696	15.368	18.333
H	0.176	16.211	17.039
H	-2.189	18.619	15.928
H	-1.304	17.653	14.724
H	-3.082	17.709	14.690
H	-3.765	17.458	18.132
H	-4.752	16.453	17.046
H	-3.920	15.711	18.432
H	-4.980	12.715	11.956
H	-3.454	12.056	12.595
H	-4.918	12.040	13.604
H	-3.996	15.507	11.333
H	-2.955	16.420	12.452
H	-2.333	14.960	11.652
H	-6.225	15.287	13.289
H	-5.997	14.690	14.951
H	-5.296	16.249	14.460
H	-0.838	11.515	15.083
H	-1.445	12.188	14.362

Silylene_Silicon(II)_H_2_rct

C	1.708	11.056	13.247
C	1.848	11.755	14.475
C	2.618	11.191	15.525
C	3.280	9.976	15.305
C	3.178	9.305	14.089
C	2.385	9.841	13.078
N	1.220	13.042	14.667
Si	2.058	14.499	14.060
C	3.793	14.010	13.492
C	2.716	11.851	16.892
C	4.153	12.273	17.239
C	0.819	11.567	12.121
C	1.590	11.769	10.807
C	2.135	10.941	17.987
C	-0.386	10.635	11.910
Si	-0.470	12.982	15.223
Si	-1.528	14.592	16.616
Si	-2.433	16.431	15.405
C	-3.452	15.798	13.926
Si	-3.320	13.122	17.238
C	-2.673	11.885	18.539
Si	-0.539	15.370	18.647
C	0.266	17.090	18.464
C	-4.814	14.059	17.965
C	-3.965	12.122	15.746
C	1.105	15.260	12.600
C	2.170	15.767	15.461
C	-1.917	15.579	19.953
C	0.756	14.151	19.319
C	-3.567	17.436	16.565
C	-1.102	17.636	14.764
H	2.285	9.302	12.132
H	3.704	8.360	13.935
H	3.884	9.545	16.108
H	0.425	12.544	12.432
H	-0.064	9.635	11.581
H	-1.061	11.043	11.142
H	-0.960	10.515	12.840
H	1.981	10.817	10.417
H	0.930	12.197	10.036
H	2.444	12.449	10.939
H	2.102	12.762	16.849
H	2.158	11.447	18.964
H	1.092	10.672	17.764
H	2.710	10.007	18.078
H	4.181	12.782	18.215
H	4.565	12.960	16.485
H	4.824	11.402	17.296
H	4.397	13.625	14.325
H	3.762	13.232	12.717
H	4.304	14.892	13.076
H	0.023	15.293	12.795
H	1.258	14.674	11.682
H	1.444	16.289	12.404
H	1.169	16.028	15.827
H	2.749	15.361	16.303
H	2.654	16.694	15.118
H	-4.819	11.505	16.068
H	-4.304	12.779	14.933
H	-3.197	11.450	15.338
H	-5.548	13.330	18.343
H	-4.531	14.721	18.795
H	-5.310	14.666	17.195
H	-3.462	11.160	18.792
H	-1.809	11.325	18.153
H	-2.364	12.388	19.466
H	1.110	14.484	20.307
H	0.336	13.141	19.425
H	1.623	14.089	18.647
H	0.617	17.424	19.453
H	1.127	17.082	17.783
H	-0.456	17.833	18.098
H	-1.481	15.989	20.877
H	-2.693	16.276	19.606
H	-2.402	14.625	20.202
H	-3.829	16.645	13.331
H	-2.846	15.159	13.267
H	-4.316	15.208	14.264
H	-1.594	18.485	14.262
H	-0.492	18.036	15.586
H	-0.425	17.164	14.040
H	-4.015	18.277	16.011
H	-4.382	16.825	16.977
H	-3.000	17.855	17.409
H	-0.581	11.653	15.924
H	-1.403	12.897	14.032

Silylene_Silicon(II)_4membered_ts (TS Si_2)

C	2.060	12.360	15.271
C	3.440	12.398	15.514

C	4.312	11.497	14.908
C	3.802	10.520	14.056
C	2.429	10.432	13.788
C	1.548	11.375	14.383
C	1.919	9.331	12.870
C	2.399	9.526	11.421
N	0.138	11.309	14.080
Si	-0.476	12.264	12.694
C	-1.867	13.414	13.282
C	1.161	13.356	15.992
C	1.572	14.816	15.739
C	2.315	7.933	13.377
Si	-0.817	10.498	15.381
Si	-2.564	8.871	14.644
Si	-2.825	7.840	16.794
C	-1.145	7.266	17.496
Si	-4.591	10.070	14.259
C	-4.716	11.576	15.422
Si	-2.298	7.074	13.089
C	-1.553	7.574	11.408
C	-4.756	10.652	12.450
C	-6.083	8.938	14.627
C	1.115	13.061	17.502
C	0.941	13.314	12.011
C	-1.154	11.139	11.332
C	-1.119	5.779	13.849
C	-3.977	6.237	12.734
C	-3.601	9.046	18.050
C	-3.960	6.310	16.671
H	4.484	9.806	13.587
H	5.384	11.550	15.106
H	3.839	13.153	16.195
H	0.820	9.396	12.873
H	3.406	7.790	13.350
H	1.861	7.153	12.746
H	1.986	7.772	14.414
H	3.496	9.453	11.355
H	1.971	8.755	10.762
H	2.107	10.510	11.028
H	0.142	13.223	15.599
H	0.423	13.750	18.011
H	0.777	12.032	17.692
H	2.110	13.182	17.958
H	0.854	15.502	16.214
H	1.607	15.048	14.666
H	2.565	15.035	16.160
H	1.298	14.043	12.751
H	1.801	12.700	11.711
H	0.589	13.869	11.127
H	-1.879	10.423	11.741
H	-0.350	10.565	10.850
H	-1.663	11.732	10.557
H	-2.711	12.856	13.709
H	-1.504	14.117	14.046
H	-2.256	14.001	12.436
H	-0.441	8.813	14.872
H	0.267	9.069	15.534
H	-1.418	6.667	10.797
H	-2.204	8.263	10.851
H	-0.573	8.055	11.524
H	-3.826	5.352	12.096
H	-4.478	5.912	13.656
H	-4.653	6.923	12.202
H	-0.952	4.962	13.129
H	-0.142	6.220	14.091
H	-1.531	5.340	14.769
H	-1.311	6.728	18.442
H	-0.622	6.588	16.807
H	-0.486	8.120	17.706
H	-3.611	8.585	19.050
H	-3.027	9.981	18.107
H	-4.638	9.294	17.783
H	-4.110	5.886	17.676
H	-4.948	6.568	16.262
H	-3.524	5.527	16.036
H	-5.756	11.087	12.294
H	-4.010	11.415	12.191
H	-4.639	9.813	11.748
H	-5.568	12.209	15.127
H	-4.875	11.253	16.460
H	-3.811	12.198	15.408
H	-7.017	9.482	14.415
H	-6.069	8.030	14.008
H	-6.103	8.632	15.683

Silylene_Silicon_sih_fragment

C	1.431	11.011	14.184
Si	2.460	12.391	15.005
C	3.960	11.600	15.874
Si	1.153	13.598	16.574
Si	2.238	15.595	17.251
C	1.457	16.247	18.863
Si	-1.019	14.037	15.730
C	-2.049	12.434	15.717
C	3.083	13.576	13.647
C	-1.917	15.332	16.804
C	-0.889	14.708	13.949
C	4.096	15.290	17.550
C	2.050	16.918	15.890
H	0.996	12.724	17.805
H	-3.058	12.629	15.320
H	-1.578	11.662	15.090
H	-2.153	12.027	16.733
H	-1.889	14.953	13.558
H	-0.275	15.619	13.908
H	-0.437	13.965	13.276
H	-2.943	15.489	16.436
H	-1.978	15.006	17.852
H	-1.397	16.301	16.780
H	1.961	17.171	19.188
H	0.389	16.469	18.727
H	1.548	15.506	19.670
H	4.581	16.209	17.916
H	4.255	14.500	18.299
H	4.604	14.985	16.623
H	2.576	17.842	16.180
H	2.471	16.574	14.935
H	0.993	17.171	15.723
H	2.058	10.424	13.495
H	1.016	10.324	14.937
H	0.592	11.428	13.608
H	4.568	11.034	15.150
H	4.602	12.364	16.335
H	3.639	10.907	16.664
H	3.657	13.022	12.887
H	2.247	14.080	13.139
H	3.741	14.353	14.065

Silylene_silicon(II)_NH_3BH_3_5m_ts (TS Si_3)

C	2.546	9.470	13.272
C	2.031	10.349	12.324
C	1.588	11.632	12.676
C	1.671	12.035	14.038
C	2.243	11.160	15.005
C	2.660	9.884	14.598
C	1.098	12.565	11.574
C	2.287	13.049	10.721
N	1.123	13.315	14.451
Si	2.136	14.793	14.268
C	1.573	15.902	12.836
C	2.475	11.567	16.456
C	3.980	11.620	16.779
C	0.031	11.949	10.657
Si	-0.453	13.042	15.260
Si	-1.790	14.931	15.979
Si	-3.953	13.893	16.065
C	-5.225	14.916	17.057
Si	-1.115	15.297	18.260
C	-2.573	15.151	19.482
Si	-2.072	16.937	14.713
C	-3.620	17.875	15.324
C	0.172	13.991	18.784
C	-0.388	17.041	18.532
C	1.758	10.650	17.460
C	2.071	15.785	15.877
C	3.937	14.273	13.977
C	-0.622	18.166	14.862
C	-2.362	16.496	12.879
C	-4.659	13.692	14.307
C	-3.843	12.184	16.908
B	-1.827	10.894	13.889
N	-1.145	10.208	15.084
H	1.962	10.032	11.281
H	2.874	8.471	12.977
H	3.095	9.207	15.337
H	0.643	13.437	12.067
H	0.427	11.093	10.089
H	-0.304	12.698	9.924
H	-0.839	11.604	11.227
H	2.745	12.203	10.187
H	1.952	13.779	9.968
H	3.073	13.519	11.327
H	2.068	12.581	16.582
H	1.938	10.998	18.489
H	0.673	10.646	17.291
H	2.124	9.614	17.390
H	4.141	12.021	17.791
H	4.527	12.250	16.065
H	4.428	10.615	16.742
H	4.439	14.064	14.931
H	4.028	13.379	13.346
H	4.478	15.096	13.486
H	0.491	16.079	12.857
H	1.828	15.468	11.860
H	2.076	16.879	12.910
H	1.038	16.041	16.147
H	2.513	15.213	16.705
H	2.635	16.724	15.772
H	-5.567	13.069	14.341
H	-4.938	14.669	13.887
H	-3.942	13.209	13.631
H	-6.224	14.486	16.880
H	-5.029	14.876	18.136
H	-5.253	15.970	16.753

H	-4.858	11.794	17.083
H	-3.311	11.472	16.265
H	-3.323	12.238	17.875
H	0.435	14.128	19.845
H	-0.223	12.973	18.657
H	1.095	14.069	18.193
H	-0.121	17.157	19.594
H	0.513	17.224	17.934
H	-1.128	17.817	18.285
H	-2.188	15.286	20.506
H	-3.330	15.926	19.300
H	-3.064	14.170	19.431
H	-2.399	17.413	12.271
H	-1.574	15.847	12.473
H	-3.317	15.966	12.758
H	-0.842	19.050	14.243
H	-0.499	18.501	15.901
H	0.332	17.747	14.525
H	-3.679	18.849	14.813
H	-4.543	17.321	15.102
H	-3.585	18.063	16.408
H	-0.670	11.328	15.709
H	-1.401	12.224	13.968
H	-0.323	9.644	14.856
H	-1.753	9.688	15.717
H	-1.401	10.567	12.812
H	-3.023	11.013	14.011

Silylene_silicon(II)_NH_3BH_3_6m_ts (TS Si_4)

C	1.578	8.477	13.425
C	1.597	9.486	14.423
C	2.618	9.491	15.413
C	3.520	8.421	15.448
C	3.454	7.379	14.528
C	2.504	7.426	13.511
N	0.583	10.511	14.452
Si	0.880	12.051	13.528
C	2.738	12.221	13.210
C	2.781	10.626	16.420
C	4.232	11.139	16.465
C	0.655	8.550	12.217
C	1.478	8.853	10.950
C	2.323	10.246	17.840
C	-0.195	7.290	12.002
Si	-0.845	10.467	15.528
Si	-3.138	9.069	14.913
Si	-4.080	10.118	16.862
C	-4.134	12.018	16.710
Si	-3.867	10.286	12.995
C	-3.118	9.570	11.394
Si	-4.192	6.898	14.843
C	-3.967	6.083	16.560
C	-5.766	10.176	12.839
C	-3.474	12.152	13.110
C	0.011	12.082	11.842
C	0.276	13.524	14.557
C	-6.063	6.900	14.464
C	-3.404	5.765	13.522
C	-5.893	9.562	17.102
C	-3.130	9.667	18.448
H	2.488	6.639	12.753
H	4.160	6.548	14.584
H	4.290	8.400	16.223
H	-0.034	9.388	12.389
H	0.426	6.387	11.907
H	-0.785	7.381	11.078
H	-0.901	7.139	12.828
H	2.133	8.005	10.700
H	0.815	9.033	10.089
H	2.120	9.735	11.083
H	2.142	11.456	16.084
H	2.498	11.086	18.529
H	1.257	9.989	17.874
H	2.882	9.375	18.213
H	4.288	12.064	17.059
H	4.624	11.348	15.460
H	4.904	10.407	16.938
H	3.286	12.507	14.117
H	3.174	11.288	12.827
H	2.896	13.007	12.455
H	-1.046	11.801	11.908
H	0.500	11.417	11.118
H	0.059	13.106	11.440
H	-0.813	13.537	14.693
H	0.740	13.528	15.554
H	0.564	14.455	14.041
H	-1.659	8.174	15.022
H	-0.341	9.173	16.433
H	-3.519	12.611	12.110
H	-4.217	12.652	13.746
H	-2.486	12.357	13.540
H	-6.101	10.858	12.042
H	-6.104	9.163	12.585
H	-6.266	10.477	13.772
H	-3.513	10.111	10.520
H	-2.024	9.651	11.381
H	-3.378	8.507	11.282
H	-3.938	4.801	13.510
H	-3.487	6.209	12.519
H	-2.341	5.558	13.705
H	-4.190	5.006	16.500
H	-2.954	6.205	16.971
H	-4.661	6.529	17.287
H	-6.468	5.902	14.693
H	-6.616	7.637	15.060
H	-6.255	7.103	13.401
H	-4.465	12.444	17.671
H	-3.147	12.434	16.467
H	-4.847	12.336	15.936
H	-3.634	10.131	19.311
H	-3.097	8.580	18.607
H	-2.093	10.030	18.422
H	-6.320	10.103	17.962
H	-6.510	9.793	16.221
H	-5.978	8.486	17.306
B	-0.194	7.790	16.746
N	-0.651	7.073	15.501
H	-0.971	7.727	17.669
H	0.985	7.797	16.985
H	0.078	6.880	14.813
H	-1.221	6.241	15.649

II_ring_TS

C	3.058	10.581	17.034
C	3.738	11.666	16.492
C	3.138	12.538	15.565
C	1.797	12.293	15.188
C	1.100	11.179	15.731
C	1.740	10.331	16.641
C	3.925	13.747	15.081
C	5.341	13.386	14.605
N	1.021	13.142	14.337
Si	-0.717	13.173	14.784
Si	-1.276	14.009	16.928
Si	-0.174	13.547	18.998
C	-1.117	14.520	20.347
C	-0.289	10.845	15.229
C	-0.182	9.995	13.959
C	3.987	14.839	16.162
Si	1.407	13.530	12.618
C	2.860	12.460	12.031
C	-0.070	13.137	11.490
C	1.764	15.381	12.387
C	-1.246	10.243	16.238
Si	-1.104	16.338	16.410
C	-2.254	16.740	14.940
Si	-3.617	13.563	17.155
C	-4.419	13.215	15.462
C	-1.568	17.467	17.876
C	0.677	16.784	15.907
C	-4.514	15.052	17.945
C	-3.947	12.069	18.296
C	1.637	14.114	18.967
C	-0.198	11.716	19.519
H	1.209	9.466	17.044
H	3.547	9.930	17.761
H	4.763	11.865	16.813
H	2.982	15.151	16.467
H	4.514	14.474	17.057
H	4.523	15.726	15.788
H	3.385	14.178	14.228
H	5.814	14.254	14.121
H	5.987	13.094	15.447
H	5.333	12.551	13.890
H	0.428	10.490	13.192
H	-0.954	9.207	16.491
H	0.310	9.039	14.209
H	-1.170	9.769	13.528
H	-2.265	10.190	15.826
H	-1.275	10.823	17.166
H	-1.278	11.814	14.377
H	2.822	12.383	10.934
H	3.837	12.875	12.306
H	2.796	11.444	12.446
H	-0.356	12.077	11.540
H	-0.958	13.733	11.741
H	0.214	13.366	10.449
H	-3.507	11.142	17.904
H	-5.034	11.915	18.389
H	-3.545	12.238	19.306
H	-4.258	14.048	14.765
H	-5.504	13.066	15.584
H	-3.997	12.312	14.997
H	-3.311	16.576	15.192
H	-4.465	15.944	17.305
H	-2.016	16.110	14.071
H	-2.134	17.795	14.646
H	-4.084	15.310	18.924
H	-2.560	17.235	18.286
H	-1.575	18.516	17.539
H	-0.832	17.382	18.688
H	-2.162	14.183	20.425

H	-1.125	15.600	20.150
H	-0.636	14.353	21.324
H	1.730	15.181	18.725
H	2.206	13.540	18.222
H	2.099	13.947	19.954
H	0.215	11.638	20.538
H	0.426	11.109	18.851
H	-1.213	11.295	19.535
H	1.999	15.583	11.330
H	0.875	15.974	12.650
H	2.603	15.745	12.996
H	1.346	16.751	16.779
H	0.711	17.805	15.494
H	1.072	16.092	15.151
H	-5.576	14.801	18.096

II_ring_pdt

C	3.710	11.920	16.139
C	3.088	12.843	15.280
C	1.739	12.611	14.919
C	1.060	11.462	15.432
C	1.715	10.580	16.288
C	3.047	10.806	16.648
C	3.868	14.072	14.835
C	3.942	15.126	15.953
N	0.925	13.489	14.126
Si	1.293	14.016	12.450
C	-0.233	13.837	11.332
C	-0.389	11.282	14.974
C	-1.288	10.556	15.973
Si	-0.753	13.153	14.703
Si	-1.488	14.363	16.609
Si	-1.278	16.634	15.922
C	-2.003	17.871	17.180
C	-0.410	10.539	13.620
C	5.280	13.736	14.327
C	1.765	15.854	12.321
C	2.646	12.905	11.723
Si	-3.809	13.828	16.807
C	-4.808	15.335	17.415
Si	-0.392	13.989	18.691
C	1.427	14.533	18.641
C	-4.099	12.417	18.058
C	-4.527	13.285	15.125
C	-0.403	12.172	19.260
C	-1.325	15.021	20.000
C	0.557	17.073	15.680
C	-2.187	16.856	14.258
H	1.185	9.707	16.677
H	3.562	10.119	17.322
H	4.747	12.096	16.433
H	2.940	15.441	16.270
H	4.463	14.724	16.835
H	4.488	16.018	15.608
H	3.320	14.530	14.004
H	5.741	14.623	13.867
H	5.939	13.415	15.147
H	5.266	12.928	13.581
H	0.222	11.032	12.869
H	-0.968	9.510	16.119
H	-0.027	9.513	13.752
H	-1.433	10.473	13.216
H	-2.324	10.520	15.603
H	-1.293	11.046	16.954
H	-1.728	13.415	13.590
H	2.716	13.089	10.640
H	3.636	13.083	12.160
H	2.399	11.844	11.873
H	-0.630	12.813	11.316
H	-1.051	14.515	11.615
H	0.073	14.099	10.307
H	-3.568	11.500	17.769
H	-5.174	12.187	18.112
H	-3.764	12.701	19.066
H	-4.386	14.061	14.358
H	-5.607	13.093	15.225
H	-4.050	12.365	14.759
H	-3.259	16.633	14.353
H	-4.794	16.153	16.680
H	-1.775	16.192	13.484
H	-2.085	17.895	13.904
H	-4.412	15.723	18.364
H	-3.069	17.693	17.374
H	-1.891	18.895	16.791
H	-1.468	17.817	18.139
H	-2.377	14.712	20.080
H	-1.307	16.093	19.759
H	-0.857	14.886	20.988
H	1.538	15.593	18.373
H	1.986	13.932	17.910
H	1.886	14.382	19.631
H	0.006	12.123	20.282
H	0.235	11.557	18.611
H	-1.412	11.736	19.280
H	1.995	16.088	11.269
H	0.917	16.486	12.623
H	2.633	16.146	12.928
H	1.069	17.162	16.650
H	0.656	18.035	15.155
H	1.075	16.302	15.094
H	-5.858	15.044	17.576

Silylene_Sulphur_rct (III)

S	10.662	3.060	11.096
Si	9.039	2.766	12.547
C	11.955	3.800	12.112
S	7.608	2.451	10.910
C	11.720	4.805	13.082
C	12.828	5.375	13.731
H	12.645	6.160	14.469
C	14.131	4.972	13.447
H	14.974	5.436	13.962
C	14.348	3.974	12.497
H	15.361	3.639	12.264
C	13.274	3.380	11.822
C	10.363	5.309	13.462
C	9.662	6.190	12.606
C	8.419	6.691	13.020
H	7.873	7.359	12.348
C	7.871	6.379	14.267
C	8.598	5.531	15.113
H	8.185	5.268	16.091
C	9.831	4.991	14.739
C	10.227	6.585	11.268
H	9.650	7.407	10.824
H	10.204	5.732	10.569
H	11.278	6.897	11.353
C	6.539	6.935	14.701
H	6.124	7.619	13.948
H	6.628	7.488	15.649
H	5.805	6.130	14.863
C	10.534	4.024	15.656
H	9.949	3.859	16.571
H	11.537	4.370	15.942
H	10.663	3.048	15.156
C	13.542	2.317	10.806
C	13.845	2.679	9.476
C	14.102	1.668	8.543
H	14.326	1.948	7.509
C	14.071	0.313	8.893
C	13.765	-0.018	10.218
H	13.726	-1.072	10.510
C	13.500	0.959	11.183
C	13.853	4.127	9.056
H	14.090	4.226	7.988
H	14.588	4.713	9.628
H	12.871	4.594	9.233
C	14.385	-0.756	7.878
H	13.870	-1.699	8.114
H	15.466	-0.971	7.851
H	14.088	-0.449	6.865
C	13.135	0.563	12.590
H	13.270	-0.515	12.743
H	12.080	0.804	12.800
H	13.741	1.099	13.335
C	6.193	1.718	11.753
C	6.298	0.732	12.762
C	5.115	0.157	13.257
H	5.199	-0.613	14.027
C	3.861	0.542	12.787
H	2.958	0.075	13.184
C	3.771	1.527	11.803
H	2.798	1.851	11.428
C	4.924	2.124	11.277
C	7.592	0.262	13.349
C	7.926	0.627	14.680
C	9.101	0.125	15.246
H	9.363	0.424	16.265
C	9.961	-0.725	14.539
C	9.605	-1.085	13.235
H	10.256	-1.757	12.669
C	8.425	-0.626	12.631
C	7.082	1.607	15.453
H	7.515	1.798	16.444
H	6.048	1.258	15.586
H	7.028	2.570	14.915
C	11.231	-1.230	15.175
H	11.740	-1.960	14.531
H	11.026	-1.714	16.142
H	11.934	-0.405	15.366
C	8.065	-1.071	11.240
H	8.730	-1.877	10.899
H	8.150	-0.233	10.528
H	7.026	-1.428	11.190
C	4.793	3.174	10.224
C	4.789	4.537	10.588
C	4.647	5.504	9.585
H	4.641	6.561	9.869
C	4.513	5.157	8.236
C	4.518	3.798	7.901
H	4.415	3.505	6.851
C	4.657	2.798	8.870
C	4.967	4.951	12.024

H	4.797	6.029	12.148
H	5.991	4.731	12.368
H	4.281	4.412	12.694
C	4.400	6.216	7.168
H	4.053	7.172	7.585
H	3.700	5.915	6.375
H	5.376	6.399	6.690
C	4.690	1.345	8.470
H	5.636	0.873	8.779
H	4.593	1.233	7.381
H	3.881	0.771	8.948

Silylene_sulphur(III)_3membered_ts (TS A)

C	8.328	0.324	14.571
C	7.011	0.726	14.257
C	6.131	1.128	15.290
C	6.606	1.173	16.605
C	7.916	0.803	16.936
C	8.754	0.370	15.904
C	6.524	0.651	12.845
C	6.264	1.789	12.048
C	5.723	1.654	10.751
C	5.488	0.368	10.243
C	5.774	-0.764	11.004
C	6.280	-0.616	12.295
C	5.367	2.845	9.920
C	6.325	3.421	9.062
C	5.958	4.525	8.284
C	4.671	5.072	8.336
C	3.736	4.478	9.192
C	4.061	3.373	9.988
C	7.731	2.891	9.006
C	3.034	2.776	10.918
S	6.451	3.486	12.666
Si	8.516	3.571	13.307
S	9.569	4.995	12.003
C	11.331	4.805	12.362
C	11.868	5.000	13.657
C	13.263	5.031	13.810
C	14.117	4.867	12.720
C	13.577	4.646	11.455
C	12.188	4.605	11.256
C	11.020	5.129	14.880
C	10.369	6.341	15.194
C	9.568	6.404	16.344
C	9.406	5.308	17.197
C	10.098	4.129	16.891
C	10.912	4.021	15.756
C	11.682	4.321	9.880
C	11.513	5.367	8.951
C	11.123	5.053	7.642
C	10.908	3.733	7.231
C	11.077	2.712	8.175
C	11.449	2.983	9.496
C	10.515	7.551	14.309
C	11.594	2.715	15.446
C	11.732	6.801	9.360
C	11.575	1.865	10.499
C	4.701	1.500	14.998
C	9.289	-0.115	13.495
C	8.393	0.848	18.365
C	4.313	6.288	7.519
C	8.487	5.370	18.390
C	10.455	3.418	5.828
H	13.671	5.191	14.810
H	15.199	4.905	12.859
H	14.230	4.490	10.593
H	9.053	7.341	16.574
H	9.993	3.259	17.545
H	10.121	8.450	14.801
H	9.965	7.405	13.365
H	11.567	7.729	14.044
H	11.418	1.985	16.246
H	12.678	2.835	15.312
H	11.200	2.293	14.506
H	10.990	5.866	6.922
H	10.898	1.674	7.879
H	11.569	7.483	8.514
H	12.751	6.964	9.742
H	11.042	7.092	10.168
H	11.358	0.892	10.038
H	10.871	2.012	11.334
H	12.581	1.824	10.943
H	6.476	-1.496	12.912
H	5.586	-1.760	10.600
H	5.076	0.271	9.236
H	5.924	1.495	17.398
H	9.779	0.067	16.140
H	4.108	1.534	15.922
H	4.230	0.784	14.308
H	4.646	2.491	14.519
H	10.309	-0.205	13.893
H	9.309	0.605	12.662
H	9.006	-1.086	13.061
H	2.723	4.888	9.246
H	6.705	4.971	7.621
H	2.069	3.291	10.821
H	3.356	2.855	11.969
H	2.876	1.705	10.719
H	8.276	3.120	9.936
H	8.298	3.351	8.187
H	7.758	1.798	8.878
H	7.964	4.729	14.384
H	8.643	3.819	14.820
H	4.851	6.300	6.560
H	3.234	6.329	7.308
H	4.578	7.214	8.054
H	9.484	0.730	18.430
H	8.123	1.799	18.849
H	7.938	0.042	18.963
H	10.904	2.484	5.460
H	9.360	3.289	5.787
H	10.717	4.224	5.129
H	8.918	4.851	19.258
H	8.273	6.408	18.681
H	7.523	4.884	18.164

Silylene_sulphur(III)_H_2_rct

C	5.415	1.710	8.436
C	5.370	2.494	9.609
C	5.502	3.895	9.534
C	5.674	4.491	8.278
C	5.722	3.737	7.101
C	5.590	2.346	7.203
C	5.166	1.839	10.935
C	6.256	1.489	11.764
C	6.038	0.885	13.023
C	4.716	0.630	13.421
C	3.634	0.960	12.608
C	3.863	1.565	11.373
S	7.899	1.737	11.049
Si	9.037	2.810	12.558
S	10.357	3.848	11.176
C	11.910	4.067	12.075
C	11.992	4.705	13.334
C	13.263	4.938	13.884
C	14.425	4.552	13.217
C	14.329	3.911	11.983
C	13.080	3.659	11.397
C	10.788	5.120	14.113
C	10.040	6.257	13.734
C	8.919	6.613	14.493
C	8.529	5.895	15.629
C	9.314	4.803	16.014
C	10.442	4.406	15.286
C	13.019	2.963	10.076
C	13.149	3.706	8.884
C	13.102	3.033	7.658
C	12.932	1.645	7.584
C	12.801	0.931	8.781
C	12.841	1.565	10.028
C	10.437	7.093	12.546
C	7.302	6.281	16.414
C	11.268	3.242	15.775
C	13.300	5.206	8.926
C	12.914	0.938	6.252
C	12.653	0.768	11.293
C	7.144	0.521	13.958
C	7.322	1.265	15.149
C	8.350	0.904	16.028
C	9.198	-0.178	15.774
C	8.982	-0.920	14.607
C	7.962	-0.604	13.701
C	6.426	2.429	15.495
C	10.283	-0.562	16.747
C	7.744	-1.467	12.486
C	5.497	4.738	10.783
C	5.928	4.394	5.760
C	5.307	0.207	8.512
H	13.326	5.441	14.851
H	15.403	4.750	13.660
H	15.228	3.589	11.453
H	8.337	7.490	14.192
H	9.046	4.240	16.913
H	9.871	8.033	12.522
H	10.245	6.552	11.606
H	11.511	7.332	12.566
H	6.891	7.240	16.071
H	7.523	6.369	17.488
H	6.510	5.522	16.308
H	10.721	2.678	16.541
H	12.217	3.582	16.216
H	11.526	2.550	14.961
H	13.192	3.611	6.734
H	12.656	-0.151	8.743
H	13.378	5.622	7.912
H	14.194	5.510	9.492
H	12.438	5.678	9.423
H	12.390	-0.024	6.315
H	13.938	0.734	5.898
H	12.419	1.547	5.481
H	12.633	-0.309	11.082

H	11.703	1.033	11.786
H	13.453	0.965	12.022
H	4.549	0.152	14.389
H	2.615	0.744	12.935
H	3.027	1.841	10.726
H	8.490	1.492	16.940
H	9.620	-1.784	14.399
H	6.841	3.000	16.335
H	5.418	2.090	15.781
H	6.298	3.115	14.644
H	11.108	-1.086	16.244
H	9.893	-1.236	17.528
H	10.699	0.318	17.256
H	8.329	-2.394	12.554
H	8.047	-0.937	11.570
H	6.683	-1.732	12.369
H	5.778	5.579	8.220
H	5.630	1.736	6.295
H	5.514	5.808	10.538
H	6.381	4.519	11.405
H	4.614	4.537	11.408
H	5.893	5.489	5.840
H	5.160	4.081	5.036
H	6.907	4.122	5.332
H	6.118	-0.217	9.126
H	5.367	-0.242	7.512
H	4.362	-0.111	8.976
H	9.879	1.949	13.445
H	8.095	3.694	13.312

Silylene_sulphur(III)_4m_ts (TS B)

C	11.237	4.502	15.807
C	11.353	5.546	14.864
C	10.844	6.830	15.158
C	10.198	7.039	16.381
C	10.054	6.014	17.325
C	10.585	4.758	17.020
C	12.032	5.286	13.560
C	11.308	5.038	12.373
C	11.970	4.774	11.155
C	13.373	4.767	11.145
C	14.103	5.013	12.307
C	13.434	5.268	13.504
C	11.232	4.507	9.884
C	11.053	3.177	9.446
C	10.398	2.949	8.230
C	9.919	3.998	7.438
C	10.103	5.308	7.897
C	10.756	5.583	9.104
C	11.545	2.014	10.271
C	10.930	7.009	9.562
C	9.257	3.731	6.111
S	9.506	5.155	12.353
Si	8.822	2.902	13.028
S	6.763	3.433	12.359
C	5.948	1.827	12.405
C	6.044	0.929	13.492
C	5.293	-0.257	13.449
C	4.463	-0.556	12.370
C	4.379	0.337	11.302
C	5.117	1.528	11.300
C	6.891	1.169	14.702
C	8.051	0.381	14.914
C	8.771	0.537	16.104
C	8.367	1.431	17.102
C	7.222	2.202	16.873
C	6.469	2.082	15.698
C	5.020	2.456	10.134
C	5.963	2.367	9.090
C	5.858	3.249	8.009
C	4.847	4.214	7.936
C	3.924	4.282	8.985
C	3.990	3.418	10.084
C	8.516	-0.621	13.887
C	9.116	1.521	18.408
C	5.225	2.910	15.515
C	7.098	1.380	9.158
C	4.745	5.139	6.750
C	2.998	3.541	11.214
C	10.967	7.956	14.163
C	9.365	6.267	18.643
C	11.775	3.124	15.517
H	13.994	5.463	14.420
H	15.195	5.012	12.280
H	13.886	4.568	10.201
H	9.793	8.031	16.601
H	10.480	3.943	17.741
H	10.678	8.914	14.614
H	10.315	7.780	13.292
H	11.994	8.046	13.779
H	8.501	6.937	18.523
H	10.049	6.742	19.364
H	9.010	5.330	19.095
H	11.525	2.428	16.328
H	12.869	3.132	15.392
H	11.357	2.713	14.584
H	9.731	6.143	7.297
H	10.257	1.918	7.894
H	10.659	7.715	8.766
H	11.966	7.214	9.870
H	10.290	7.226	10.433
H	8.845	2.713	6.063
H	9.976	3.833	5.282
H	8.439	4.441	5.919
H	11.263	1.059	9.807
H	11.121	2.036	11.287
H	12.640	2.029	10.384
H	5.363	-0.945	14.294
H	3.882	-1.480	12.363
H	3.742	0.116	10.443
H	6.893	2.909	17.639
H	9.672	-0.064	16.256
H	4.947	3.417	16.448
H	4.377	2.291	15.186
H	5.382	3.675	14.737
H	10.203	1.442	18.259
H	8.823	0.700	19.084
H	8.907	2.465	18.930
H	9.547	-0.938	14.092
H	8.479	-0.204	12.870
H	7.879	-1.520	13.885
H	3.132	5.037	8.954
H	6.597	3.186	7.205
H	2.284	4.353	11.024
H	3.509	3.750	12.168
H	2.429	2.610	11.360
H	4.284	6.098	7.026
H	4.129	4.695	5.951
H	5.736	5.349	6.319
H	7.837	1.697	9.913
H	7.618	1.310	8.194
H	6.752	0.377	9.446
H	9.116	4.600	13.853
H	8.775	3.756	14.464

Silylene_S_SiH_fragment

Si	16.917	4.483	11.249
S	17.139	3.983	9.175
C	18.596	4.916	8.632
C	19.890	4.622	9.118
C	20.975	5.332	8.580
C	20.793	6.303	7.596
C	19.508	6.581	7.129
C	18.397	5.893	7.635
C	20.150	3.592	10.169
C	20.448	3.997	11.490
C	20.679	3.015	12.462
C	20.649	1.649	12.159
C	20.382	1.275	10.836
C	20.135	2.220	9.833
C	17.030	6.211	7.124
C	16.253	7.196	7.770
C	14.978	7.486	7.271
C	14.456	6.830	6.149
C	15.246	5.855	5.528
C	16.526	5.533	5.993
C	20.518	5.457	11.865
C	20.933	0.613	13.216
C	19.850	1.767	8.425
C	16.772	7.903	8.994
C	13.094	7.185	5.608
C	17.336	4.455	5.318
H	21.978	5.103	8.947
H	21.653	6.840	7.191
H	19.348	7.341	6.361
H	20.364	0.213	10.575
H	20.888	3.330	13.489
H	20.096	0.704	8.296
H	20.423	2.349	7.688
H	18.784	1.898	8.178
H	20.662	0.976	14.218
H	22.004	0.355	13.238
H	20.377	-0.316	13.027
H	20.586	5.577	12.955
H	19.631	6.006	11.516
H	21.396	5.946	11.415
H	14.852	5.324	4.656
H	14.374	8.246	7.775
H	16.812	4.061	4.437
H	17.527	3.615	6.005
H	18.320	4.828	4.996
H	12.632	6.333	5.091
H	13.162	8.012	4.882
H	12.415	7.509	6.409
H	16.906	7.198	9.833
H	16.079	8.689	9.322
H	17.757	8.361	8.815
H	15.723	3.498	11.293

Silylene_S_SH_fragment

C	12.554	2.536	10.573
C	11.983	3.812	10.369

C	11.405	4.143	9.123
C	11.400	3.184	8.103
C	11.950	1.908	8.285
C	12.526	1.607	9.524
C	11.985	4.811	11.477
C	13.045	5.728	11.653
C	13.024	6.659	12.713
C	11.933	6.662	13.591
C	10.878	5.763	13.430
C	10.911	4.847	12.378
C	14.147	7.624	12.902
C	15.255	7.265	13.698
C	16.294	8.189	13.868
C	16.263	9.454	13.270
C	15.157	9.783	12.476
C	14.097	8.891	12.279
C	15.330	5.902	14.339
C	12.930	9.268	11.402
C	17.378	10.446	13.490
S	14.465	5.773	10.562
C	10.821	5.513	8.893
C	11.901	0.884	7.180
C	13.201	2.188	11.889
H	10.093	4.137	12.240
H	10.033	5.776	14.121
H	11.925	7.385	14.409
H	10.954	3.443	7.138
H	12.970	0.620	9.681
H	10.428	5.609	7.871
H	11.580	6.297	9.045
H	10.005	5.727	9.599
H	12.103	1.339	6.200
H	10.906	0.414	7.122
H	12.635	0.082	7.343
H	13.593	1.163	11.878
H	12.490	2.279	12.724
H	14.035	2.873	12.112
H	15.119	10.763	11.990
H	17.154	7.908	14.483
H	13.054	10.280	10.994
H	11.980	9.233	11.956
H	12.831	8.567	10.558
H	18.296	9.950	13.834
H	17.099	11.191	14.254
H	17.612	10.999	12.568
H	16.253	5.791	14.924
H	15.310	5.108	13.576
H	14.474	5.721	15.006
H	14.021	4.749	9.775

Silylene_sulphur(III)_NH_3BH_3_5membered_ts (TS C)

C	6.504	-1.907	12.693
C	6.005	-0.688	13.205
C	5.974	-0.468	14.596
C	6.485	-1.451	15.454
C	7.005	-2.654	14.970
C	6.992	-2.867	13.585
C	5.469	0.347	12.272
C	6.320	1.236	11.570
C	5.778	2.183	10.671
C	4.382	2.241	10.518
C	3.536	1.379	11.212
C	4.083	0.434	12.079
C	6.597	3.114	9.837
C	7.296	2.633	8.705
C	7.955	3.550	7.876
C	7.921	4.927	8.112
C	7.210	5.382	9.229
C	6.553	4.506	10.098
C	7.344	1.167	8.369
C	5.793	5.066	11.276
C	8.625	5.898	7.198
S	8.099	0.997	11.765
Si	8.908	2.959	12.354
S	10.503	2.799	10.866
C	11.944	3.860	11.114
C	12.051	4.970	11.979
C	13.270	5.669	12.025
C	14.356	5.303	11.233
C	14.228	4.223	10.360
C	13.036	3.495	10.286
C	10.938	5.508	12.814
C	9.979	6.359	12.214
C	9.012	6.967	13.021
C	8.990	6.784	14.411
C	9.964	5.960	14.985
C	10.943	5.318	14.212
C	12.930	2.360	9.318
C	12.438	2.596	8.017
C	12.353	1.524	7.122
C	12.742	0.228	7.481
C	13.220	0.019	8.780
C	13.322	1.062	9.708
C	10.030	6.632	10.735
C	7.950	7.475	15.260
C	11.995	4.463	14.869
C	11.966	3.969	7.612
C	12.673	-0.905	6.490
C	13.793	0.795	11.113
C	5.388	0.792	15.185
C	7.591	-3.682	15.905
C	6.523	-2.175	11.209
H	13.343	6.529	12.694
H	15.290	5.866	11.286
H	15.059	3.927	9.716
H	8.271	7.621	12.554
H	9.970	5.808	16.069
H	9.282	7.382	10.446
H	9.831	5.715	10.159
H	11.024	6.994	10.435
H	8.097	8.566	15.257
H	7.994	7.139	16.305
H	6.932	7.288	14.882
H	11.765	4.302	15.930
H	12.989	4.929	14.796
H	12.070	3.479	14.384
H	11.966	1.706	6.115
H	13.515	-0.988	9.087
H	11.677	3.990	6.552
H	12.740	4.733	7.776
H	11.089	4.268	8.208
H	12.454	-1.861	6.987
H	13.632	-1.025	5.959
H	11.898	-0.728	5.731
H	14.099	-0.252	11.236
H	12.989	1.003	11.837
H	14.643	1.438	11.388
H	3.438	-0.257	12.625
H	2.456	1.433	11.067
H	3.968	2.969	9.817
H	6.479	-1.266	16.532
H	7.378	-3.810	13.185
H	5.957	1.109	16.071
H	4.343	0.635	15.498
H	5.376	1.609	14.451
H	7.401	-4.705	15.548
H	7.175	-3.589	16.918
H	8.683	-3.562	15.985
H	6.764	-3.226	11.003
H	7.279	-1.552	10.703
H	5.554	-1.942	10.742
H	7.166	6.456	9.434
H	8.503	3.170	7.008
H	6.175	6.061	11.544
H	5.880	4.418	12.159
H	4.718	5.165	11.056
H	9.430	6.432	7.727
H	7.930	6.659	6.812
H	9.076	5.383	6.339
H	8.088	0.654	9.000
H	7.627	1.015	7.319
H	6.377	0.675	8.546
H	9.543	2.543	13.866
H	7.852	3.779	13.391
N	7.668	3.564	14.806
B	8.802	2.586	15.082
H	9.693	3.004	15.779
H	8.461	1.435	15.180
H	7.771	4.503	15.195
H	6.721	3.213	14.941

Silylene_sulphur(III)_NH_3BH_3_6membered_ts (TS D)

C	-1.225	4.741	0.352
C	0.091	4.331	0.655
C	0.585	4.434	1.974
C	-0.251	4.946	2.972
C	-1.561	5.362	2.699
C	-2.030	5.245	1.384
C	0.997	3.891	-0.443
C	0.970	2.608	-1.031
C	1.792	2.304	-2.140
C	2.672	3.287	-2.616
C	2.737	4.546	-2.024
C	1.894	4.842	-0.955
C	1.720	1.003	-2.872
C	0.697	0.811	-3.827
C	0.659	-0.387	-4.548
C	1.605	-1.398	-4.350
C	2.637	-1.163	-3.434
C	2.720	0.021	-2.694
C	-0.348	1.870	-4.070
C	3.845	0.215	-1.710
C	1.494	-2.718	-5.068
S	-0.142	1.293	-0.472
Si	1.107	-0.322	1.013
S	-0.732	-1.479	1.454
C	-0.725	-2.933	0.385
C	0.289	-3.914	0.458
C	0.178	-5.056	-0.350
C	-0.914	-5.243	-1.196
C	-1.929	-4.288	-1.230

C	-1.854	-3.130	-0.444
C	1.450	-3.808	1.392
C	1.274	-4.063	2.771
C	2.381	-3.977	3.623
C	3.658	-3.652	3.152
C	3.815	-3.436	1.778
C	2.737	-3.516	0.889
C	-2.967	-2.134	-0.484
C	-3.957	-2.135	0.519
C	-4.966	-1.164	0.476
C	-5.021	-0.196	-0.532
C	-4.037	-0.227	-1.527
C	-3.018	-1.188	-1.528
C	-0.078	-4.414	3.333
C	4.823	-3.512	4.099
C	2.957	-3.275	-0.581
C	-3.921	-3.139	1.642
C	-6.132	0.822	-0.573
C	-1.981	-1.191	-2.617
C	1.977	3.968	2.315
C	-2.432	5.924	3.793
C	-1.770	4.633	-1.048
B	-0.674	1.287	3.234
N	-1.633	1.863	2.329
H	1.908	5.834	-0.499
H	3.424	5.302	-2.409
H	3.300	3.045	-3.476
H	-3.051	5.561	1.150
H	0.125	5.002	3.996
H	-2.740	5.141	-1.134
H	-1.915	3.579	-1.340
H	-1.081	5.072	-1.785
H	-3.493	5.922	3.505
H	-2.152	6.965	4.022
H	-2.328	5.347	4.723
H	2.161	4.039	3.394
H	2.743	4.559	1.792
H	2.126	2.919	2.016
H	-0.138	-0.538	-5.280
H	3.404	-1.929	-3.287
H	-0.954	1.628	-4.953
H	0.103	2.862	-4.222
H	-1.028	1.960	-3.207
H	0.948	-3.448	-4.447
H	2.483	-3.147	-5.282
H	0.947	-2.619	-6.016
H	4.625	-0.543	-1.853
H	3.471	0.122	-0.675
H	4.306	1.209	-1.799
H	0.962	-5.815	-0.288
H	-0.986	-6.145	-1.807
H	-2.804	-4.433	-1.869
H	2.239	-4.173	4.690
H	4.806	-3.192	1.384
H	0.011	-4.821	4.350
H	-0.602	-5.150	2.707
H	-0.718	-3.518	3.381
H	5.773	-3.771	3.610
H	4.704	-4.156	4.982
H	4.913	-2.475	4.461
H	3.980	-2.921	-0.769
H	2.259	-2.518	-0.970
H	2.798	-4.188	-1.175
H	-5.731	-1.165	1.259
H	-4.061	0.515	-2.330
H	-4.865	-3.138	2.203
H	-3.108	-2.906	2.348
H	-3.737	-4.158	1.270
H	-6.519	1.037	0.433
H	-6.979	0.460	-1.178
H	-5.793	1.768	-1.020
H	-0.962	-1.113	-2.210
H	-2.133	-0.351	-3.306
H	-2.009	-2.123	-3.204
H	-0.757	1.887	0.657
H	0.678	0.629	2.208
H	-1.762	2.873	2.277
H	-2.461	1.339	2.053
H	-0.873	0.185	3.669
H	0.118	2.031	3.755

Silylene_sulphur(III)_dimer

C	6.392	2.789	8.453
C	5.644	3.335	9.517
C	4.965	4.561	9.355
C	5.029	5.212	8.117
C	5.757	4.687	7.043
C	6.434	3.476	7.233
C	5.561	2.627	10.830
C	4.582	1.635	11.070
C	4.474	1.030	12.343
C	5.370	1.421	13.351
C	6.356	2.378	13.117
C	6.443	2.978	11.861
C	3.461	-0.019	12.683
C	3.667	-1.362	12.274
C	2.759	-2.343	12.692
C	1.673	-2.046	13.524
C	1.514	-0.724	13.960
C	2.391	0.293	13.572
C	4.842	-1.734	11.410
C	2.176	1.699	14.062
C	0.686	-3.113	13.922
S	3.574	1.143	9.654
C	4.160	5.149	10.486
C	5.838	5.422	5.728
C	7.115	1.476	8.615
Si	0.404	2.571	10.284
S	-1.317	2.683	11.645
C	-1.776	4.421	11.506
C	-2.127	5.065	12.715
C	-2.572	6.393	12.677
C	-2.656	7.087	11.470
C	-2.281	6.453	10.286
C	-1.839	5.120	10.276
C	-1.997	4.362	14.026
C	-3.100	3.685	14.584
C	-2.942	3.031	15.813
C	-1.724	3.036	16.501
C	-0.643	3.715	15.925
C	-0.756	4.380	14.699
C	-1.444	4.504	8.973
C	-2.298	3.566	8.340
C	-1.904	3.007	7.121
C	-0.701	3.358	6.494
C	0.105	4.319	7.110
C	-0.248	4.913	8.329
C	-4.418	3.632	13.852
C	-1.582	2.351	17.837
C	0.436	5.069	14.088
C	-3.606	3.164	8.966
C	-0.302	2.738	5.180
C	0.647	5.975	8.916
H	-2.841	6.880	13.617
H	-3.005	8.121	11.452
H	-2.334	6.988	9.336
H	-3.797	2.497	16.240
H	0.320	3.726	16.444
H	-5.165	3.066	14.425
H	-4.305	3.149	12.868
H	-4.819	4.639	13.664
H	-2.333	1.559	17.965
H	-1.715	3.066	18.665
H	-0.585	1.900	17.954
H	1.307	5.019	14.756
H	0.227	6.126	13.869
H	0.713	4.596	13.132
H	-2.557	2.271	6.645
H	1.050	4.606	6.642
H	-4.223	2.597	8.256
H	-4.177	4.042	9.304
H	-3.433	2.534	9.853
H	0.789	2.725	5.060
H	-0.721	3.305	4.333
H	-0.669	1.705	5.096
H	1.670	5.872	8.530
H	0.683	5.926	10.012
H	0.287	6.983	8.651
H	7.198	3.743	11.663
H	7.050	2.657	13.911
H	5.289	0.945	14.331
H	4.496	6.159	7.990
H	7.007	3.048	6.405
H	3.719	6.113	10.199
H	4.776	5.305	11.384
H	3.340	4.473	10.780
H	5.952	4.726	4.885
H	6.705	6.103	5.708
H	4.940	6.031	5.552
H	7.714	1.242	7.725
H	6.403	0.650	8.773
H	7.784	1.489	9.489
H	0.676	-0.471	14.616
H	2.914	-3.375	12.365
H	1.186	1.809	14.523
H	2.246	2.417	13.230
H	2.939	1.990	14.801
H	0.303	-2.946	14.939
H	1.137	-4.114	13.881
H	-0.181	-3.113	13.243
H	4.743	-1.290	10.406
H	4.921	-2.823	11.301
H	5.784	-1.354	11.833
Si	1.672	0.732	10.647
H	1.168	-0.580	10.100
H	1.258	3.752	10.706

Silylene_sulphur(III)_sih3_silane

C	4.640	2.774	9.045
C	4.875	3.117	10.393
C	4.739	4.454	10.822
C	4.378	5.431	9.887
C	4.150	5.118	8.541

C	4.281	3.782	8.143
C	5.305	2.067	11.366
C	4.372	1.287	12.089
C	4.819	0.327	13.024
C	6.202	0.148	13.194
C	7.129	0.903	12.479
C	6.675	1.862	11.575
S	2.641	1.706	11.781
Si	1.463	-0.124	11.811
C	3.902	-0.501	13.859
C	3.251	0.070	14.976
C	2.440	-0.742	15.777
C	2.262	-2.106	15.513
C	2.937	-2.656	14.417
C	3.762	-1.883	13.590
C	3.423	1.528	15.314
C	1.357	-2.953	16.371
C	4.485	-2.535	12.437
C	4.956	4.824	12.268
C	3.802	6.196	7.545
C	4.740	1.341	8.591
H	6.541	-0.593	13.921
H	8.199	0.752	12.634
H	7.384	2.469	11.007
H	1.938	-0.296	16.641
H	2.821	-3.722	14.198
H	2.996	1.757	16.300
H	2.921	2.164	14.568
H	4.484	1.817	15.318
H	1.218	-2.510	17.367
H	1.760	-3.968	16.500
H	0.360	-3.054	15.913
H	4.035	-3.506	12.193
H	5.546	-2.708	12.676
H	4.465	-1.906	11.536
H	4.267	6.467	10.221
H	4.094	3.515	7.099
H	4.793	5.898	12.429
H	5.975	4.577	12.602
H	4.267	4.272	12.927
H	3.256	5.787	6.684
H	4.712	6.682	7.155
H	3.184	6.982	8.001
H	4.573	1.254	7.509
H	3.989	0.719	9.105
H	5.724	0.908	8.826
H	2.155	-1.211	11.045
H	1.027	-0.600	13.161
H	0.253	0.325	11.042

Silylene_sulphur(III) (silane_TS1)

C	0.163	2.039	15.072
C	1.107	0.987	15.070
C	0.674	-0.351	15.204
C	-0.698	-0.615	15.289
C	-1.653	0.407	15.271
C	-1.198	1.727	15.168
C	2.569	1.286	14.983
C	3.212	1.650	13.777
C	4.594	1.933	13.752
C	5.327	1.842	14.946
C	4.707	1.479	16.141
C	3.340	1.203	16.153
C	5.300	2.320	12.495
C	5.418	3.680	12.144
C	6.111	4.019	10.975
C	6.685	3.048	10.147
C	6.556	1.704	10.520
C	5.874	1.322	11.680
C	4.790	4.753	12.998
C	5.739	-0.134	12.042
C	7.394	3.433	8.873
S	2.272	1.920	12.248
Si	1.606	-0.077	11.734
C	1.660	-1.490	15.235
C	-3.123	0.101	15.401
C	0.599	3.477	14.969
H	2.843	0.928	17.085
H	5.287	1.416	17.064
H	6.397	2.059	14.919
H	-1.925	2.544	15.164
H	-1.029	-1.654	15.375
H	-0.224	4.158	15.221
H	0.931	3.708	13.943
H	1.446	3.691	15.637
H	-3.442	0.139	16.455
H	-3.360	-0.903	15.025
H	-3.736	0.828	14.849
H	1.142	-2.458	15.218
H	2.292	-1.458	16.136
H	2.339	-1.451	14.368
H	6.201	5.075	10.702
H	7.001	0.929	9.889
H	5.015	5.753	12.604
H	5.142	4.703	14.039
H	3.694	4.641	13.031
H	6.708	3.390	8.011
H	8.231	2.754	8.657
H	7.789	4.457	8.926
H	6.253	-0.774	11.312
H	4.679	-0.439	12.075
H	6.153	-0.346	13.040
H	1.618	-0.241	10.241
H	0.186	-0.388	12.247
H	0.055	0.448	11.405

Silylene_sulphur(III) (silane_TS2)

C	0.620	8.349	12.098
C	1.756	8.826	12.789
C	2.773	9.515	12.085
C	2.653	9.672	10.702
C	1.546	9.187	9.991
C	0.538	8.543	10.710
C	1.846	8.673	14.273
C	2.711	7.744	14.898
C	2.741	7.630	16.306
C	1.920	8.467	17.075
C	1.072	9.395	16.471
C	1.034	9.486	15.080
S	3.857	6.737	13.938
Si	2.518	5.557	12.594
C	3.608	6.628	16.996
C	4.960	6.920	17.270
C	5.738	5.964	17.934
C	5.210	4.731	18.337
C	3.861	4.473	18.070
C	3.049	5.399	17.405
C	5.568	8.231	16.839
C	6.078	3.696	19.007
C	1.607	5.073	17.107
C	3.969	10.080	12.805
C	1.463	9.345	8.494
C	-0.523	7.667	12.811
C	-1.325	4.268	14.418
C	-1.718	2.815	14.438
C	-2.087	2.148	13.250
C	-2.504	0.801	13.295
C	-2.525	0.139	14.529
C	-2.127	0.768	15.715
C	-1.728	2.107	15.646
C	-2.113	2.892	11.953
C	-1.105	2.753	10.972
C	-1.206	3.423	9.725
C	-2.308	4.265	9.509
C	-3.292	4.434	10.482
C	-3.198	3.742	11.689
S	0.273	1.620	11.268
Si	1.900	3.051	11.658
S	3.397	2.409	10.200
C	4.928	2.565	11.148
C	5.992	3.287	10.567
C	7.194	3.404	11.280
C	7.344	2.817	12.536
C	6.296	2.078	13.084
C	5.079	1.926	12.404
C	5.891	3.877	9.196
C	6.165	3.057	8.080
C	6.102	3.612	6.796
C	5.763	4.953	6.586
C	5.502	5.747	7.708
C	5.568	5.238	9.011
C	6.504	1.598	8.253
C	5.254	6.134	10.179
C	5.651	5.516	5.192
C	3.999	1.083	12.999
C	3.713	-0.183	12.429
C	2.693	-0.961	12.981
C	1.942	-0.535	14.084
C	2.270	0.691	14.663
C	3.301	1.501	14.162
C	4.489	-0.709	11.251
C	0.806	-1.368	14.614
C	3.664	2.748	14.924
C	-0.211	3.235	8.624
C	-0.186	2.016	7.905
C	0.763	1.843	6.893
C	1.692	2.838	6.566
C	1.620	4.051	7.255
C	0.671	4.278	8.261
C	-2.916	0.070	12.042
C	-2.100	0.017	17.022
C	-1.159	0.904	8.203
C	2.749	2.605	5.518
C	0.612	5.645	8.894
H	-3.978	3.846	12.447
H	-4.145	5.089	10.291
H	-2.387	4.781	8.550
H	-2.860	-0.901	14.563
H	-1.428	2.625	16.562
H	-3.403	-0.883	12.286
H	-2.039	-0.151	11.412
H	-3.604	0.668	11.429
H	-2.806	-0.824	17.018

H	-2.349	0.672	17.869
H	-1.097	-0.398	17.215
H	-0.935	4.586	15.394
H	-2.179	4.916	14.167
H	-0.552	4.464	13.662
H	0.777	0.898	6.344
H	2.333	4.846	7.016
H	-1.219	0.203	7.360
H	-2.169	1.287	8.410
H	-0.842	0.333	9.091
H	2.821	3.456	4.823
H	2.541	1.701	4.929
H	3.739	2.490	5.986
H	1.617	6.073	9.008
H	0.139	5.633	9.883
H	0.030	6.338	8.264
H	8.017	3.964	10.830
H	8.283	2.923	13.083
H	6.415	1.593	14.055
H	5.249	6.803	7.569
H	6.329	2.976	5.935
H	5.254	7.193	9.886
H	5.961	6.002	11.010
H	4.251	5.908	10.581
H	4.611	5.461	4.828
H	6.274	4.958	4.480
H	5.951	6.573	5.158
H	6.824	1.152	7.302
H	5.631	1.030	8.615
H	7.304	1.449	8.993
H	1.710	1.038	15.537
H	2.477	-1.937	12.536
H	2.764	3.273	15.266
H	4.266	3.454	14.341
H	4.249	2.495	15.823
H	0.757	-1.329	15.712
H	0.901	-2.420	14.310
H	-0.155	-0.989	14.235
H	4.136	-0.244	10.316
H	4.363	-1.796	11.155
H	5.563	-0.487	11.337
H	1.511	4.612	11.330
H	3.327	4.231	12.444
H	1.403	5.138	13.536
H	1.957	8.377	18.164
H	0.442	10.045	17.081
H	0.373	10.206	14.594
H	6.787	6.191	18.143
H	3.427	3.518	18.382
H	0.918	5.765	17.615
H	1.399	5.159	16.029
H	1.359	4.050	17.423
H	6.582	8.349	17.246
H	5.635	8.289	15.741
H	4.960	9.087	17.167
H	5.502	3.083	19.714
H	6.518	3.011	18.263
H	6.911	4.161	19.554
H	3.444	10.201	10.162
H	-0.341	8.169	10.180
H	4.542	10.751	12.150
H	3.672	10.639	13.704
H	4.639	9.270	13.136
H	-1.269	8.402	13.153
H	-1.038	6.962	12.142
H	-0.187	7.116	13.698
H	1.737	10.364	8.181
H	2.153	8.652	7.986
H	0.451	9.133	8.123

III_ring_TS

C	10.027	4.433	7.083
C	8.996	3.678	7.683
C	7.750	4.280	7.960
C	7.562	5.631	7.639
C	8.568	6.397	7.041
C	9.792	5.777	6.771
C	9.207	2.227	7.972
C	9.869	1.760	9.123
C	10.050	0.381	9.364
C	9.553	-0.535	8.430
C	8.903	-0.091	7.275
C	8.731	1.273	7.053
S	10.628	2.913	10.299
Si	9.076	3.031	11.804
C	8.582	0.487	11.816
C	9.941	-0.006	11.827
C	10.705	-0.067	10.628
C	12.038	-0.510	10.655
C	12.605	-0.884	11.882
C	11.881	-0.817	13.084
C	10.561	-0.374	13.045
C	12.510	-1.235	14.390
C	12.868	-0.529	9.395
C	6.638	3.508	8.625
C	8.332	7.841	6.677
C	11.372	3.816	6.800
S	10.035	2.887	13.726
C	9.071	4.082	14.690
C	8.991	5.448	14.337
C	8.272	6.309	15.180
C	7.664	5.840	16.345
C	7.757	4.489	16.683
C	8.454	3.592	15.861
C	9.649	5.979	13.107
C	11.047	6.184	13.096
C	11.654	6.652	11.926
C	10.919	6.916	10.763
C	9.533	6.737	10.804
C	8.879	6.284	11.959
C	11.885	5.899	14.316
C	7.373	6.167	11.956
C	11.611	7.344	9.495
C	8.524	2.138	16.198
C	9.607	1.632	16.945
C	9.683	0.253	17.177
C	8.718	-0.634	16.686
C	7.646	-0.104	15.957
C	7.528	1.267	15.708
C	10.697	2.549	17.439
C	8.829	-2.115	16.943
C	6.379	1.799	14.890
H	8.206	7.366	14.912
H	7.118	6.529	16.992
H	7.281	4.110	17.590
H	12.736	6.809	11.921
H	8.943	6.928	9.904
H	12.893	6.322	14.206
H	11.990	4.813	14.469
H	11.431	6.312	15.228
H	12.558	7.860	9.707
H	10.976	8.011	8.895
H	11.838	6.466	8.869
H	6.998	6.048	10.930
H	6.908	7.072	12.380
H	7.023	5.314	12.553
H	10.531	-0.139	17.747
H	6.885	-0.782	15.559
H	11.399	2.014	18.091
H	10.287	3.405	17.996
H	11.271	2.968	16.596
H	8.439	-2.375	17.941
H	9.876	-2.450	16.904
H	8.258	-2.694	16.204
H	5.725	0.985	14.550
H	6.740	2.345	14.003
H	5.769	2.513	15.465
H	9.680	-1.602	8.622
H	8.529	-0.813	6.547
H	8.223	1.626	6.153
H	9.979	-0.315	13.968
H	13.646	-1.219	11.901
H	7.994	0.297	10.914
H	7.840	2.203	11.582
H	8.026	0.382	12.751
H	11.959	-0.817	15.244
H	13.556	-0.900	14.458
H	12.512	-2.332	14.498
H	13.883	-0.896	9.597
H	12.948	0.481	8.965
H	12.421	-1.167	8.617
H	6.597	6.096	7.863
H	10.594	6.358	6.305
H	5.705	4.088	8.629
H	6.893	3.277	9.672
H	6.448	2.547	8.127
H	7.578	8.303	7.330
H	7.971	7.936	5.640
H	9.257	8.431	6.754
H	11.916	3.617	7.739
H	11.992	4.483	6.187
H	11.278	2.852	6.279

III_ring_pdt

C	12.885	1.732	12.585
C	13.004	2.524	11.423
C	13.453	1.948	10.216
C	13.745	0.579	10.185
C	13.605	-0.234	11.316
C	13.180	0.364	12.508
C	12.625	3.968	11.480
C	11.345	4.404	11.071
C	10.964	5.761	11.186
C	11.901	6.673	11.696
C	13.177	6.260	12.081
C	13.532	4.915	11.979
S	10.232	3.200	10.294
Si	8.902	2.708	11.928
C	9.097	0.897	12.487
C	8.727	0.012	11.331
C	7.371	-0.208	11.002
C	7.045	-0.938	9.839
C	8.082	-1.435	9.037

C	9.431	-1.236	9.356
C	9.735	-0.501	10.506
C	5.609	-1.147	9.422
C	6.297	0.304	11.905
C	6.035	1.683	12.075
C	5.031	2.127	12.963
C	4.284	1.174	13.671
C	4.535	-0.188	13.518
C	5.537	-0.614	12.648
C	10.533	-1.797	8.494
S	6.912	2.927	11.094
C	4.759	3.580	13.186
C	3.856	4.271	12.351
C	3.596	5.624	12.604
C	4.215	6.313	13.654
C	5.104	5.605	14.472
C	5.385	4.249	14.259
C	3.202	3.578	11.183
C	3.966	7.784	13.869
C	6.365	3.531	15.151
C	9.596	6.225	10.806
C	9.256	6.381	9.444
C	7.946	6.742	9.109
C	6.962	6.948	10.082
C	7.332	6.829	11.424
C	8.636	6.493	11.808
C	10.269	6.145	8.353
C	5.545	7.298	9.704
C	8.967	6.446	13.281
C	13.577	2.777	8.963
C	13.918	-1.707	11.253
C	12.427	2.334	13.891
H	11.612	7.723	11.783
H	13.894	6.988	12.466
H	14.523	4.579	12.291
H	7.684	6.850	8.052
H	6.578	6.973	12.203
H	9.930	6.579	7.403
H	10.424	5.066	8.193
H	11.248	6.578	8.605
H	5.350	7.094	8.642
H	5.336	8.366	9.882
H	4.828	6.721	10.305
H	8.093	6.116	13.861
H	9.248	7.446	13.648
H	9.806	5.775	13.503
H	14.082	0.133	9.244
H	13.065	-0.252	13.404
H	14.129	2.235	8.184
H	14.089	3.730	9.155
H	12.581	3.024	8.561
H	13.385	-2.264	12.037
H	14.996	-1.891	11.392
H	13.636	-2.135	10.280
H	12.259	1.554	14.646
H	11.495	2.908	13.772
H	13.172	3.039	14.292
H	5.752	-1.679	12.536
H	3.953	-0.919	14.083
H	3.507	1.521	14.356
H	10.779	-0.301	10.761
H	7.824	-1.982	8.125
H	10.145	0.751	12.786
H	8.454	0.737	13.367
H	9.195	3.653	13.055
H	10.201	-1.940	7.456
H	10.869	-2.778	8.870
H	11.409	-1.132	8.489
H	5.555	-1.530	8.395
H	5.040	-0.207	9.472
H	5.090	-1.866	10.075
H	5.592	6.121	15.304
H	2.888	6.155	11.961
H	6.701	4.180	15.971
H	7.257	3.218	14.585
H	5.932	2.618	15.584
H	4.102	8.066	14.922
H	2.950	8.071	13.563
H	4.669	8.392	13.274
H	3.946	3.340	10.406
H	2.431	4.214	10.727
H	2.738	2.627	11.481