Electronic Supplementary Information for Dalton Transactions

SUPPORTING INFORMATION

COMBINING THE CHEMISTRIES OF SILYLENE AND SULFUR-NITROGEN COMPOUNDS – SiS_2N_2 AND RELATED SYSTEMS

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Table S1. Calculated singlet-triplet energy gaps at CCSD(T) level with cc-pVDZ, cc-pVTZ, and cc-pVQZ basis sets and extrapolated to the infinite basis set limit using HF and KS-B3LYP reference wavefunctions. Numbers shown in read are presented in Table 1 of the manuscript. All values are given in kJ/mol. In Italics those results are presented where the CCSD(T) calculation resulted in singles or doubles excitations larger than 0.1.

silylene	wavefunction	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-V∞Z
SiH_2	HF	79.5	85.8	86.2	87.5
	KS	84.6	93.4	96.3	97.6
9a	HF	*213.9*	*224.4*	*229.4*	229.4
	KS	206.0	215.2	219.8	220.2
9b	HF	*116.0*	*128.5*	*134.4*	135.2
	KS	113.5	126.0	131.9	133.6
10	HF	258.3	276.7	280.9	283.0
	KS	257.9	276.7	280.5	282.2
11	HF	313.2	315.3	315.7	316.9
	KS	313.6	315.3	315.3	316.5
12	HF	249.1	264.6	269.6	272.1
	KS	248.7	263.3	268.4	270.9
13	HF	279.3	278.0	277.6	278.8
	KS	279.3	277.6	276.7	277.6
14	HF	*	*252.9*	*	
	KS	238.2	244.9	248.7	250.8
15	HF	*237.8*	*238.2*	*	
	KS	237.4	237.8	238.2	239.1

* the calculation could not be converged

Cartesian coordinates and optimized structures of the molecules investigated in the

paper

NH_3			
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	0	0.115411	0
H	-0.937922	-0.269068	0
H	0.468961	-0.269405	0.812227
H	0.468961	-0.269405	-0.81223
Total	**energy**	**-56.5847254**	
BH_3			
level:	**B3LYP/cc-pVTZ**		
Geometry:			
B	0	0	0
H	0	1.188096	0
H	1.028921	-0.594048	0
H	-1.028921	-0.594048	0
Total	**energy**	**-26.62421755**	
SiH_4			
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	0	0	0.000035
H	0	0	1.482256
H	0	1.39772	-0.49425
H	1.210461	-0.69886	-0.49425
H	-1.210461	-0.69886	-0.49425
Total	**energy**	**-291.9183344**	
SiH_2		**singlet**	**silylene**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	0	0	0.133139
H	0	1.093152	-0.93197
H	0	-1.093152	-0.93197
Total	**energy**	**-290.6443319**	
Si H_2		**triplet**	**silylene**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	0	0	0.094879
H	0	1.279129	-0.66416
H	0	-1.279129	-0.66416
Total	**energy**	**-290.6115901**	
SiH_2	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	0.837207	0.000037	-0.13341

H	0.849009	-1.111536	0.915696
H	0.85236	1.109879	0.917335
N	-1.234302	0.000259	-0.00046
H	-1.61462	-0.816248	-0.46655
H	-1.551369	-0.00523	0.962564
H	-1.61616	0.820804	-0.45811
Total	**energy**	**-347.2740119**	
SiH_2	**disilene**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	-1.080999	-0.000083	0.06801
Si	1.081032	-0.000083	-0.06807
H	-1.829344	-1.229487	-0.28134
H	-1.827111	1.230657	-0.28153
H	1.826903	1.230645	0.281937
H	1.829096	-1.229503	0.281741
Total	**energy**	**-581.3854988**	
9a	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	0.447221	-1.352576	-8.3E-05
S	1.487657	-0.178155	-3.2E-05
N	0.752632	1.232883	0.000206
S	-0.907759	1.168722	-8.4E-05
Si	-1.262667	-1.07223	0.000072
Total	**energy**	**-1195.49288**	
9a	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	-0.096722	-1.376053	-3.1E-05
Si	1.150665	-0.201307	-9.1E-05
B	3.129358	-0.246675	0.000085
S	-1.589962	-0.901665	0.000023
N	-1.695537	0.683902	0.000052
S	-0.248172	1.508613	-9E-06
H	3.369115	-0.861833	-1.00889
H	3.461933	0.907103	-0.00105
H	3.368813	-0.859716	1.010434
Total	**energy**	**-1222.150214**	
9a	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	-0.399227	-1.409893	-0.00008
Si	1.245705	-0.849243	0.000018
S	0.747156	1.327106	-1.2E-05
N	-0.938056	1.1537	-2E-06

S	-1.504026	-0.3161	0.000021
H	2.015604	-1.246673	-1.20339
H	2.015421	-1.246675	1.203551
Total	**energy**	**-1196.701926**	
9a	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	-2.241708	-0.36124	0.998547
Si	-1.105872	0.052217	-0.95304
S	0.358786	1.549949	0.003843
N	1.55756	0.499913	0.559148
S	1.348234	-1.020059	0.174004
N	0.024738	-1.267096	-0.61614
H	-2.091444	-1.334369	1.247261
H	-1.883597	0.223385	1.74817
H	-3.239184	-0.19932	0.910672
Total	**energy**	**-1252.08806**	
9a	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	-0.826282	1.191358	-0.12461
S	-1.538653	-0.22264	-0.02908
N	-0.252186	-1.434883	0.244577
S	1.257876	-0.888342	-0.10728
Si	0.860122	1.391457	0.095857
Total	**energy**	**-1195.421049**	
9a	**(μ-N)$_2$**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	-0.681595	-1.08292	-0.71386
S	-2.875884	-1.207762	0.214145
N	-3.276566	0.399858	0.325453
S	-2.232662	1.464928	-0.19452
N	-0.858857	0.732759	-0.59182
Si	0.681603	1.082925	0.713864
N	0.858867	-0.732757	0.591846
S	2.232667	-1.464928	0.194539
N	3.276558	-0.399862	-0.32547
S	2.875872	1.207759	-0.21418
Total	**energy**	**-2390.973584**	
9b	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	-0.539206	1.297101	-0.00019
Si	-1.754257	-0.000156	0
N	-0.538919	-1.297196	0.000191

S	1.003457	-1.065752	-0.0001
S	1.003197	1.06593	0.000101
Total	**energy**	**-1195.481129**	
9b	**+**	**BH3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	-0.114509	-1.306327	-0.00954
S	1.426188	-1.067594	0.006
S	1.43984	1.056303	0.006241
N	-0.098837	1.314227	-0.00945
Si	-1.26018	0.011594	-0.01985
B	-3.234472	0.000407	0.018951
H	-3.548753	1.125806	-0.26005
H	-3.53544	-0.846994	-0.78142
H	-3.463961	-0.317807	1.161706
Total	**energy**	**-1222.142173**	
9b	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	0.46759	-1.346543	-0.00064
Si	1.605769	-0.000019	0.000022
N	0.467983	1.346402	0.000022
S	-1.062415	1.051649	-5.1E-05
S	-1.062555	-1.051503	0.000189
H	2.484598	-0.001477	1.198498
H	2.485146	0.000392	-1.19667
Total	**energy**	**-1196.688487**	
9b	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	-0.023157	1.303161	0.527919
Si	1.010303	-0.004043	1.172621
N	-0.026094	-1.306225	0.522535
S	-1.27934	-1.060821	-0.37414
S	-1.276817	1.06427	-0.37002
N	2.635371	0.001477	-1.10606
H	3.576536	-0.053444	-0.73515
H	2.504471	-0.785509	-1.73134
H	2.570402	0.851482	-1.65455
Total	**energy**	**-1252.070312**	
9b	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	0.556809	1.325964	0.125646
Si	1.724702	-0.001481	-0.07154
N	0.554043	-1.326823	0.125173

S	-0.998572	-1.232732	-0.02345
S	-0.99654	1.234404	-0.02368
Total	**energy**	**-1195.44394**	
9b	**disilene**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	2.067737	1.393404	0.000284
S	3.681061	1.13896	0.000038
S	3.68117	-1.13887	-0.00031
N	2.067839	-1.393484	-0.00013
Si	1.141292	-0.000078	0.000453
Si	-1.141294	0.000066	-0.00014
N	-2.067839	1.393476	-0.00021
S	-3.681155	1.138939	-0.0002
S	-3.681073	-1.139021	0.000139
N	-2.067739	-1.39339	0.0002
Total	**energy:**	**-2390.944426**	
9b	**(μ-N)$_2$**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
N	0.819463	0.885498	0.293207
S	2.403013	1.427731	0.189517
S	3.280101	-0.583558	-0.29213
N	2.032141	-1.517346	-0.02301
Si	0.637827	-0.869437	0.74908
Si	-0.637831	0.869459	-0.74901
N	-0.819435	-0.885467	-0.29319
S	-2.403013	-1.427674	-0.1895
S	-3.280088	0.583457	0.292072
N	-2.032188	1.51737	0.022961
Total	**energy**	**-2390.972177**	
9c	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
S	-1.5224	-0.002131	-6.1E-05
Si	-0.003193	-1.519737	0.000103
S	1.522363	-0.00723	-0.00012
N	0.608317	1.528895	0.000269
N	-0.601846	1.531974	-6.5E-05
Total	**energy**	**-1195.500992**	
9c	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
S	0.405451	1.5564	-0.01999
Si	-1.048274	-0.000869	-0.08407
S	0.406705	-1.556475	-0.01992

N	1.90856	-0.606324	0.061165
N	1.907629	0.608118	0.061111
B	-3.038813	0.000007	0.090952
H	-3.027295	-0.001203	1.305226
H	-3.406355	-1.027811	-0.40137
H	-3.404253	1.029791	-0.39901
Total	**energy**	**-1222.150646**	
9c	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
S	-1.601843	-0.065328	0.000181
Si	0.006145	1.390448	-0.00025
S	1.601579	-0.075806	0.000263
N	0.59778	-1.552538	-2E-06
N	-0.611284	-1.546297	-0.00055
H	0.004529	2.241302	1.211032
H	0.008208	2.242416	-1.2107
Total	**energy**	**-1196.707115**	
9c	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
S	-0.392635	-1.543701	-0.25309
Si	1.04384	-0.005355	-0.85405
S	-0.382853	1.544259	-0.25647
N	-1.675108	0.607125	0.619222
N	-1.679598	-0.595233	0.620847
N	2.081992	-0.002096	1.04805
H	1.767191	-0.798789	1.595715
H	1.845039	0.849349	1.550749
H	3.090816	-0.053097	0.946305
Total	**energy**	**-1252.104949**	
9d	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	-1.745174	-0.442845	0
N	-1.006918	1.323932	-3E-06
N	-0.056703	1.929101	0.000004
S	1.730799	0.153652	-1E-06
S	0.261562	-1.189365	0.000001
Total	**energy**	**-1195.496599**	
9d	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	-1.260788	-0.040614	-0.00015
N	-0.295216	1.520895	-7.2E-05
N	0.832307	1.773596	0.000001

S	2.068392	-0.060449	0.000096
S	0.463682	-1.278395	-5.2E-05
B	-3.229582	-0.141025	0.000187
H	-3.503569	-1.306978	0.000298
H	-3.48476	0.470327	1.009784
H	-3.48556	0.470427	-1.00911
Total	**energy**	**-1222.148856**	
9d	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	1.551148	-0.010025	0.000103
N	0.62595	1.53174	-0.00017
N	-0.583565	1.593797	-0.00011
S	-1.575535	0.075845	0.000114
S	-0.100727	-1.424932	-0.00011
H	2.403929	-0.07668	-1.20802
H	2.403492	-0.076332	1.208557
Total	**energy**	**-1196.709452**	
9d	**(μ-N)$_2$**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	0.872485	-1.194168	0.508992
S	3.021881	-1.159644	-0.18456
N	0.882106	0.674466	0.572836
Si	-0.871214	1.200089	-0.48941
N	1.850693	1.457638	0.409771
S	3.319593	0.896474	-0.1249
N	-0.872514	-0.669148	-0.54989
N	-1.841161	-1.45617	-0.40027
S	-3.319313	-0.900694	0.108953
S	-3.03164	1.155713	0.169173
Total	**energy**	**-2390.988468**	
10	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.254919	-0.67559	0
N	0.028814	-1.196308	0.000001
C	-1.254919	0.67559	0
Si	1.330302	0	-1E-06
N	0.028814	1.196308	0.000001
H	0.140135	2.1963	0.000001
H	-2.124433	-1.31216	0
H	0.140135	-2.1963	0.000001
H	-2.124433	1.31216	0
Total	**energy**	**-477.742772**	
10	**+**	**BH_3**	**complex**

level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.763892	-0.663164	0.003505
N	0.480796	-1.210285	-0.0014
Si	-0.767798	-0.012177	-0.00517
B	-2.747075	0.002419	0.005428
C	1.751661	0.683749	0.003398
N	0.458536	1.206549	-0.00181
H	0.331069	2.203987	-0.00441
H	2.635472	-1.294938	0.005251
H	0.374117	-2.210137	-0.00379
H	2.611436	1.331426	0.005135
H	-3.011379	1.162682	-0.1927
H	-3.070688	-0.74084	-0.88637
H	-3.05412	-0.39116	1.103094
Total	**energy**	**-504.407653**	

10	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.330667	0.669006	0.000197
N	-0.036514	1.238335	-0.00054
C	-1.330667	-0.669006	0.000183
Si	1.184822	0	0.000184
N	-0.036513	-1.238335	-0.00057
H	0.055739	-2.23609	0.000272
H	-2.201098	1.302765	0.000442
H	0.055736	2.23609	0.000155
H	-2.201098	-1.302766	0.000422
H	2.090474	-0.000019	1.187383
H	2.09194	0.00002	-1.1858
Total	**energy**	**-478.9394272**	

10	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	0.157616	0.34007	1.181694
N	-0.539367	-0.819029	0.877006
Si	-1.581413	-0.721974	-0.54677
N	-1.003897	0.943861	-0.67432
C	-0.104101	1.335175	0.304317
H	-1.269723	1.615267	-1.37512
H	0.820636	0.394021	2.029262
H	-0.404398	-1.623886	1.465923
H	0.301627	2.333199	0.332041
N	3.366696	-0.398652	-0.41897
H	3.314759	-1.064314	-1.18182
H	2.417549	-0.085222	-0.24341

H	3.874226	0.403842	-0.77417
Total	**energy**	**-534.3295311**	
10	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.236496	-0.700059	-0.0706
C	-1.23648	0.700077	-0.07061
N	-0.05181	1.255767	0.184504
Si	1.412479	-0.000011	-0.10224
N	-0.051826	-1.255763	0.184444
H	0.022106	2.258133	0.107164
H	-2.127794	-1.283688	-0.2592
H	0.022038	-2.258148	0.107321
H	-2.127751	1.283719	-0.2593
Total	**energy**	**-477.6454334**	
11	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.234605	0.755324	0.140244
C	-1.234622	-0.755318	-0.14024
N	0.13642	-1.210004	0.115487
Si	1.376739	-0.000008	0.000001
N	0.136444	1.210008	-0.1155
H	0.295039	-2.202438	0.064275
H	-1.522514	0.946156	1.180719
H	0.295014	2.202447	-0.06424
H	-1.957022	-1.265319	0.500236
H	-1.957007	1.265343	-0.50022
H	-1.522542	-0.946144	-1.18071
Total	**energy**	**-478.9440126**	
11	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.714524	-0.766116	0.151704
C	1.729573	0.75208	-0.12143
N	0.357216	1.227305	0.097866
Si	-0.829356	0.008974	-0.02654
N	0.345649	-1.223528	-0.12028
H	0.198098	2.219105	0.053903
H	1.989493	-0.965387	1.192634
H	0.173793	-2.213679	-0.089
H	2.434776	1.250795	0.544679
H	2.438119	-1.274304	-0.48693
H	2.04615	0.948121	-1.15102
B	-2.7913	0.000165	0.024151
H	-3.127026	-0.912019	-0.68961

H	-3.02455	-0.212735	1.193278
H	-3.145998	1.091423	-0.34191
Total	**energy**	**-505.6156523**	
11	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.287258	-0.745482	0.178499
C	1.287258	0.745481	-0.1785
N	-0.043952	1.249322	0.18601
Si	-1.234498	0	0
N	-0.043952	-1.249322	-0.18601
H	-0.2086	2.216306	-0.03839
H	1.498338	-0.863938	1.248906
H	-0.208602	-2.216305	0.03839
H	2.06977	1.267735	0.376616
H	2.069769	-1.267736	-0.37662
H	1.49834	0.863938	-1.24891
H	-2.133902	-0.119673	1.183998
H	-2.133903	0.119673	-1.184
Total	**energy**	**-480.1584289**	
11	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.306835	0.843786	-0.68278
N	-0.546025	1.159016	0.525668
Si	0.460826	-0.131975	1.134422
N	-0.37557	-1.23105	0.044425
C	-1.551229	-0.66855	-0.62747
H	-0.370906	2.135857	0.694655
H	-2.254204	1.386906	-0.72372
H	-1.684308	-1.073386	-1.63465
H	-0.398704	-2.226962	0.193189
H	-2.470357	-0.874451	-0.06448
H	-0.743373	1.096043	-1.5923
N	2.44006	0.112813	-0.80792
H	3.324067	-0.223836	-0.44574
H	2.03511	-0.619685	-1.37875
H	2.630233	0.910289	-1.40384
Total	**energy**	**-535.5310686**	
11	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.169356	-0.739032	-0.20799
N	0.121214	-1.308157	0.223279
Si	1.308558	-0.00001	0.000039
N	0.121228	1.30813	-0.2234

C	-1.169308	0.739063	0.208042
H	0.315298	2.203707	0.200502
H	-1.32003	-0.810149	-1.29176
H	0.315255	-2.203672	-0.20076
H	-1.987791	1.264386	-0.28939
H	-1.987801	-1.264327	0.289541
H	-1.319851	0.810196	1.291837
Total	**energy**	**-478.8254639**	
11	**(μ-N)$_2$**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	0.604381	-1.179169	0.697417
N	2.095938	-1.121476	-0.23376
C	2.652902	0.17725	-0.59559
C	2.117879	1.172864	0.438426
N	0.726597	0.756983	0.746859
H	2.705578	-1.913537	-0.33281
H	2.350126	0.496735	-1.60039
H	2.136268	2.195471	0.053646
H	0.419391	1.164336	1.622806
Si	-0.60438	1.179195	-0.6974
N	-0.726567	-0.756965	-0.74682
N	-2.095998	1.121442	0.233654
C	-2.652934	-0.177268	0.595561
C	-2.117845	-1.172882	-0.43842
H	-2.705477	1.913572	0.333142
H	-2.350191	-0.496717	1.600379
H	-2.136214	-2.195482	-0.05362
H	-0.419324	-1.16432	-1.62275
H	3.744435	0.166458	-0.5769
H	2.721808	1.125653	1.346669
H	-2.721746	-1.1257	-1.34668
H	-3.744468	-0.166513	0.576811
Total	**energy**	**-957.9018104**	
12	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.245034	-0.979879	0
N	-0.060139	-1.429517	0
C	1.439798	0.350607	0
Si	-1.425316	-0.313807	0
S	0	1.342728	0
H	2.050051	-1.701665	0
H	-0.191417	-2.429827	0
H	2.407771	0.823395	0
Total	**energy**	**-820.5956014**	

12	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.462796	1.229256	0.001945
N	-0.089749	1.413447	-0.00201
Si	0.93798	0.022682	-0.00388
B	2.917266	-0.055963	0.004015
C	-1.92339	-0.030874	0.003245
S	-0.723473	-1.319953	-0.00066
H	-2.103795	2.099007	0.003242
H	0.257282	2.360252	-0.0043
H	-2.964631	-0.304771	0.005327
H	3.220899	-0.731125	-0.94432
H	3.188032	1.116827	-0.09953
H	3.205083	-0.543095	1.067248
Total	**energy**	**-847.2571794**	

12	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-0.49948	1.552581	-0.00002
N	0.854049	1.215581	-0.00101
C	-1.417663	0.58437	0.000448
Si	1.21292	-0.492797	0.000239
S	-0.855928	-1.116385	-0.00018
H	-0.757707	2.602416	0.000276
H	1.520558	1.967076	0.001598
H	-2.48159	0.746577	0.000694
H	1.97868	-0.943871	-1.19201
H	1.978536	-0.941654	1.193491
Total	**energy**	**-821.7986478**	

12	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.202913	1.233079	0.446395
N	0.122018	1.431607	-0.40074
Si	-0.805666	0.059128	-1.03508
S	0.705267	-1.305041	-0.15068
C	1.595614	-0.026402	0.685819
H	1.700365	2.09684	0.86853
H	-0.118438	2.387344	-0.6091
H	2.432665	-0.292991	1.309721
N	-2.120347	-0.123165	1.039716
H	-2.431488	-1.084105	1.125801
H	-1.467275	0.060269	1.793606
H	-2.923636	0.486347	1.147253
Total	**energy**	**-877.1839879**	

12	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-0.345868	1.534963	0.04307
N	-1.316294	0.689185	-0.25753
C	0.957021	1.056598	0.192699
Si	-1.004448	-1.168952	0.154421
S	1.291323	-0.587292	-0.13086
H	-0.561616	2.590565	0.176749
H	-2.247613	1.073053	-0.33276
H	1.757478	1.724714	0.475938
Total	**energy**	**-820.503097**	

12	**(μ-N)$_2$**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-2.762317	0.915634	0.209007
C	-1.76717	1.633215	-0.3
N	-0.56384	0.954565	-0.70948
Si	0.712596	0.978012	0.864978
S	2.685038	0.850686	-0.22731
C	2.762305	-0.915677	-0.20895
C	1.767147	-1.633213	0.300101
N	0.563819	-0.954522	0.709506
Si	-0.712562	-0.977968	-0.865
S	-2.685038	-0.850728	0.227237
H	0.150659	-1.380503	1.534338
H	-3.653457	1.375868	0.609594
H	-1.772281	2.713112	-0.34542
H	-0.150724	1.38058	-1.53431
H	1.772248	-2.713107	0.34559
H	3.653446	-1.375945	-0.6095
Total	**energy**	**-1641.164999**	

12	**(μ-N) (μ-S)**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
Si	0.644233	-0.895901	0.93976
S	2.623526	-0.91886	-0.09681
C	2.712964	0.832855	-0.31576
C	1.743299	1.614267	0.146728
N	0.570656	1.007338	0.714224
H	3.583145	1.229987	-0.8173
H	1.750371	2.691104	0.048251
H	0.281231	1.477301	1.568779
Si	-0.978999	1.306753	-0.71206
S	-0.978924	-1.021674	-0.97656
C	-2.364111	-1.273884	0.11852

C	-2.917105	-0.177561	0.646265
N	-2.405664	1.07507	0.341514
H	-2.694473	-2.280747	0.307925
H	-3.776208	-0.232885	1.303707
H	-2.976204	1.860934	0.610199
Total	**energy**	**-1641.164477**	
13	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.297301	0.963807	-0.21198
C	1.409509	-0.480577	0.25363
S	-0.17637	-1.375991	-0.09664
Si	-1.44012	0.396155	0.046845
N	-0.06107	1.437162	0.067702
H	1.512166	1.029252	-1.28469
H	-0.171863	2.440442	0.070569
H	2.214779	-1.002989	-0.25791
H	2.034109	1.579094	0.311028
H	1.581041	-0.535639	1.327677
Total	**energy**	**-821.8036874**	
13	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.505707	1.224402	-0.18272
C	1.892053	-0.169349	0.302677
S	0.556895	-1.397515	-0.10816
Si	-0.981355	0.076498	-0.02129
N	0.069932	1.41405	0.032494
H	1.75365	1.335797	-1.24312
H	-0.266028	2.364549	0.009656
H	2.809354	-0.514283	-0.16743
H	2.076214	1.971287	0.373258
H	2.019389	-0.188619	1.38319
B	-2.944937	0.015242	0.075349
H	-3.299324	-0.873279	-0.65404
H	-3.124566	-0.236158	1.246032
H	-3.29144	1.125101	-0.24294
Total	**energy**	**-848.4705752**	
13	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.03413	1.270085	-0.25506
C	1.5145	-0.067736	0.293901
S	0.279784	-1.399207	-0.10619
Si	-1.34925	0.005205	0.039094
N	-0.371286	1.434271	0.113313

H	1.1936	1.297198	-1.34013
H	-0.748222	2.354759	-0.04485
H	2.45721	-0.36953	-0.15675
H	1.630956	2.072557	0.187915
H	1.633152	-0.023018	1.374716
H	-2.201298	-0.140918	1.246916
H	-2.245204	-0.130602	-1.14228
Total	**energy**	**-823.0198058**	
13	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.484486	1.136918	0.205566
C	1.494522	-0.264441	0.795978
S	0.508444	-1.389637	-0.29432
Si	-0.929849	0.195642	-0.91407
N	0.123683	1.448205	-0.23604
H	2.199196	1.182229	-0.62537
H	0.035835	2.375098	-0.62674
H	2.506328	-0.659331	0.861969
H	1.820753	1.851935	0.964975
H	1.059865	-0.268273	1.796354
N	-2.100146	-0.026353	0.987038
H	-3.102431	0.051572	0.856491
H	-1.886701	-0.931216	1.394801
H	-1.788866	0.705362	1.617466
Total	**energy**	**-878.3965048**	
13	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.15025	1.107341	-0.16178
C	0.262393	1.319684	0.40906
S	1.440064	0.024895	-0.22568
Si	-0.182011	-1.356575	0.20149
N	-1.550171	-0.307449	-0.09906
H	-1.162611	1.450953	-1.19989
H	-2.228055	-0.558374	-0.8017
H	0.655924	2.284844	0.093603
H	-1.842731	1.73258	0.411449
H	0.262945	1.273719	1.496326
Total	**energy**	**-821.6993538**	
13	**(μ-N)(μ-S)**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	1.845733	1.563554	-0.14315
N	0.591906	1.078259	0.505125
Si	0.549288	-0.81495	0.915747

S	2.482493	-1.105967	-0.16363
C	3.011274	0.631543	0.141907
H	1.673217	1.606208	-1.2198
H	0.424195	1.597932	1.360501
H	3.845505	0.844042	-0.52533
H	2.058367	2.580731	0.192893
H	3.364754	0.732953	1.168306
Si	-0.984683	1.373665	-0.753
S	-0.946276	-1.028347	-0.94386
C	-2.53288	-1.249954	-0.0237
C	-2.769253	-0.085663	0.942151
N	-2.34877	1.169397	0.327143
H	-3.310263	-1.300914	-0.78402
H	-2.484742	-2.202888	0.50173
H	-2.217865	-0.279917	1.867059
H	-3.829085	-0.043772	1.203799
H	-3.039227	1.902149	0.347101
Total	**energy**	**-1643.609002**	
14	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-0.669839	1.464398	0.000001
C	0.669807	1.464416	0
S	1.574505	-0.029109	0
Si	0.000022	-1.528287	0.000001
S	-1.574509	-0.02914	-1E-06
H	-1.249174	2.377532	0.000006
H	1.249115	2.377566	-4E-06
Total	**energy**	**-1163.442638**	
14	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.851889	-0.668391	0.025232
C	-1.851888	0.668393	0.025233
S	-0.369377	1.603639	-0.01024
Si	1.040766	-0.000001	-0.03538
S	-0.369379	-1.603639	-0.01024
H	-2.765342	-1.245586	0.043821
H	-2.76534	1.24559	0.043821
B	3.022977	-0.000001	0.040116
H	3.345751	1.022793	-0.50268
H	3.196309	0.000005	1.237307
H	3.345762	-1.022794	-0.50268
Total	**energy**	**-1190.099918**	
14	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		

Geometry:			
C	-0.665151	1.493567	0.000007
C	0.665155	1.493565	0.000007
S	1.660676	0.026363	-8E-06
Si	-0.000002	-1.365402	0.000008
S	-1.660676	0.026366	-8E-06
H	-1.233407	2.413091	0.000015
H	1.233412	2.413089	0.000017
H	-0.000001	-2.238487	1.198661
H	-0.000005	-2.238511	-1.19862
Total	**energy**	**-1164.650388**	
14	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.57421	0.667716	0.543759
C	-1.574245	-0.667632	0.543763
S	-0.345602	-1.613086	-0.30285
Si	1.089781	-0.000033	-0.83556
S	-0.345514	1.613101	-0.30286
H	-2.358392	1.236373	1.02572
H	-2.358456	-1.236244	1.025728
N	1.904606	-0.000041	1.181896
H	2.471454	0.826166	1.347958
H	1.133421	-0.000009	1.843327
H	2.471397	-0.826285	1.347969
Total	**energy**	**-1220.03888**	
14	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-0.685163	1.357419	0.244371
C	0.685188	1.357409	0.244371
S	1.625053	0.009082	-0.2625
Si	-0.000019	-1.504003	0.308099
S	-1.625049	0.009106	-0.2625
H	-1.221114	2.238045	0.577106
H	1.221151	2.238028	0.577105
Total	**energy**	**-1163.355496**	
15	**singlet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	0.694145	-1.461932	-0.29875
S	1.59871	0.106675	0.078724
Si	0	1.557833	0
S	-1.59871	0.106674	-0.07872
C	-0.694144	-1.461931	0.298746
H	0.659678	-1.562846	-1.38234

H	-1.291072	-2.277194	-0.11032
H	1.291073	-2.277193	0.110319
H	-0.659678	-1.562846	1.382342
Total	**energy**	**-1164.659813**	
15	**+**	**BH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.848723	-0.683481	-0.25918
S	-0.290052	-1.629365	0.057326
Si	1.078797	-0.007007	-0.07355
B	3.040488	-0.005869	0.078131
C	-1.814135	0.700496	0.355846
S	-0.279376	1.628481	-0.10128
H	-1.989189	-0.635366	-1.33714
H	-2.651616	1.298097	-0.00287
H	-2.656885	-1.272339	0.1737
H	-1.856872	0.653922	1.442202
H	3.423709	1.024889	-0.4044
H	3.074532	-0.000181	1.295606
H	3.438719	-1.029521	-0.40478
Total	**energy**	**-1191.321859**	
15	**silane**	**derivative**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	0.6758	1.469867	0.345456
S	1.663977	-0.034119	-0.08204
Si	-0.00002	-1.405819	0.000012
S	-1.663977	-0.034082	0.082009
C	-0.675759	1.469896	-0.34543
H	0.562858	1.527325	1.426041
H	-1.275644	2.316541	-0.01019
H	1.275705	2.316513	0.010256
H	-0.562813	1.527386	-1.42601
H	0.027092	-2.276849	-1.20001
H	-0.027174	-2.276813	1.200055
Total	**energy**	**-1165.879684**	
15	**+**	**NH_3**	**complex**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	-1.846889	-0.514117	0.235995
S	-0.413349	-1.611046	-0.16445
Si	1.097347	-0.125761	-0.86261
N	2.114541	-0.111963	1.065849
C	-1.40595	0.833829	0.765034
S	-0.168853	1.61885	-0.36145
H	-2.437972	-0.396397	-0.67048

H	-2.252344	1.519645	0.822548
H	-2.448312	-1.041919	0.977597
H	-0.977394	0.738958	1.76296
H	3.096945	-0.352779	0.987976
H	2.032685	0.816778	1.468985
H	1.654021	-0.783017	1.6742
Total	**energy**	**-1221.259703**	
15	**triplet**	**silylene**	
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	0.714678	1.302147	0.467653
S	1.66117	-0.103148	-0.2935
Si	0.032104	-1.403956	0.254014
S	-1.698282	-0.148954	-0.13857
C	-0.699522	1.431134	-0.09856
H	0.704707	1.167111	1.547104
H	-1.269432	2.144261	0.496413
H	1.28008	2.204287	0.229533
H	-0.661949	1.773681	-1.1306
Total	**energy**	**-1164.570347**	
15	**disilene**	**dimer**	**derivative**
level:	**B3LYP/cc-pVTZ**		
Geometry:			
C	3.613557	-0.681393	0.733981
C	3.905977	0.663463	0.102247
S	2.363694	1.63605	-0.21288
Si	1.024601	0.004715	-0.70307
S	2.360604	-1.630725	-0.23774
H	3.237354	-0.56799	1.749408
H	4.518128	1.273387	0.767312
H	4.51374	-1.296413	0.757995
H	4.427124	0.547329	-0.8459
Si	-1.024579	0.004712	0.703009
S	-2.360603	-1.630724	0.23773
C	-3.613608	-0.681384	-0.73392
C	-3.905987	0.663469	-0.10216
S	-2.363681	1.636051	0.212868
H	-3.237461	-0.567978	-1.74937
H	-4.513794	-1.296401	-0.75789
H	-4.518181	1.273397	-0.76719
H	-4.427071	0.547332	0.846013
Total	**energy**	**-2329.329481**	