Supplementary Material (ESI) for PCCP

Supplementary data for:

Kinetic Correlations for H_2 Addition and Elimination Reaction Mechanisms during Silicon Hydride Pyrolysis

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Table S1: Rate coefficients of all reactions from G3//B3LYP and using the full parameter TSGA model: (a) H_2 addition and (b) H_2 elimination. The rate coefficient units are cm^3 $molecule^{-1}$ s^{-1} for H_2 addition and s^{-1} for H_2 elimination.

(a)

	G3//B3LYP			**TSGA**		
	Temperature (K)					
Reaction	800	1000	1200	800	1000	1200
1	5.49E-12	1.04E-11	1.59E-11	5.49E-12	1.04E-11	1.59E-11
2	8.12E-12	8.99E-12	9.63E-12	1.13E-11	1.46E-11	1.73E-11
3	5.04E-12	6.55E-12	7.80E-12	5.94E-12	8.69E-12	1.12E-11
4	1.02E-10	9.55E-11	9.13E-11	9.24E-11	8.17E-11	7.52E-11
5	2.79E-11	3.35E-11	3.78E-11	2.57E-11	2.91E-11	3.16E-11
6	1.39E-11	1.67E-11	1.88E-11	1.22E-11	1.41E-11	1.54E-11
7	6.08E-12	8.91E-12	1.15E-11	6.48E-12	9.69E-12	1.27E-11
8	1.52E-12	2.29E-12	3.01E-12	1.52E-12	2.29E-12	3.01E-12

9	1.64E-12	4.85E-12	1.00E-11	1.64E-12	4.85E-12	1.00E-11
10	3.87E-11	4.54E-11	5.04E-11	3.87E-11	4.54E-11	5.04E-11
11	4.50E-11	4.91E-11	5.20E-11	4.50E-11	4.91E-11	5.20E-11
12	1.25E-11	1.78E-11	2.25E-11	1.25E-11	1.78E-11	2.25E-11
13	1.01E-15	1.42E-14	8.24E-14	1.01E-15	1.42E-14	8.24E-14
14	7.84E-13	2.13E-12	4.14E-12	7.84E-13	2.13E-12	4.14E-12
15	6.03E-13	9.87E-13	1.37E-12	6.03E-13	9.87E-13	1.37E-12
16	8.58E-13	1.44E-12	2.02E-12	8.58E-13	1.44E-12	2.02E-12
17	2.93E-16	5.67E-15	4.09E-14	1.01E-15	1.42E-14	8.24E-14
18	5.05E-16	8.25E-15	5.32E-14	1.01E-15	1.42E-14	8.24E-14
19	9.66E-13	1.87E-12	2.91E-12	4.12E-13	1.62E-12	4.02E-12
20	7.58E-12	1.17E-11	1.56E-11	9.75E-12	1.51E-11	2.02E-11
21	2.21E-12	4.09E-12	6.17E-12	6.55E-13	9.54E-13	1.23E-12
22	1.97E-15	2.88E-14	1.72E-13	1.10E-15	1.37E-14	7.37E-14
23	3.10E-12	5.19E-12	7.32E-12	3.14E-12	5.13E-12	7.13E-12
24	3.12E-11	3.85E-11	4.43E-11	1.22E-11	1.41E-11	1.54E-11
25	1.16E-11	1.49E-11	1.77E-11	5.94E-12	8.69E-12	1.12E-11

(b)

	G3//B3LYP			TSGA		
	Temperature (K)					
Reaction	800	1000	1200	800	1000	1200
1	9.83E-02	1.34E+02	1.64E+04	9.83E-02	1.34E+02	1.64E+04
2	1.04E+00	7.25E+02	5.69E+04	6.26E-01	4.89E+02	4.15E+04
3	2.75E-01	1.86E+02	1.43E+04	1.70E-01	1.27E+02	1.04E+04
4	1.84E+00	8.63E+02	5.21E+04	2.66E+00	1.19E+03	6.99E+04
5	1.38E+00	5.93E+02	3.37E+04	1.76E+00	7.19E+02	3.96E+04
6	2.36E+00	1.08E+03	6.39E+04	1.88E+00	8.36E+02	4.87E+04
7	4.74E+00	2.06E+03	1.19E+05	5.31E+00	2.34E+03	1.36E+05
8	2.04E+00	8.90E+02	5.12E+04	2.04E+00	8.90E+02	5.12E+04
9	3.46E+02	8.73E+04	3.49E+06	3.46E+02	8.73E+04	3.49E+06
10	3.59E+01	1.33E+04	6.88E+05	3.59E+01	1.33E+04	6.88E+05
11	8.22E+00	2.92E+03	1.47E+05	8.22E+00	2.92E+03	1.47E+05
12	1.91E+01	9.05E+03	5.50E+05	1.91E+01	9.05E+03	5.50E+05
13	1.95E-01	1.25E+02	9.27E+03	1.95E-01	1.25E+02	9.27E+03

14	1.64E-01	1.10E+02	8.44E+03	1.64E-01	1.10E+02	8.44E+03
15	1.45E-01	9.11E+01	6.68E+03	1.45E-01	9.11E+01	6.68E+03
16	1.87E-01	1.25E+02	9.59E+03	1.87E-01	1.25E+02	9.59E+03
17	5.15E-01	3.36E+02	2.53E+04	5.86E-01	3.75E+02	2.78E+04
18	3.02E-01	1.91E+02	1.41E+04	1.95E-01	1.25E+02	9.27E+03
19	6.30E+01	1.50E+04	5.75E+05	1.74E+02	4.74E+04	1.99E+06
20	7.77E+00	3.35E+03	1.91E+05	2.71E+01	1.09E+04	5.91E+05
21	2.60E+00	1.18E+03	6.97E+04	2.61E+00	9.35E+02	4.71E+04
22	2.67E+00	1.06E+03	5.73E+04	3.52E+00	1.28E+03	6.54E+04
23	2.08E+01	8.50E+03	4.68E+05	1.11E+01	5.44E+03	3.40E+05
24	7.25E+00	3.06E+03	1.73E+05	1.88E+00	8.36E+02	4.87E+04
25	3.96E-01	2.62E+02	1.99E+04	1.70E-01	1.27E+02	1.04E+04

Table S2: External symmetry numbers for all species.

	Reactants		Transition	Product
	Silylene	H_2	State	Silane
Reaction	σ_{rot}	σ_{rot}	σ_{rot}	σ_{rot}
1	2	2	1	12
2	1	2	1	6
3	1	2	1	2
4	2	2	1	2
5	2	2	1	2
6	1	2	1	1
7	2	2	1	2
8	1	2	1	1
9	2	2	1	6
10	2	2	1	8
11	2	2	1	10
12	2	2	1	12
13	1	2	1	1
14	1	2	1	1
15	1	2	1	1
16	1	2	1	1
17	1	2	1	3
18	1	2	1	1
19	2	2	1	1
20	2	2	1	2
21	1	2	1	1
22	1	2	1	1
23	1	2	1	4
24	1	2	1	1
25	1	2	1	2

Table S3: B3LYP/6-31G(d) geometries and frequencies for all silylenes, silanes and rate-determining transition states, as well as dihydrogen.

Dihydrogen

Atomic Symbol	Coordinates (Angtroms) X	Y	Z	Frequency cm^{-1}
H	0.0000	0.0000	-0.0714	4453
H	0.0000	0.0000	0.6714	

Reaction 1

Reactant Silylene Atomic Symbol	Coordinates (Angtroms) X	Y	Z	Frequency cm^{-1}	Transition State Atomic Symbol	Coordinates (Angtroms) X	Y	Z	Frequency cm^{-1}	Product Silane Atomic Symbol	Coordinates (Angtroms) X	Y	Z	Frequency cm^{-1}
Si	-0.1346	0.0000	-0.0915	1040	Si	0.0000	0.1855	0.0000	-1215	Si	0.0591	0.0087	0.0128	916
H	0.1359	0.0000	1.4149	2053	H	-0.7844	-0.2051	1.2062	745	H	-0.0457	-0.0431	1.4941	916
H	1.3659	0.0000	-0.3933	2058	H	0.3457	-1.4458	0.0000	782	H	1.4914	0.0286	-0.3822	917
					H	-0.7844	-0.2051	-1.2062	983	H	-0.5995	-1.1878	-0.5725	975
					H	1.2230	-0.7407	0.0000	1037	H	-0.6101	1.2372	-0.4883	975
									1641					2252
									2111					2265
									2214					2265
									2238					2265

Reaction 2

Reactant					Transition State					Product				
Silylene										Silane				
Atomic	Coordinates (Angtroms)			Frequency	Atomic	Coordinates (Angtroms)			Frequency	Atomic	Coordinates (Angtroms)			Frequency
Symbol	X	Y	Z	cm^{-1}	Symbol	X	Y	Z	cm^{-1}	Symbol	X	Y	Z	cm^{-1}
Si	-0.0351	-0.5007	0.1460	60	Si	0.5956	0.3007	-0.2306	-1086	Si	-0.0394	-0.0345	-0.0152	134
H	0.1592	0.6470	1.1418	375	H	0.5992	0.0155	1.2414	147	H	0.6752	0.2750	1.2542	379
Si	2.1910	-0.1079	-0.6784	389	H	0.1529	-1.0933	-0.7755	336	H	0.9745	-0.3715	-1.0527	383
H	3.1709	-0.3135	0.4330	430	H	-0.6965	-0.7569	-0.2331	413	H	-0.8946	-1.2328	0.2096	433
H	2.5979	-0.9974	-1.8027	729	Si	-1.2380	1.7111	-0.7043	428	Si	-1.3455	1.7961	-0.6986	638
H	2.3359	1.3047	-1.1462	869	H	-2.3171	1.7392	0.3208	582	H	-2.3598	2.1330	0.3385	639
				931	H	-0.7398	3.1062	-0.8560	699	H	-0.4916	2.9951	-0.9242	856
				954	H	-1.8212	1.2880	-2.0081	833	H	-2.0598	1.4852	-1.9679	931
				2046					895					943
				2191					936					944
				2204					972					957
				2232					1022					958
									1677					2225
									2024					2235
									2176					2238
									2228					2239
									2238					2248
									2242					2249

Reaction 3

Reactant					Transition State					Product				
Silylene										Silane				
Atomic	Coordinates (Angtroms)			Frequency	Atomic	Coordinates (Angtroms)			Frequency	Atomic	Coordinates (Angtroms)			Frequency
Symbol	X	Y	Z	cm^{-1}	Symbol	X	Y	Z	cm^{-1}	Symbol	X	Y	Z	cm^{-1}

Si	-0.2734	0.0013	-0.0071	61
Si	-0.1767	-0.0269	2.3602	69
H	0.7431	1.0334	2.8568	152
H	-1.5218	0.2181	2.9523	369
H	0.3121	-1.3462	2.8482	378
Si	-1.2685	2.0651	-0.6941	418
H	0.0411	2.7970	-0.3869	454
H	1.1274	-0.1943	-0.4935	473
H	-1.0578	-1.1989	-0.4249	646
				667
				759
				884
				937
				947
				957
				2049
				2191
				2209
				2225
				2237
				2242

Si	-1.9546	-0.4122	-0.0068	-1103
H	-2.0267	-1.2482	1.2239	97
H	-1.9653	-1.3226	-1.1857	100
H	-3.1745	0.4425	-0.0684	122
Si	0.0140	0.8739	0.0102	322
H	0.0861	1.6853	1.2612	372
H	-0.0317	1.8426	-1.1245	377
Si	2.0475	-0.3281	-0.1514	461
H	2.4466	-0.6356	1.3244	467
H	1.4205	-0.9194	1.2795	540
H	1.7484	-1.7143	-0.6387	627
				728
				764
				829
				895
				932
				947
				951
				1018
				1668
				2026
				2177
				2205
				2216
				2223
				2235
				2240

Si	-0.0810	-0.0830	-0.0853	77
H	1.0375	0.2872	0.8258	96
H	0.4923	-0.8015	-1.2571	101
H	-0.9874	-1.0162	0.6397	320
Si	-1.2428	1.8404	-0.7866	383
H	-1.8320	2.5187	0.4052	427
H	-2.3770	1.4335	-1.6674	443
Si	0.1260	3.3649	-1.9455	466
H	-0.6513	4.5636	-2.3659	570
H	1.2523	3.8154	-1.0813	600
H	0.7007	2.7279	-3.1629	718
				733
				886
				898
				934
				947
				950
				951
				957
				2208
				2218
				2225
				2231
				2240
				2240
				2243
				2246

Reaction 4

Reactant		Product
Silylene	Transition State	Silane

Atomic	Coordinates (Angtroms)			Frequency	Atomic	Coordinates (Angtroms)			Frequency	Atomic	Coordinates (Angtroms)			Frequency
Symbol	X	Y	Z	cm^{-1}	Symbol	X	Y	Z	cm^{-1}	Symbol	X	Y	Z	cm^{-1}
Si	0.2017	-0.3202	-0.2046	84	Si	-1.9551	-0.4035	0.0161	-806	Si	-0.0810	-0.0830	-0.0853	77
Si	0.0773	0.2270	2.1269	97	H	-1.7532	-1.7450	0.6317	84	H	1.0375	0.2872	0.8258	96
H	1.2063	-0.3270	2.9269	138	H	-2.5520	-0.6240	-1.3305	91	H	0.4923	-0.8015	-1.2571	101
H	-0.0759	1.6687	2.4808	317	H	-2.9426	0.3533	0.8371	118	H	-0.9874	-1.0162	0.6397	320
H	-1.1694	-0.4770	2.5693	338	Si	0.0000	0.9118	-0.2358	357	Si	-1.2428	1.8404	-0.7866	383
Si	-1.1434	1.5648	-0.8275	416	H	0.0001	0.8189	1.4546	369	H	-1.8320	2.5187	0.4052	427
H	-2.1582	2.0309	0.1624	423	H	0.0001	1.7444	1.1201	400	H	-2.3770	1.4335	-1.6674	443
H	-0.1328	2.6603	-0.9820	496	Si	1.9551	-0.4035	0.0161	455	Si	0.1260	3.3649	-1.9455	466
H	-1.8241	1.4006	-2.1432	566	H	2.9424	0.3532	0.8374	505	H	-0.6513	4.5636	-2.3659	570
				855	H	1.7532	-1.7452	0.6314	568	H	1.2523	3.8154	-1.0813	600
				886	H	2.5523	-0.6237	-1.3305	597	H	0.7007	2.7279	-3.1629	718
				915					628					733
				924					838					886
				957					912					898
				959					916					934
				2179					935					947
				2182					938					950
				2211					965					951
				2215					969					957
				2228					1691					2208
				2231					1992					2218
									2218					2225
									2223					2231
									2231					2240
									2234					2240
									2236					2243
									2238					2246

Reaction 5

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-1.6436	-0.3818	-0.4452	23	959	Si	3.6491	-0.7878	-0.1875	-835	948	Si	-0.4153	0.3452	-0.0265	21	948
H	-2.1439	0.2184	0.8227	34	2188	H	3.1881	-2.0075	-0.9096	26	948	H	0.2232	0.6070	1.2931	24	949
H	-0.5449	0.4769	-0.9675	64	2193	H	4.8739	-0.2801	-0.8662	29	959	H	0.2794	1.1680	-1.0559	45	952
H	-2.7591	-0.3800	-1.4302	74	2201	H	4.0075	-1.1831	1.2023	66	965	H	-1.8356	0.7865	0.0471	84	954
Si	-0.8592	-2.5874	-0.0878	86	2206	Si	1.9538	0.8467	-0.1759	89	1687	Si	-0.2941	-1.9454	-0.5570	89	2206
H	0.3963	-2.4763	0.7146	104	2226	H	1.7220	1.3338	-1.5678	90	1982	H	1.1381	-2.3524	-0.6619	105	2206
H	-0.4762	-3.1316	-1.4268	136	2229	H	2.4470	2.0251	0.5970	107	2203	H	-0.9128	-2.1754	-1.8956	120	2209
Si	-2.5163	-3.8893	1.0440	345	2239	Si	0.0000	0.0787	0.9303	127	2207	Si	-1.3675	-3.3164	1.0322	301	2212
Si	-3.9496	-4.1121	-0.8583	365	2242	H	0.0002	-1.0555	-0.3249	344	2212	H	-0.7480	-3.0919	2.3717	321	2217
H	-4.4277	-5.5271	-0.9363	373	2245	H	0.0002	-1.4710	0.5726	355	2214	H	-2.7990	-2.9082	1.1460	371	2225
H	-3.4074	-3.7560	-2.2049	385	2249	Si	-1.9535	0.8464	-0.1768	374	2225	Si	-1.2564	-5.6104	0.5005	379	2227
Si	-5.8821	-2.8023	-0.4649	423		H	-1.7214	1.3320	-1.5692	383	2226	H	0.1757	-6.0147	0.3857	403	2229
H	-6.7989	-2.8611	-1.6369	423		H	-2.4463	2.0257	0.5949	398	2238	H	-1.8812	-5.8304	-0.8369	450	2240
H	-6.6062	-3.3067	0.7340	472		Si	-3.6495	-0.7876	-0.1870	443	2239	Si	-2.3252	-6.9761	2.0930	471	2241
H	-5.5265	-1.3765	-0.2230	475		H	-4.8743	-0.2797	-0.8656	444	2244	H	-2.2296	-8.4131	1.7123	473	2243
				505		H	-3.1891	-2.0078	-0.9086	484	2244	H	-1.6963	-6.8023	3.4316	492	2244
				551		H	-4.0075	-1.1819	1.2031	504		H	-3.7655	-6.6145	2.2040	529	
				657						530						570	
				662						573						651	
				693						585						656	
				711						688						715	
				878						704						739	
				890						705						747	
				932						748						797	
				940						886						886	
				947						897						893	

					947							901							931	
					954							946							932	
												946							937	

Reaction 6

Reactant												Product								
Silylene							Transition State						Silane							
Atomic	Coordinates (Angtroms)			Frequency			Atomic	Coordinates (Angtroms)			Frequency			Atomic	Coordinates (Angtroms)			Frequency		
Symbol	X	Y	Z	cm^{-1}			Symbol	X	Y	Z	cm^{-1}			Symbol	X	Y	Z	cm^{-1}		
Si	0.2681	-0.7665	-0.0759	19	948		Si	-3.2293	0.0139	0.3077	-898	909		Si	0.3309	-0.0594	-0.1965	23	906	
H	0.4557	-0.9937	1.3859	51	950		H	-4.2114	-1.0905	0.1136	15	912		H	1.4243	-0.5176	0.7054	61	935	
H	1.2783	-1.5912	-0.8009	66	953		H	-3.0783	0.2677	1.7677	65	935		H	0.9268	0.3030	-1.5121	74	947	
H	0.5810	0.6730	-0.3443	79	957		H	-3.7994	1.2494	-0.2978	76	945		H	-0.2800	1.1647	0.3915	81	947	
Si	-2.0046	-1.0358	-0.8006	86	2169		Si	-1.2279	-0.5371	-0.8346	81	948		Si	-1.2924	-1.7429	-0.4655	87	949	
Si	-1.3965	-1.2627	-3.0926	89	2185		H	-1.3052	-1.8795	0.1824	87	949		H	-0.6316	-2.9805	-0.9765	96	950	
H	0.0170	-0.9396	-3.4693	104	2214		H	-1.2545	-2.1231	-0.7845	89	952		H	-1.8765	-2.0794	0.8664	116	952	
Si	-1.6704	-3.5889	-3.4776	140	2223		Si	0.6829	0.0089	0.4714	113	967		Si	-3.0395	-1.1341	-1.9337	131	954	
H	-0.9334	-4.3965	-2.4655	343	2225		H	0.4191	0.0464	1.9434	141	1686		H	-2.4273	-0.7332	-3.2383	329	2194	
H	-3.1099	-3.9597	-3.4059	349	2227		Si	2.3949	-1.5596	0.0654	332	1975		Si	-4.4698	-2.9647	-2.3361	343	2207	
H	-1.1501	-3.9456	-4.8263	396	2236		H	1.9214	-2.9408	0.3659	348	2185		H	-3.7119	-4.1063	-2.9195	410	2218	
Si	-2.8519	-0.1202	-4.5561	419	2239		H	2.8142	-1.5147	-1.3622	392	2220		H	-5.0940	-3.4198	-1.0628	440	2225	
H	-2.7261	1.3538	-4.3808	442	2242		H	3.5855	-1.2802	0.9159	425	2220		H	-5.5585	-2.5901	-3.2816	449	2227	
H	-2.5490	-0.4455	-5.9780	448	2247		Si	1.3970	2.1676	-0.1504	445	2225		Si	-4.2474	0.7142	-1.1074	462	2231	
H	-4.2612	-0.5063	-4.2716	494			H	0.3110	3.1666	0.0605	451	2233		H	-3.3590	1.8970	-0.9348	472	2239	
				504			H	2.5780	2.5907	0.6527	463	2234		H	-5.3461	1.0855	-2.0420	488	2240	
				550			H	1.7738	2.1939	-1.5911	508	2236		H	-4.8499	0.3877	0.2150	543	2242	
				573							535	2238						566	2243	
				677							564	2239						574	2244	
				725							572	2244						667	2246	

866	598	714
872	709	722
901	727	770
924	851	878
944	879	890

Reaction 7

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-0.3518	0.4557	0.2557	15	952	Si	1.9634	-0.0840	-0.4790	-954	948	Si	0.1268	0.1052	0.0641	17	947
H	-0.1534	1.0582	-1.1006	22	953	H	1.7429	-0.0889	-1.9584	13	948	H	0.3811	0.7671	-1.2524	20	949
Si	-2.3526	-0.7957	0.6061	42	2169	Si	0.0000	-0.5706	0.7726	23	948	Si	-1.4796	-1.6040	-0.2509	46	950
Si	-2.8794	-1.0227	-1.7098	54	2178	H	0.0000	-1.9717	-0.1576	50	950	H	-0.7836	-2.9043	-0.4880	72	951
H	-1.7807	-0.7429	-2.6879	62	2222	H	0.0000	-2.1547	0.8332	70	951	H	-2.2659	-1.7674	1.0077	76	951
Si	-3.8449	-3.1119	-2.2314	72	2222	Si	-1.9634	-0.0840	-0.4789	76	953	Si	-2.9609	-1.2096	-2.0469	78	952
H	-2.8649	-4.2148	-2.0236	76	2225	H	-1.7429	-0.0887	-1.9583	77	1682	H	-2.1383	-1.0892	-3.2903	79	2191
H	-5.0195	-3.3610	-1.3507	83	2228	Si	-3.6334	-1.6700	0.0255	77	1966	Si	-4.4330	-3.0316	-2.3224	89	2194
H	-4.2997	-3.1579	-3.6496	87	2234	H	-3.1435	-3.0511	-0.2479	86	2185	H	-3.6749	-4.2960	-2.5333	92	2200
Si	-4.5266	0.6456	-2.0782	94	2235	H	-4.0112	-1.5889	1.4631	90	2189	H	-5.2837	-3.1931	-1.1107	98	2215
H	-4.0126	1.9968	-1.7191	105	2239	H	-4.8531	-1.4363	-0.7970	97	2221	H	-5.3271	-2.8177	-3.4948	116	2223
H	-4.9230	0.6614	-3.5133	124	2240	Si	-2.7011	2.0782	0.1025	126	2222	Si	-4.1637	0.8013	-1.7882	121	2224
H	-5.7372	0.3764	-1.2547	137	2241	H	-1.6455	3.0934	-0.1725	128	2224	H	-3.2440	1.9707	-1.7271	141	2227
Si	1.3722	-1.1532	0.5238	347	2241	H	-3.9173	2.4507	-0.6730	142	2226	H	-5.0970	0.9990	-2.9321	333	2230
H	1.3681	-1.6941	1.9107	349	2246	H	-3.0323	2.1373	1.5535	332	2233	H	-4.9640	0.7696	-0.5328	355	2237
H	1.1990	-2.2933	-0.4191	397	2246	Si	2.7010	2.0783	0.1022	354	2236	Si	-0.6683	1.7398	1.5645	383	2238
H	2.6975	-0.5270	0.2622	401		H	1.6453	3.0933	-0.1728	355	2237	H	-0.8048	1.1557	2.9276	425	2239
Si	-0.0219	2.1292	1.8866	439		H	3.0324	2.1375	1.5531	418	2238	H	0.2734	2.8913	1.6410	440	2240
H	-0.0958	1.5305	3.2480	441		H	3.9171	2.4508	-0.6735	431	2238	H	-2.0016	2.2515	1.1430	443	2241

H	1.3082	2.7819	1.7295	446		Si	3.6335	-1.6699	0.0257	445	2240	Si	2.1653	-0.8081	0.8176	449	2243
H	-1.0696	3.1836	1.7845	446		H	3.1437	-3.0510	-0.2478	446	2245	H	1.9535	-1.5579	2.0870	450	2244
				492		H	4.8533	-1.4361	-0.7965	450	2245	H	2.7220	-1.7489	-0.1937	462	2245
				497		H	4.0110	-1.5888	1.4634	451		H	3.1714	0.2613	1.0700	497	
				509						468						506	
				540						514						534	
				568						530						551	
				574						544						569	
				670						553						577	
				679						569						630	
				725						575						688	
				730						689						716	
				870						713						721	
				874						724						724	
				891						742						785	
				909						862						877	
				944						881						881	
				945						881						899	
				947						907						909	
				948						912						939	
				949						945						946	
				950						946						946	

Reaction 8

Reactant												Product					
Silylene						Transition State						Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-0.4665	-1.0067	1.2081	11	942	Si	-0.5229	-0.5237	1.2773	-957	875	Si	-0.3824	-0.9650	0.8797	13	881
Si	1.5680	0.0914	0.5842	19	944	Si	1.6357	0.2433	0.6157	8	881	Si	1.6971	0.0901	0.4798	22	904

Si	1.5619	2.4332	0.2571	34	945	Si	1.7902	2.5060	1.2727	24	909	Si	1.5233	2.4364	0.6624	44	915
H	2.8842	2.8843	-0.2608	48	947	H	3.1425	3.0500	0.9647	44	920	H	2.8675	3.0615	0.5171	56	939
H	0.5103	2.8481	-0.7090	59	948	H	0.7832	3.3373	0.5549	60	943	H	0.6360	2.9882	-0.3985	70	944
H	1.3129	3.1278	1.5514	65	949	H	1.5480	2.6448	2.7359	72	945	H	0.9677	2.8249	1.9884	74	945
Si	3.2837	-0.4564	2.1132	73	950	Si	3.2115	-0.9893	1.8704	75	945	Si	3.2557	-0.6940	2.0716	76	946
H	2.9406	0.0210	3.4827	76	951	H	3.0424	-0.7356	3.3275	79	947	H	2.8600	-0.2712	3.4439	79	947
H	3.4746	-1.9332	2.1727	84	953	H	3.0380	-2.4503	1.6296	86	948	H	3.3304	-2.1813	2.0431	82	948
H	4.5810	0.1647	1.7215	86	953	H	4.6017	-0.6189	1.4837	88	948	H	4.6149	-0.1523	1.7901	92	950
Si	2.1250	-0.9195	-1.4913	90	2182	Si	2.1394	0.0687	-1.6820	91	949	Si	2.4534	-0.4730	-1.6838	94	950
H	1.3614	-0.2900	-2.6028	92	2218	H	1.1330	0.7967	-2.5034	93	950	H	1.4694	-0.0484	-2.7179	97	951
H	3.5817	-0.7738	-1.7644	95	2220	H	3.4820	0.6442	-1.9803	101	952	H	3.7527	0.1955	-1.9738	101	952
H	1.8050	-2.3752	-1.4786	101	2223	H	2.1392	-1.3611	-2.1016	103	953	H	2.6490	-1.9449	-1.8019	107	953
Si	-1.9469	0.0698	-0.3286	114	2224	Si	-2.1660	-0.3820	-0.4356	113	1675	Si	-2.1714	-0.1712	-0.4503	117	2195
H	-1.3656	0.9702	-1.3725	140	2228	H	-1.6266	-0.4906	-1.8259	130	1965	H	-1.6282	0.2551	-1.7764	148	2199
Si	-3.2798	-1.5473	-1.4195	295	2232	Si	-3.7397	-2.1089	-0.1181	151	2187	Si	-3.7327	-1.8963	-0.8326	298	2211
H	-3.9838	-2.3905	-0.4147	350	2233	H	-4.4540	-1.9304	1.1754	294	2218	H	-4.2362	-2.4292	0.4636	348	2222
H	-4.2983	-0.8957	-2.2897	392	2235	H	-4.7455	-2.1152	-1.2168	346	2220	H	-4.8979	-1.4000	-1.6173	390	2223
H	-2.4430	-2.4382	-2.2711	406	2237	H	-3.0638	-3.4374	-0.0965	351	2222	H	-3.1008	-3.0155	-1.5848	415	2224
Si	-3.3944	1.3976	0.9971	431	2237	Si	-3.2272	1.7166	-0.2705	407	2224	Si	-3.2106	1.6917	0.5523	435	2228
H	-4.1366	0.5440	1.9645	433	2240	H	-3.8559	1.8712	1.0708	425	2227	H	-3.8828	1.2793	1.8156	437	2230
H	-2.6317	2.4186	1.7685	438	2243	H	-2.2499	2.8260	-0.4545	433	2232	H	-2.2175	2.7517	0.8791	442	2236
H	-4.3791	2.1056	0.1331	448	2244	H	-4.2881	1.8540	-1.3070	440	2233	H	-4.2373	2.2746	-0.3557	450	2236
				474	2247	H	-0.3162	-2.0878	1.4412	445	2235	H	-0.7501	-0.8041	2.3182	457	2238
				495	2250	H	-0.0965	-1.9394	0.4712	450	2237	H	-0.2080	-2.4303	0.6467	473	2238
				497						466	2238					500	2240
				510						471	2239					507	2241
				533						515	2239					533	2242
				568						530	2242					544	2242
				570						536	2243					570	2244
				572						547	2246					575	2246
				582						570						577	
				683						575						584	

715	577	652
866	581	690
872	705	718
874	724	769
894	854	872
916	874	874

Reaction 9

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-0.5007	-0.0107	-0.1241	179		Si	-0.1814	0.1326	-0.5277	-1185	1953	Si	-0.2138	0.0347	-0.4846	229	2225
Si	-0.2576	0.7849	1.9864	357		Si	-0.1820	0.9124	1.7064	81	2217	Si	-0.2966	-0.0215	1.8584	229	2228
Si	1.7168	-0.0103	1.2024	413		Si	1.8026	0.0927	0.7123	348	2220	Si	1.7743	-0.0049	0.7590	351	2249
H	-0.0477	-1.2514	-0.8164	417		H	-0.7130	-1.1980	-0.9273	363	2239	H	-0.6053	-1.1819	-1.2435	374	2251
H	-1.2088	0.8302	-1.1334	440		H	-0.4590	1.1449	-1.5829	367	2247	H	-0.5994	1.2876	-1.1855	374	2262
H	2.9419	0.8296	1.3476	442		H	-0.3029	-0.7327	1.8399	368		H	-0.7412	-1.2698	2.5320	415	
H	2.1111	-1.2519	0.4766	498		H	-0.7973	-0.1657	2.6549	435		H	-0.7289	1.1999	2.5871	504	
				548		H	2.9009	1.0778	0.5160	490		H	2.6110	1.2221	0.8188	605	
				582		H	2.3570	-1.2595	0.9900	491		H	2.5902	-1.2473	0.7560	605	
				955						550						645	
				975						613						646	
				2200						679						669	
				2209						739						897	
				2217						926						898	
				2230						928						899	
										1667						2224	

Reaction 10

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	0.0808	-0.0064	0.0620	85	921	Si	-1.6549	-0.0131	0.1694	-965	935	Si	-0.4773	-0.0309	-0.1801	78	924
Si	-0.0982	-0.2697	2.4722	198	938	Si	0.0008	-1.6546	-0.4000	65	953	Si	-0.3577	0.3179	2.1612	196	946
Si	2.3033	-0.0066	2.1979	238	2179	Si	1.6549	-0.0115	0.1694	227	1708	Si	1.9833	-0.0150	1.9961	299	2206
Si	2.2184	-0.9952	0.0620	320	2188	Si	-0.0008	1.6526	-0.1494	301	1942	Si	1.5755	-1.2039	-0.0139	300	2207
H	3.2296	-0.4917	3.2619	364	2201	H	2.8507	0.0299	-0.7207	357	2204	H	2.7033	-0.6943	3.1100	381	2208
H	2.5571	1.4558	2.0016	389	2212	H	2.1517	-0.0386	1.5762	373	2205	H	2.6726	1.2764	1.7053	404	2214
H	0.2667	1.4560	-0.1993	407	2215	H	0.0009	-1.8498	1.2575	390	2212	H	-0.8743	1.5920	2.7360	415	2225
H	-1.0197	-0.4915	-0.8208	419	2221	H	0.0013	-2.7356	0.7630	400	2218	H	-0.9918	-0.8206	2.8884	415	2227
H	2.0933	-2.4769	0.1917	445		H	-2.1515	-0.0405	1.5762	413	2219	H	-0.2820	1.2568	-0.9088	432	2228
H	3.2307	-0.6977	-0.9920	457		H	-2.8508	0.0273	-0.7206	426	2229	H	-1.6671	-0.7218	-0.7528	459	2235
				576		H	-0.0010	2.1565	-1.5543	430		H	1.3260	-2.6461	0.2779	534	
				628		H	-0.0013	2.8242	0.7719	499		H	2.5608	-1.1113	-1.1281	561	
				635						548						631	
				702						577						661	
				710						634						662	
				905						665						729	
										708						730	
										744						739	
										843						917	
										921						917	

Reaction 11

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	

Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-0.1691	0.1675	-0.1368	81	2205	Si	0.3636	-2.0312	-0.1085	-894	931	Si	-0.6459	0.1475	-0.2884	11	927
Si	0.1263	0.1123	2.2419	82	2207	Si	1.9454	-0.2512	-0.2567	54	945	Si	-0.5224	0.2971	2.0781	69	947
Si	2.3554	0.0958	3.0241	156	2211	Si	0.8485	1.7567	0.3263	73	1683	Si	1.7528	-0.0371	2.6358	167	2206
Si	3.3690	-1.1600	1.3101	156	2217	Si	-1.4064	1.3763	-0.2616	174	1972	Si	2.5821	-1.3879	0.8851	188	2207
Si	2.1305	-0.3757	-0.5426	259	2223	Si	-1.7511	-0.9372	0.1092	216	2201	Si	1.5030	-0.5242	-1.0320	324	2209
H	2.5908	1.0479	-0.7266	310	2230	H	-2.3444	-1.1825	1.4567	331	2202	H	2.2510	0.6753	-1.5110	331	2210
H	2.3970	-1.0731	-1.8351	362		H	-2.7083	-1.4922	-0.8912	343	2205	H	1.4395	-1.5002	-2.1572	351	2217
H	-0.8196	0.9691	3.0160	366		H	0.4740	-1.6092	1.5187	361	2209	H	-1.0364	1.4527	-0.8949	371	2218
H	-0.3458	-1.3080	2.4204	379		H	0.6187	-2.5867	1.3550	362	2215	H	-1.6738	-0.8586	-0.6835	399	2225
H	2.4888	-0.4986	4.3849	409		H	3.1309	-0.5329	0.6048	391	2217	H	-1.0429	1.5988	2.5856	402	2226
H	2.9242	1.4744	3.0582	423		H	2.4290	-0.1849	-1.6671	399	2222	H	-1.3481	-0.7880	2.6844	420	2227
H	3.1410	-2.6172	1.5329	442		H	1.4207	2.9803	-0.3070	423	2227	H	1.9377	-0.6353	3.9886	443	2234
H	4.8355	-0.9330	1.1661	457		H	0.9391	1.9176	1.8082	434		H	2.4628	1.2759	2.6135	460	
				504		H	-1.6000	1.6781	-1.7109	456		H	2.1450	-2.7983	1.1050	465	
				609		H	-2.3593	2.2247	0.5106	462		H	4.0689	-1.3782	0.7786	574	
				616						521						595	
				629						570						604	
				674						608						634	
				705						640						662	
				741						652						705	
				762						683						732	
				897						735						749	
				897						759						750	
				922						772						769	
				940						858						917	
				2135						916						918	
				2135						923						927	

Reaction 12

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	0.0207	0.0312	0.0220	43	2195	Si	1.9916	1.1205	-0.2258	-872	922	Si	0.0400	0.0000	-0.0272	60	935
Si	-0.0245	-0.0512	2.3766	66	2201	Si	-0.0041	2.3947	-0.0142	51	934	H	0.0908	0.0000	1.4646	62	935
Si	2.1906	0.0310	3.1769	95	2203	Si	-1.9954	1.1136	-0.2259	58	948	H	1.4485	0.0000	-0.5207	105	954
Si	3.3466	1.8545	2.1782	98	2207	Si	-1.9239	-1.1635	0.3838	96	1666	Si	-1.0832	1.9445	-0.7519	117	2202
Si	3.6278	1.3101	-0.1325	127	2209	Si	0.0038	-2.2152	-0.4735	125	1984	H	-1.0582	1.9868	-2.2437	117	2204
Si	1.3688	1.8540	-0.6971	166	2215	Si	1.9280	-1.1569	0.3837	125	2195	H	-0.3793	3.1651	-0.2599	168	2204
H	2.2372	0.1554	4.6630	327	2217	H	-3.0567	1.8163	0.5560	199	2195	Si	-1.0832	-1.9445	-0.7519	336	2209
H	-0.7864	1.1186	2.9009	341	2218	H	-0.0031	1.8140	1.5787	306	2201	H	-0.3793	-3.1651	-0.2599	336	2209
H	-0.7077	-1.2914	2.8474	354	2230	H	-0.0049	2.8056	1.5188	323	2202	H	-1.0582	-1.9868	-2.2437	342	2214
H	0.6008	-1.2465	-0.4881	374		H	2.3799	1.2180	-1.6643	328	2209	Si	-3.3292	1.9445	-0.0281	380	2217
H	-1.3503	0.1568	-0.5530	381		H	3.0504	1.8267	0.5563	370	2209	H	-4.0331	3.1651	-0.5201	381	2218
H	2.5384	3.0780	2.4696	414		H	-1.8773	-1.2445	1.8743	374	2210	H	-3.3541	1.9868	1.4637	394	2220
H	4.6548	2.0099	2.8816	418		H	-3.1601	-1.8739	-0.0625	384	2215	Si	-3.3292	-1.9445	-0.0281	395	2222
H	0.8068	3.0773	-0.0468	429		H	0.0063	-3.6688	-0.1345	396	2216	H	-3.3541	-1.9868	1.4637	412	2222
H	1.1817	2.0105	-2.1704	439		H	0.0036	-2.1065	-1.9627	414	2222	H	-4.0331	-3.1651	-0.5201	458	2229
H	2.8745	-1.2465	2.8167	467		H	1.8818	-1.2380	1.8742	440		Si	-4.4524	0.0000	-0.7528	459	
				500		H	3.1666	-1.8629	-0.0627	459		H	-5.8609	0.0000	-0.2593	485	
				521		H	-2.3840	1.2097	-1.6645	473		H	-4.5031	0.0000	-2.2446	511	
				566						499						528	
				601						514						576	
				635						582						629	
				644						602						644	
				655						635						645	
				708						650						675	
				719						690						675	
				755						691						758	

771	757	759
919	763	768
922	785	768
937	791	789
940	870	919
955	913	920
2187	915	920

Reaction 13

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-2.9526	2.3457	-4.6691	104	2038	Si	-1.4627	-1.1501	-0.2500	-1122	901	Si	-0.2465	0.1269	-0.4634	80	907
H	-1.9421	2.7771	-5.7330	178	2149	Si	0.3526	-0.0666	0.7691	79	904	Si	-0.1990	-0.0376	1.8829	82	944
Si	-4.7117	2.9114	-6.0722	274	2233	Si	-1.4051	1.1886	-0.1587	80	1020	Si	1.8044	-0.0045	0.6492	97	951
H	-6.0237	2.9609	-5.3346	310	2246	H	-1.2363	-1.8225	-1.5555	130	1667	H	-0.7067	-1.0487	-1.2480	289	2213
Si	-3.7025	4.8517	-4.8552	386	2265	H	-2.4714	-1.8593	0.5817	316	2025	H	-0.6582	1.4143	-1.0818	308	2225
H	-2.3044	5.3429	-4.9110	400	2279	H	0.3625	-0.1125	2.2590	318	2183	H	-0.5109	1.2271	2.6074	335	2226
H	-4.4828	5.4167	-3.7287	426		H	-2.3442	1.8802	0.7633	335	2210	H	2.6716	1.2003	0.7216	365	2230
Si	-4.6718	5.0259	-7.0244	460		H	-1.1529	1.9818	-1.3909	371	2224	H	2.5911	-1.2609	0.5398	421	2240
H	-5.9426	5.7635	-7.2497	472		Si	2.5165	0.0050	-0.1429	390	2226	Si	-0.9034	-1.9943	2.9582	449	2245
H	-3.6542	5.3146	-8.0659	484		H	2.4428	1.0666	-1.2810	417	2249	H	-0.2625	-2.1331	4.2951	454	2251
				530		H	2.7687	-1.2381	-0.9393	456	2257	H	-2.3812	-2.0062	3.1413	525	2259
				558		H	1.6142	0.4267	-1.4817	525		H	-0.5193	-3.1650	2.1237	553	
				625						546						583	
				642						609						614	
				695						634						642	
				823						640						661	
				899						662						706	

				918						720					885		
										821					900		

Reaction 14

Reactant												Product					
Silylene							Transition State					Silane					
Atomic	Coordinates (Angtroms)			Frequency			Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}			Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-3.0578	2.7305	-5.0981	43	2031		Si	-0.6742	-1.6453	0.1330	-1129	918	Si	-0.4480	-0.1005	-0.4602	49	921
H	-3.9381	1.6891	-4.4004	84	2161		Si	0.8024	0.0704	-0.5902	49	921	Si	-0.3257	0.1626	1.8985	86	941
Si	-5.0203	3.5889	-5.8943	126	2208		Si	-0.7979	1.6493	0.1766	89	940	Si	2.0247	-0.1314	1.6968	90	948
H	-6.3608	3.0299	-5.5123	180	2217		Si	-2.4318	-0.0599	0.0173	109	1015	Si	1.6335	-1.2277	-0.3656	114	948
Si	-4.2800	4.7332	-3.7083	270	2228		H	-0.3881	-2.0215	1.5495	132	1669	H	-0.3036	1.2216	-1.1376	187	2192
H	-3.0283	5.5393	-3.7309	340	2235		H	-0.7696	-2.8973	-0.6694	187	2027	H	-1.6268	-0.7989	-1.0468	308	2204
H	-4.4769	4.1225	-2.3671	346	2244		H	0.7659	0.0866	-2.0865	315	2176	H	-0.9083	-1.0518	2.5491	322	2206
Si	-5.5088	5.7693	-6.6743	381	2249		H	-3.0447	-0.0723	-1.3432	318	2185	H	1.4138	-2.6856	-0.1345	373	2211
H	-6.6148	5.8692	-7.6649	406			H	-3.5264	-0.1233	1.0278	362	2203	H	2.6088	-1.0700	-1.4820	398	2222
H	-4.2989	6.4615	-7.1962	418			H	-1.0062	2.9087	-0.5938	377	2207	H	2.7560	-0.8538	2.7759	414	2225
Si	-5.9478	6.2800	-4.4256	438			H	-0.5459	2.0086	1.6029	401	2212	H	2.6946	1.1844	1.4789	420	2227
H	-7.3091	5.7936	-4.0671	494			Si	3.0706	-0.0487	0.0552	416	2223	Si	-1.1824	2.1036	2.9122	440	2231
H	-5.7740	7.6682	-3.9095	512			H	2.3254	0.0241	1.5445	421	2226	H	-0.6042	3.3109	2.2610	468	2237
				541			H	3.0622	-0.7505	1.4446	473	2232	H	-2.6651	2.1636	2.7803	485	2245
				572			H	3.5592	1.3159	0.4378	480		H	-0.8395	2.1421	4.3614	532	
				592							496						534	
				629							571						587	
				631							608						648	
				671							640						649	
				683							651						702	
				724							699						705	

					785							717							738	
					907							736							748	
					922							762							890	
					935							824							918	

Reaction 15

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	3.5759	0.0014	-0.0913	9	921	Si	1.3603	-0.0268	-0.8199	-1125	833	Si	-0.6368	0.0156	-0.1670	6	918
H	3.1186	-0.0647	-1.5507	23	926	Si	-0.1601	-1.8403	-0.8306	20	919	Si	-0.4923	-0.1561	2.1914	61	923
Si	1.3000	-0.0318	0.6004	42	941	Si	-1.8852	-1.1764	0.6446	45	924	Si	1.8116	0.0699	2.6573	86	928
H	1.1211	-0.0201	2.0871	116	2048	Si	-1.9792	1.1883	0.5018	86	928	Si	2.8578	-1.1006	0.8911	98	945
Si	0.0529	1.8110	-0.2382	153	2184	Si	-0.0626	1.8635	-0.7192	92	941	Si	1.4282	-0.8331	-0.9831	117	949
H	0.3507	1.9719	-1.6918	175	2205	H	-0.4552	2.2613	-2.1032	114	1006	H	2.0160	0.1138	-1.9744	163	949
H	0.3973	3.0965	0.4352	217	2208	H	0.6150	3.0365	-0.0929	192	1682	H	1.2309	-2.1385	-1.6780	183	2190
Si	-0.0049	-1.8305	-0.2367	322	2209	H	2.1960	-0.0321	-2.0577	209	2014	H	-0.7007	1.4691	-0.5135	324	2205
H	0.2908	-1.9994	-1.6898	336	2216	H	-0.7165	-2.0217	-2.2044	299	2176	H	-1.3422	0.8506	2.8896	337	2206
H	0.2977	-3.1263	0.4372	346	2217	H	0.4718	-3.1294	-0.4245	329	2189	H	-0.9505	-1.5115	2.6180	351	2208
Si	-2.2229	1.2093	0.0358	385	2223	H	-1.5384	-1.5783	2.0383	341	2202	H	2.1992	-0.4359	4.0053	388	2213
H	-2.7239	1.7262	1.3420	395	2225	H	-3.1909	-1.8097	0.3013	349	2205	H	2.1823	1.5138	2.5822	390	2219
H	-3.0785	1.7859	-1.0414	405	2232	H	-1.9820	1.8004	1.8613	384	2210	H	2.9400	-2.5490	1.2411	404	2223
Si	-2.2619	-1.1598	0.0299	434		H	-3.2202	1.6326	-0.1964	398	2215	H	4.2425	-0.6191	0.6191	442	2226
H	-3.1309	-1.6996	-1.0558	435		Si	2.5498	-0.1259	1.2254	409	2217	Si	-2.5132	-1.0695	-1.0845	450	2227
H	-2.7899	-1.6650	1.3300	445		H	3.1275	1.3087	1.4314	438	2221	H	-2.4593	-2.5241	-0.7713	453	2231
				465		H	3.8160	-0.8989	1.0094	452	2224	H	-3.7773	-0.5164	-0.5230	469	2238
				532		H	3.3543	1.0769	0.4069	465	2233	H	-2.5483	-0.9105	-2.5651	483	2242
				579						468						543	
				616						545						570	

617	585	593
657	604	621
692	631	643
712	648	685
727	670	708
747	703	726
769	723	732
782	733	757
917	749	767
	758	891

Reaction 16

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-1.1770	-2.6082	0.0000	18	920	Si	-1.4701	-1.9008	0.5077	-1126	783	Si	-0.6482	-0.3541	-0.3649	36	894
H	-1.1088	-4.0993	0.0000	37	920	Si	-2.7139	0.0814	0.2128	36	834	Si	-0.6228	-0.3024	1.9935	54	920
H	-2.6208	-2.2297	0.0000	65	928	Si	-1.3434	1.9851	0.4615	56	920	Si	1.5878	-0.2927	2.8178	78	920
Si	-0.1693	-1.7380	1.9481	90	936	Si	0.5124	1.8949	-0.9919	79	921	Si	2.8203	1.5032	1.9101	81	929
H	-0.8758	-2.2393	3.1645	104	950	Si	1.7800	-0.0821	-0.7176	95	929	Si	2.8206	1.4472	-0.4534	98	935
H	1.2432	-2.2127	2.0244	112	2048	Si	0.3768	-1.9706	-0.9595	102	935	Si	0.5987	1.4368	-1.2627	107	948
Si	-0.1693	0.6223	1.9023	119	2189	H	-2.1298	3.2266	0.1985	111	949	H	1.5855	-0.2143	4.3083	123	950
H	-1.5758	1.1181	1.8544	171	2199	H	-3.2916	0.0863	-1.1639	128	1011	H	-1.3098	0.9407	2.4530	137	951
H	0.4418	1.1608	3.1541	195	2200	H	-3.8539	0.1341	1.1745	140	1681	H	-1.3806	-1.4621	2.5487	194	2189
Si	0.9859	1.4421	0.0000	325	2203	H	-0.9802	-1.9605	1.9158	203	2016	H	-0.0516	-1.6413	-0.8277	321	2202
H	2.3372	0.7982	0.0000	342	2207	H	-2.3386	-3.0949	0.2885	315	2173	H	-2.0519	-0.3073	-0.8698	339	2203
Si	-0.1693	-1.7380	-1.9481	359	2214	H	0.0285	1.9547	-2.4031	336	2185	H	2.2054	2.7857	2.3641	358	2206
H	1.2432	-2.2127	-2.0244	368	2215	H	1.3872	3.0865	-0.7759	340	2200	H	4.2222	1.4757	2.4221	365	2208
H	-0.8758	-2.2393	-3.1645	379	2216	H	2.8031	-0.1495	-1.8062	360	2202	H	3.5011	2.6807	-0.9575	379	2214
Si	-0.1693	0.6223	-1.9023	400	2219	H	-0.1243	-2.0265	-2.3651	371	2205	H	-0.0614	2.7198	-0.8789	404	2215

H	-1.5758	1.1181	-1.8544	403	2222	H	1.1617	-3.2193	-0.7232	379	2208	H	0.5992	1.3652	-2.7537	409	2217
H	0.4418	1.1608	-3.1541	430	2229	H	-0.8538	2.0571	1.8687	405	2213	H	2.2513	-1.5752	2.4405	433	2219
Si	1.1074	3.8246	0.0000	447		Si	2.6734	-0.1201	1.4781	412	2214	Si	4.0225	-0.4149	-1.2552	451	2221
H	-0.4221	3.8966	0.0000	457		H	3.2283	1.3169	1.7220	425	2215	H	3.3994	-1.6811	-0.7802	459	2226
				479		H	3.9541	-0.8991	1.4475	456	2218	H	4.0353	-0.4335	-2.7444	476	2228
				487		H	3.5955	1.0562	0.7467	464	2222	H	5.4311	-0.3810	-0.7723	480	2240
				523						484	2228					512	2243
				580						503						525	
				598						536						575	
				638						578						578	
				652						584						630	
				656						630						636	
				676						636						672	
				721						670						675	
				756						678						699	
				761						705						708	
				767						722						755	
				786						758						760	
				787						761						769	
										771						783	

Reaction 17

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-3.1630	2.9862	-5.0129	53	955	Si	-5.3186	2.1284	-6.6255	-1137	943	Si	-5.3365	2.2889	-6.3338	48	944
H	-2.3429	3.4044	-6.2365	64	2021	H	-6.0917	1.2512	-5.7000	48	945	H	-6.1465	1.5733	-5.3072	58	945
Si	-4.9297	2.3287	-6.3771	75	2151	Si	-6.4448	4.0812	-7.3203	58	951	Si	-6.3889	4.1889	-7.2415	64	950
H	-6.1858	2.0609	-5.5927	89	2223	Si	-6.1758	2.2862	-8.8094	66	953	Si	-6.2103	2.2205	-8.5163	65	951

Si	-4.8045	4.7850	-5.8859	97	2227	Si	-5.2867	6.0954	-7.6129	69	1015	Si	-5.1796	6.1058	-7.8276	88	953
Si	-5.6470	3.8766	-7.9468	122	2232	H	-5.1044	6.8094	-6.3183	94	1673	H	-4.9545	6.9827	-6.6448	94	2210
Si	-3.2356	6.4627	-6.3873	151	2234	H	-3.9443	5.8048	-8.1854	95	2029	H	-3.8570	5.6969	-8.3729	98	2212
H	-2.3016	6.6964	-5.2553	210	2246	H	-6.0146	6.9993	-8.5465	114	2182	H	-5.8993	6.8945	-8.8655	120	2217
H	-2.4668	6.0627	-7.5919	259	2252	Si	-7.8791	0.8771	-9.5998	129	2203	Si	-8.0982	0.9328	-9.0229	134	2227
H	-3.9647	7.7311	-6.6683	305	2257	H	-8.2371	0.8907	-7.9736	145	2207	H	-7.7257	-0.4850	-9.2853	325	2227
Si	-7.8941	4.0816	-8.5970	367	2268	H	-9.1660	1.6370	-9.6968	323	2214	H	-9.0330	0.9731	-7.8662	329	2231
H	-8.2122	3.1125	-9.6812	421		H	-8.1944	-0.0838	-8.4168	334	2226	H	-8.8028	1.4621	-10.2236	353	2239
H	-8.7643	3.8019	-7.4249	452		H	-5.1187	2.5216	-9.8341	350	2228	H	-5.1812	2.2732	-9.5933	423	2240
H	-8.1713	5.4574	-9.0930	466		H	-7.8125	4.2301	-6.7484	386	2238	H	-7.7458	4.4582	-6.6865	445	2241
H	-4.6634	4.1716	-9.0257	494		Si	-3.0066	2.1047	-6.2571	429	2239	Si	-3.0240	2.2113	-5.9781	455	2245
H	-5.8863	5.2115	-4.9577	502		H	-2.4569	0.7294	-6.4132	452	2245	H	-2.5336	0.8053	-5.9711	461	2248
				511		H	-2.3453	2.9962	-7.2476	458	2251	H	-2.3398	2.9476	-7.0749	481	2250
				526		H	-2.6743	2.5885	-4.8878	463		H	-2.6557	2.8432	-4.6805	506	
				528						512						547	
				549						531						549	
				611						549						550	
				624						556						556	
				698						581						594	
				708						613						649	
				727						649						692	
				821						696						702	
				880						704						729	
				891						735						884	
				939						819						884	
				943						885						905	
				948						899						943	

Reaction 18

Reactant												Product					

Silylene						Transition State						Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-3.4023	3.4518	-4.6565	37	943	Si	-5.3048	2.6190	-6.0952	-1139	914	Si	-5.1851	2.7869	-6.0857	39	942
H	-2.4359	3.7890	-5.7946	44	945	H	-6.5512	2.0913	-5.4688	43	942	H	-6.3650	2.1951	-5.3918	48	943
Si	-4.9810	2.6462	-6.1523	55	946	Si	-5.1835	4.9676	-5.9764	46	944	Si	-5.1493	5.1408	-6.0751	58	944
H	-6.3044	2.3651	-5.4951	60	949	Si	-5.7240	3.8954	-8.0243	53	945	Si	-5.7203	3.9648	-8.0521	62	946
Si	-4.9903	5.1460	-5.9221	63	950	Si	-3.0849	5.9989	-5.7728	64	947	Si	-3.0636	6.2153	-6.0002	66	947
Si	-5.5250	3.9964	-7.9717	79	956	H	-2.0295	5.1467	-6.3873	64	948	H	-2.0504	5.4313	-6.7566	70	948
Si	-3.2795	6.7214	-6.3091	90	2028	H	-3.0703	7.3241	-6.4521	69	949	H	-3.1483	7.5778	-6.5962	75	950
H	-2.3669	6.2493	-7.3803	91	2152	H	-2.7385	6.2089	-4.3387	71	951	H	-2.5995	6.3534	-4.5913	83	951
H	-3.9145	7.9984	-6.7432	103	2223	Si	-7.9430	4.0380	-8.7790	78	953	Si	-7.9772	3.9399	-8.6984	87	952
H	-2.4941	6.9895	-5.0763	107	2226	H	-8.2470	2.9197	-9.7153	86	1014	H	-8.2666	2.7409	-9.5336	89	955
Si	-7.7618	4.0022	-8.7059	116	2227	H	-8.8796	3.9576	-7.6259	91	1676	H	-8.8507	3.9018	-7.4949	93	2209
H	-8.0064	2.8544	-9.6222	126	2231	H	-8.1870	5.3206	-9.4972	94	2032	H	-8.3195	5.1518	-9.4943	96	2222
H	-8.6751	3.8900	-7.5377	144	2239	Si	-4.0837	3.9046	-9.7025	97	2181	Si	-4.1669	3.9578	-9.8124	108	2223
H	-8.0694	5.2612	-9.4393	189	2241	H	-4.2978	2.7738	-10.6484	109	2204	H	-4.3685	2.7641	-10.6805	121	2225
Si	-3.9054	4.1980	-9.6674	236	2243	H	-4.1324	5.1742	-10.4806	132	2221	H	-4.3214	5.1761	-10.6554	146	2226
H	-4.2028	3.1968	-10.7293	260	2249	H	-2.7273	3.7718	-9.1054	162	2222	H	-2.7783	3.9251	-9.2797	267	2231
H	-3.9442	5.5538	-10.2806	320	2250	Si	-6.9234	6.0185	-4.8004	266	2224	Si	-6.8779	6.1991	-4.8902	284	2234
H	-2.5448	3.9431	-9.1291	396	2253	H	-8.1838	5.2437	-4.9556	285	2228	H	-8.1161	5.3773	-4.9570	328	2236
Si	-6.8235	6.0142	-4.7307	442	2259	H	-6.5934	6.1047	-3.3503	326	2234	H	-6.4983	6.3707	-3.4600	422	2238
H	-7.8176	4.9473	-4.4400	452	2266	H	-7.1529	7.4017	-5.3048	384	2235	H	-7.1722	7.5456	-5.4558	445	2240
H	-6.3554	6.6004	-3.4449	455		Si	-3.4988	1.1622	-5.7280	423	2237	Si	-3.2384	1.5005	-5.8834	455	2240
H	-7.4945	7.0894	-5.5141	485		H	-2.2777	2.0705	-5.4072	438	2237	H	-3.4443	0.1366	-6.4449	461	2241
				500		H	-3.0646	0.5566	-7.0273	456	2240	H	-2.1308	2.1582	-6.6265	482	2243
				510		H	-2.6748	2.4857	-6.3119	463	2243	H	-2.8384	1.3647	-4.4552	487	2246
				516						488	2245					507	2250
				529						505	2251					511	2254
				537						517						521	
				545						520						540	

549	533	547
568	545	552
586	556	558
597	566	570
669	605	599
794	611	610
865	611	711
875	727	869
881	821	877
910	869	884
939	877	884
941	884	921

Reaction 19

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	0.6021	0.6885	0.2008	32	2195	Si	0.2790	0.9350	0.2208	-1196	926	Si	0.4374	0.8815	0.2225	65	924
Si	0.4839	0.5151	2.5645	42	2207	Si	0.1662	0.7592	2.5813	66	934	Si	0.3236	0.7122	2.5842	83	933
Si	2.6873	0.0953	3.3124	70	2210	Si	2.3592	0.8119	3.4142	79	945	Si	2.5003	0.9938	3.4174	111	947
Si	4.1271	0.7486	1.5692	152	2217	Si	3.7155	0.3490	1.5300	113	1625	Si	3.8900	0.5640	1.5526	150	2205
Si	2.8717	0.3911	-0.3893	172	2221	Si	2.5403	1.0882	-0.3880	162	1955	Si	2.6798	1.2703	-0.3525	192	2206
H	3.0986	-0.9790	-0.9325	280	2224	H	2.8763	0.2687	-1.5881	206	2200	H	3.1082	0.5577	-1.5904	338	2212
H	3.2053	1.3597	-1.4732	309	2232	H	2.9007	2.5038	-0.6964	217	2201	H	2.8880	2.7315	-0.5757	342	2216
H	2.9107	0.8694	4.5674	356		H	2.6767	2.1684	3.9514	330	2206	H	2.6800	2.4051	3.8693	345	2220
H	2.8644	-1.3480	3.6438	366		H	2.5900	-0.1699	4.5131	334	2207	H	2.8138	0.1049	4.5729	361	2221
H	4.3878	2.2110	1.6994	377		H	5.0350	1.0356	1.6425	357	2213	H	5.2076	1.2528	1.6662	384	2222
H	5.4387	0.0367	1.5770	412		H	3.9835	-1.1156	1.4359	370	2216	H	4.1484	-0.9022	1.4563	394	2227
Si	-0.8385	-0.9074	1.2044	424		Si	-0.6074	-1.0080	1.2234	397	2218	Si	-0.0438	-1.1682	1.2424	419	2230

H	-0.2875	1.3619	3.5227	454		H	-0.8810	1.4614	3.3783	400	2226	H	-0.8210	1.2652	3.3602	426	2255
H	-0.0920	1.6648	-0.6913	478		H	-0.6934	1.7538	-0.5598	424		H	-0.6341	1.5448	-0.5714	444	
				489		H	1.0342	-1.2407	1.2847	429		H	0.9112	-2.3067	1.2082	485	
				501		H	0.4059	-2.1896	1.1844	444		H	-1.4565	-1.6189	1.1406	499	
				542						482						503	
				544						490						517	
				620						515						561	
				624						566						591	
				637						573						600	
				682						607						643	
				701						644						652	
				743						652						654	
				751						696						670	
				919						715						717	
				930						735						745	
				945						747						756	
				2192						757						905	

Reaction 20

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	0.0393	-0.6630	1.5890	45	931	Si	-0.0800	-0.3898	1.6262	-1028	735	Si	0.0890	-0.6622	1.6241	31	732
Si	1.8205	-1.1340	0.0000	48	945	Si	1.5692	-0.2243	-0.0715	25	824	Si	1.7229	-0.9368	-0.0816	78	890
Si	0.0393	-0.6630	-1.5890	61	949	Si	-0.1346	-0.3560	-1.7174	80	891	Si	0.0324	-0.6244	-1.7248	81	895
Si	-1.6529	-1.1160	0.0000	83	951	Si	-1.6892	0.3436	-0.0126	93	895	Si	-1.5815	-1.0333	-0.0271	99	919
H	0.0734	-1.5161	-2.8199	84	951	H	-0.2975	-1.7747	-2.1614	98	928	H	0.0420	-1.6102	-2.8477	106	938
H	0.0734	-1.5161	2.8199	90	2167	H	-0.2285	-1.8176	2.0457	101	947	H	0.1360	-1.6705	2.7258	106	948
H	-2.0067	-2.5663	0.0000	112	2169	H	-2.0385	-1.2842	-0.0240	104	948	H	-2.0427	-2.4528	-0.0352	114	949

H	-2.9239	-0.3324	0.0000	239	2194	H	-2.8829	-0.6987	-0.0038	129	948	H	-2.7891	-0.1584	0.0043	237	950
Si	0.0393	1.5607	2.3901	326	2213	Si	0.1327	0.9449	3.5525	192	948	Si	0.0451	1.4954	2.5640	337	951
H	-0.0214	2.5447	1.2768	340	2226	H	0.2939	2.3740	3.1648	312	1704	H	0.0018	2.5237	1.4881	345	2197
H	-1.1370	1.7818	3.2766	361	2228	H	-1.0759	0.8306	4.4171	331	1935	H	-1.1555	1.6721	3.4278	354	2199
H	1.2771	1.8208	3.1768	376	2239	H	1.3202	0.5425	4.3583	366	2189	H	1.2596	1.7366	3.3919	402	2203
Si	0.0393	1.5607	-2.3901	414	2240	Si	0.0130	1.0200	-3.6206	389	2191	Si	-0.0424	1.5512	-2.6198	410	2210
H	-1.1370	1.7818	-3.2766	422	2247	H	-1.2256	0.9252	-4.4442	391	2207	H	-1.2667	1.7429	-3.4464	424	2220
H	-0.0214	2.5447	-1.2768	456	2261	H	0.1892	2.4401	-3.2071	402	2220	H	-0.0570	2.5583	-1.5232	445	2223
H	1.2771	1.8208	-3.1768	464		H	1.1708	0.6354	-4.4768	411	2222	H	1.1483	1.8106	-3.4763	471	2226
				486		H	2.6412	-1.2600	-0.0990	458	2227	H	2.2692	-2.3256	-0.1075	481	2229
				494		H	2.2213	1.1187	-0.0690	477	2232	H	2.8756	0.0097	-0.0902	491	2240
				544						480	2233					528	2240
				559						513	2239					548	2241
				631						516	2240					549	2248
				658						540						631	
				679						549						638	
				686						629						663	
				715						666						690	
				874						691						698	
				892						731						724	

Reaction 21

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-0.2389	-0.0485	-0.3155	11	900	Si	0.5274	0.4166	0.8070	-968	753	Si	0.1243	0.5181	0.7466	10	763
Si	-2.0267	-1.6024	-0.5119	19	917	Si	-0.0035	2.3760	2.0437	7	759	Si	-0.2811	2.5767	1.8486	17	770
Si	-3.9015	-0.5297	0.4604	27	921	Si	0.7527	4.2278	0.7733	13	859	Si	1.3283	4.0545	0.9533	27	880
Si	-3.4951	1.7920	0.2208	29	926	Si	1.1318	3.3772	-1.3973	23	879	Si	1.4220	3.4455	-1.3272	38	907

Si	-1.3905	1.9572	-0.8543	56	942	Si	1.8625	1.1664	-1.0021	47	912	Si	1.0293	1.1071	-1.3720	61	917
H	-1.5935	2.0074	-2.3321	63	946	H	1.7380	0.2929	-2.2053	57	918	H	0.0883	0.7551	-2.4746	73	922
H	-0.6302	3.1787	-0.4620	83	949	H	3.3008	1.1854	-0.6021	74	924	H	2.2976	0.3598	-1.6113	82	927
H	0.1159	0.0248	1.1379	91	950	H	1.3058	-0.5444	1.6454	81	929	H	1.1891	-0.2016	1.5113	93	931
H	-2.2905	-1.8446	-1.9608	93	953	H	-1.4798	2.4522	2.2552	96	944	H	-1.6468	3.0656	1.4955	98	943
H	-1.7158	-2.9193	0.1149	95	2171	H	0.6344	2.3421	3.3918	101	945	H	-0.2144	2.4465	3.3324	104	946
H	-3.9900	-0.8874	1.9055	114	2173	H	2.0458	4.7072	1.3439	107	948	H	2.6488	3.7810	1.5930	119	949
H	-5.1752	-0.9477	-0.1933	144	2205	H	-0.2097	5.3660	0.8021	124	949	H	1.0014	5.4938	1.1638	152	951
H	-3.4317	2.4416	1.5617	173	2207	H	2.1076	4.1894	-2.1789	157	952	H	2.7119	3.8156	-1.9770	170	953
H	-4.5676	2.4680	-0.5646	188	2209	H	-0.1546	3.3485	-2.1525	173	1675	H	0.3248	4.1384	-2.0644	190	2187
Si	1.4292	-0.5408	-1.9368	326	2217	Si	-1.4850	-0.4561	-0.0980	215	1971	Si	-1.7947	-0.8489	0.6279	319	2188
Si	3.2580	-0.8264	-0.4196	330	2218	Si	-1.5261	-2.8317	-0.2618	315	2185	Si	-1.3837	-3.0750	-0.0535	334	2202
H	4.4941	-1.1756	-1.1914	333	2222	H	-2.9587	-3.2222	-0.0681	334	2190	H	-2.6960	-3.7946	-0.0215	346	2205
Si	3.7724	1.1544	0.7673	356	2223	Si	-0.9403	-3.4305	-2.4664	349	2202	Si	-0.5571	-3.2068	-2.2567	352	2207
H	2.6754	1.5028	1.7101	385	2226	H	0.4488	-2.9867	-2.7728	349	2204	H	0.7730	-2.5449	-2.3537	379	2209
H	5.0312	0.9835	1.5456	396	2227	H	-1.0039	-4.9073	-2.6518	354	2207	H	-0.3980	-4.6299	-2.6671	390	2213
H	3.9602	2.2979	-0.1695	409	2233	H	-1.8579	-2.7896	-3.4491	384	2212	H	-1.4827	-2.5411	-3.2146	399	2214
Si	2.9398	-2.5840	1.1305	423	2236	Si	-0.2289	-4.0316	1.2975	401	2218	Si	0.0637	-4.1664	1.4533	420	2222
H	4.1671	-2.7836	1.9511	430	2238	H	-0.3620	-5.5019	1.0894	408	2220	H	0.1962	-5.6081	1.1029	431	2224
H	1.8040	-2.2826	2.0430	434	2246	H	1.2110	-3.6765	1.1633	423	2221	H	1.4190	-3.5510	1.4116	443	2225
H	2.6430	-3.8617	0.4238	440	2250	H	-0.6611	-3.7123	2.6872	431	2225	H	-0.4507	-4.0669	2.8476	448	2226
				444		H	-2.5560	-0.1476	1.0269	443	2226	H	-2.7654	-0.2122	-0.3106	449	2230
				455		H	-1.8769	-0.7083	1.5183	445	2230	H	-2.4467	-0.8834	1.9715	456	2231
				464						456	2234					466	2239
				494						461	2238					478	2241
				525						467	2240					509	2242
				557						494	2242					522	2245
				573						522						556	
				575						544						575	
				615						564						589	
				654						573						615	
				674						604						630	

691	627	639
706	641	683
712	658	692
721	689	697
734	696	720
754	709	727
765	722	732
873	742	755

Reaction 22

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	2.2096	-1.6770	1.1709	22	901	Si	0.6082	2.0777	1.6468	-898	767	Si	-0.2279	2.5899	0.5812	15	766
Si	3.1469	-0.7220	-1.0454	32	920	Si	2.8798	2.4280	-1.9453	13	779	Si	3.8932	2.4791	0.5434	21	780
Si	3.8191	1.5470	-0.5892	51	921	Si	2.1401	4.5484	-1.2772	23	793	Si	3.2302	2.4033	-1.6965	27	789
Si	3.6225	0.1663	1.2538	65	921	Si	2.4030	2.8392	0.3179	37	887	Si	1.8483	3.4455	-0.1034	43	900
H	1.8956	-0.6112	-1.8330	67	931	H	1.9379	1.5979	-2.7397	39	903	H	3.8684	1.2087	1.3143	61	901
H	4.1805	-1.5622	-1.6956	84	937	H	4.2907	2.2499	-2.3811	60	905	H	5.0071	3.3705	0.9600	70	919
H	2.7533	2.5174	-0.9332	94	951	H	0.7571	4.9522	-1.6479	74	918	H	2.8157	1.0896	-2.2539	82	919
H	5.1755	2.0223	-0.9675	106	2133	H	3.0720	5.7065	-1.2696	80	919	H	3.9169	3.2518	-2.7053	95	928
H	5.0416	-0.3424	1.2870	123	2155	H	3.6402	3.0070	1.1347	92	928	H	1.8983	4.9353	-0.1698	103	935
Si	-1.2791	-2.0028	-0.5364	144	2191	Si	0.6180	-1.3247	-0.6291	101	934	Si	-0.8879	-0.5232	-1.6956	118	939
Si	0.0243	-0.6718	0.9240	144	2195	Si	-0.0718	-0.1790	1.3186	120	949	Si	-0.3449	0.2313	0.4774	125	949
Si	-0.3949	1.6009	0.4127	165	2199	Si	-2.4230	-0.3101	1.5439	124	1676	Si	-1.9194	-0.5982	2.0336	147	2194
Si	-2.6859	2.1438	0.5871	213	2202	Si	-3.1843	-2.5447	1.5403	153	1970	Si	-2.0787	-2.9517	1.9522	169	2200
Si	-3.9808	0.7794	-0.8358	260	2204	Si	-2.4544	-3.6914	-0.3876	193	2186	Si	-2.6040	-3.6865	-0.2271	285	2201
Si	-3.5817	-1.5048	-0.4027	298	2208	Si	-0.1083	-3.5716	-0.6002	294	2200	Si	-1.0283	-2.8774	-1.7852	308	2203
H	0.4054	2.4941	1.3046	315	2210	H	-2.8575	0.3821	2.7926	306	2201	H	-1.5534	-0.1502	3.4094	318	2206

H	-0.5943	-0.8752	2.2764	339	2213	H	0.5053	-0.9285	2.4789	316	2204	H	0.9897	-0.3359	0.8433	335	2208
H	-0.8284	-1.7794	-1.9439	358	2217	H	0.0305	-0.6455	-1.8210	331	2207	H	-2.2101	0.0562	-2.0753	336	2209
H	-1.0613	-3.4514	-0.2433	365	2224	H	2.1023	-1.2701	-0.7705	336	2208	H	0.1129	-0.0266	-2.6842	361	2214
H	-3.1268	1.9333	1.9975	383	2238	H	-2.6437	-3.2316	2.7498	357	2213	H	-0.7660	-3.5356	2.3562	364	2216
H	-2.9084	3.5856	0.2653	391	2246	H	-4.6737	-2.5781	1.6360	363	2215	H	-3.1014	-3.4346	2.9265	372	2216
H	-5.4317	1.0983	-0.6857	395	2275	H	-2.9076	-5.1128	-0.3451	371	2216	H	-2.6671	-5.1768	-0.2741	383	2217
H	-3.6077	1.0765	-2.2508	398	2283	H	-3.0804	-3.0596	-1.5865	382	2218	H	-3.9548	-3.1702	-0.5966	396	2220
H	-4.0682	-1.8232	0.9722	406		H	0.5178	-4.2710	0.5603	387	2221	H	0.3112	-3.4516	-1.4632	401	2221
H	-4.3616	-2.3510	-1.3549	426		H	0.3346	-4.2789	-1.8383	396	2222	H	-1.3844	-3.3220	-3.1650	418	2227
H	0.0486	1.8915	-0.9845	448		H	-3.0479	0.4208	0.4006	401	2225	H	-3.2544	-0.0092	1.7179	420	2228
				458		H	-0.2908	2.3715	0.2491	414	2227	H	-1.3074	3.1610	-0.2773	447	2230
				464		H	-0.6027	2.9002	1.0329	435	2247	H	-0.4983	3.0457	1.9772	461	2252
				469						456	2257					466	2260
				482						466						479	
				493						472						486	
				498						481						505	
				512						486						516	
				519						513						520	
				529						517						535	
				557						524						595	
				597						551						602	
				623						596						616	
				638						616						637	
				639						631						640	
				654						637						649	
				676						639						655	
				693						653						664	
				719						661						675	
				760						674						682	
				766						706						690	
				778						721						726	
				782						737						756	

792 760 762

Reaction 23

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	0.0363	-0.8619	0.9389	23	928	Si	0.0760	-1.0681	0.5963	-896	879	Si	-0.0714	-0.9202	0.9245	25	919
H	-0.6101	-0.5983	2.2653	29	932	H	0.0011	-0.6306	2.0268	14	919	H	-0.5519	-0.5804	2.3005	33	920
Si	0.0044	1.1810	-0.2699	37	941	Si	-0.1065	0.8854	-0.7290	30	921	Si	0.0036	1.1059	-0.3015	46	923
H	-0.0405	0.8275	-1.7229	56	947	H	-0.5317	0.4159	-2.0863	41	924	H	0.0515	0.7249	-1.7489	57	926
Si	2.0306	2.3217	0.1151	66	2169	Si	1.9387	2.0546	-0.9991	64	929	Si	1.9793	2.2989	0.1883	69	929
H	2.1065	2.6788	1.5624	74	2184	H	1.7181	3.5224	-0.8420	68	931	H	2.0493	2.4879	1.6673	84	933
H	2.1200	3.5890	-0.6669	80	2192	H	2.4362	1.8325	-2.3891	84	942	H	1.9612	3.6567	-0.4309	91	942
Si	3.8272	0.8742	-0.4222	111	2200	Si	3.5782	1.3138	0.5220	89	947	Si	3.8901	1.0960	-0.5228	112	948
H	4.8427	0.8979	0.6713	116	2202	H	3.0818	1.5485	1.9108	115	1676	H	5.0254	1.3835	0.4023	119	2179
H	4.5068	1.3359	-1.6680	133	2203	H	4.8384	2.0989	0.3641	122	1975	H	4.2941	1.5654	-1.8806	135	2188
Si	3.0515	-1.3482	-0.7645	149	2206	Si	4.0061	-0.9913	0.2653	134	2176	Si	3.5023	-1.2350	-0.6016	148	2201
H	4.2099	-2.1892	-1.1896	166	2206	H	5.0004	-1.4079	1.2982	164	2180	H	4.7980	-1.9733	-0.5450	169	2202
H	2.1158	-1.2701	-1.9283	198	2211	H	4.6392	-1.2467	-1.0627	169	2199	H	2.8617	-1.5618	-1.9098	193	2203
Si	2.0369	-2.1199	1.2568	300	2213	Si	2.0695	-2.3616	0.5043	209	2200	Si	2.0601	-1.9395	1.1260	302	2205
Si	-3.8053	0.7909	0.3303	330	2215	Si	-3.6451	0.9426	0.9413	292	2201	Si	-3.8514	0.8811	0.3416	330	2206
Si	-2.0042	2.3247	0.2144	344	2217	Si	-1.8567	2.2443	0.1006	335	2203	Si	-1.9991	2.3209	0.0317	342	2208
H	-1.8842	3.0525	1.5111	357	2218	H	-1.3376	3.1245	1.1884	341	2206	H	-1.8576	3.2071	1.2239	356	2211
H	-2.2726	3.3409	-0.8456	359	2223	H	-2.3495	3.1357	-0.9908	351	2207	H	-2.2339	3.2017	-1.1502	358	2214
Si	-1.4933	-2.3319	-0.1432	366	2225	Si	-1.8230	-2.4297	0.2211	357	2211	Si	-1.6926	-2.3461	-0.0400	366	2215
H	-0.8274	-3.0385	-1.2765	377	2229	H	-1.5781	-3.3079	-0.9618	365	2213	H	-1.0814	-3.1063	-1.1695	371	2216
H	-1.9330	-3.3770	0.8270	381		H	-2.0263	-3.3232	1.3988	373	2214	H	-2.1290	-3.3459	0.9788	384	2218
Si	-3.3709	-1.1383	-0.9572	394		Si	-3.7716	-1.1389	-0.1604	380	2215	Si	-3.5678	-1.1414	-0.8389	398	2218
H	-4.5624	-2.0368	-0.9881	410		H	-4.9826	-1.8980	0.2693	387	2216	H	-4.7975	-1.9824	-0.7515	401	2220

H	-3.0876	-0.7244	-2.3626	423	H	-3.8982	-0.8947	-1.6276	395	2220	H	-3.3489	-0.8229	-2.2807	410	2223
H	-3.9976	0.3793	1.7516	434	H	-3.4116	0.6943	2.3947	406	2222	H	-3.9682	0.5690	1.7967	443	2226
H	-5.0715	1.4392	-0.1211	443	H	-4.9332	1.6866	0.8191	435	2226	H	-5.1126	1.5650	-0.0694	448	2229
				456	H	1.9640	-3.0712	-0.9112	442		H	2.6533	-1.5511	2.4401	452	
				462	H	1.9098	-2.1047	-1.1552	454		H	1.9274	-3.4259	1.1224	470	
				472					462						476	
				480					471						483	
				483					479						487	
				535					483						492	
				540					488						535	
				594					504						549	
				598					532						597	
				605					575						605	
				622					599						618	
				626					620						624	
				681					623						635	
				688					634						656	
				698					648						683	
				706					676						694	
				722					693						707	
				730					704						716	
				744					716						733	
				747					730						739	
				767					750						749	
				775					754						760	
				783					763						764	
				917					769						767	
				921					774						780	
				923					787						785	

Reaction 24

Reactant						Transition State						Product					
Silylene												Silane					
Atomic Symbol	Coordinates (Angtroms) X	Y	Z	Frequency cm^{-1}		Atomic Symbol	Coordinates (Angtroms) X	Y	Z	Frequency cm^{-1}		Atomic Symbol	Coordinates (Angtroms) X	Y	Z	Frequency cm^{-1}	
Si	0.6360	-1.3378	0.0934	16	2178	Si	0.3381	-1.1348	0.1466	-810	952	Si	0.2313	-1.2411	0.1274	24	952
Si	-0.3473	-0.5031	2.1092	30	2183	Si	-0.7463	-0.5321	2.1693	11	954	Si	-0.6777	-0.2621	2.0843	26	953
Si	0.0458	1.7738	2.5798	38	2188	Si	-0.1835	1.6234	2.9431	20	967	Si	0.2434	1.8351	2.6466	35	955
H	-0.5681	2.1251	3.8906	46	2217	H	-0.7885	1.8680	4.2816	29	1680	H	-0.4469	2.3857	3.8463	49	2173
H	1.5078	2.0482	2.6623	50	2223	H	1.2941	1.7773	3.0700	49	1986	H	1.6945	1.7126	2.9562	58	2187
H	-0.5384	2.6556	1.5353	64	2225	H	-0.6750	2.6719	2.0085	54	2174	H	0.0837	2.8070	1.5311	62	2188
Si	-2.6471	-1.0283	2.1744	73	2226	Si	-3.0913	-0.7778	2.0928	61	2185	Si	-3.0322	-0.1339	2.0187	74	2203
H	-3.3761	-0.3214	1.0870	77	2228	H	-3.7068	0.2913	1.2603	76	2190	H	-3.4753	0.8602	1.0029	78	2215
H	-2.8439	-2.4936	2.0063	80	2230	H	-3.4715	-2.0991	1.5218	78	2220	H	-3.6288	-1.4541	1.6750	86	2225
H	-3.2334	-0.6137	3.4799	87	2237	H	-3.6528	-0.6781	3.4691	87	2223	H	-3.5583	0.2908	3.3462	89	2226
Si	2.9439	-1.2223	0.6411	94	2239	Si	2.6876	-1.1379	0.5327	93	2224	Si	2.5937	-1.3681	0.2068	94	2229
H	0.2063	-2.7740	0.1260	95	2240	H	-0.0020	-2.5812	-0.0468	95	2227	H	-0.2535	-2.6587	0.1429	96	2230
Si	3.3732	0.9561	-0.2677	96	2242	Si	3.9868	-0.4927	-1.3413	98	2229	Si	3.7307	0.6028	-0.3975	102	2233
H	4.4101	1.6873	0.5152	111	2245	H	4.4746	-1.7300	-2.0115	102	2236	H	3.4308	0.9665	-1.8097	108	2237
H	3.9662	0.6563	-1.6100	115	2248	H	3.3101	0.3325	-2.3789	106	2237	H	3.3312	1.7422	0.4725	119	2239
H	2.2281	1.8859	-0.4867	127	2254	H	5.1695	0.2607	-0.8357	116	2238	H	5.2013	0.4060	-0.2673	121	2241
Si	-1.7817	-2.0191	-2.8062	168	2257	Si	-2.5319	-0.8081	-2.5216	128	2239	Si	-2.5745	-1.2594	-2.5705	170	2242
Si	-0.2676	-0.4427	-1.9186	206		Si	-0.4150	-0.0428	-1.8164	175	2240	Si	-0.5118	-0.3152	-1.9263	210	2242
Si	-1.2783	1.6842	-1.7971	291		Si	-0.3655	2.3089	-1.6652	200	2240	Si	-0.6270	2.0395	-1.9512	288	2244
H	-1.8309	2.0395	-3.1345	337		H	-0.5064	2.9138	-3.0187	284	2242	H	-0.9386	2.5137	-3.3283	336	2245
H	-2.3998	1.6800	-0.8185	348		H	-1.4804	2.8071	-0.8134	351	2245	H	-1.6996	2.5208	-1.0379	358	2248
H	-0.3032	2.7329	-1.3957	389		H	0.9173	2.7811	-1.0725	366	2247	H	0.6611	2.6505	-1.5237	379	2249
H	-2.9194	-2.2274	-1.8680	418		H	-3.5752	-0.4896	-1.5092	371	2252	H	-3.6185	-0.9833	-1.5462	423	2251
H	-1.1060	-3.3290	-3.0180	434		H	-2.5122	-2.2834	-2.7244	416		H	-2.4463	-2.7351	-2.7219	440	
H	-2.3338	-1.5574	-4.1111	439		H	-2.9221	-0.1627	-3.8068	431		H	-3.0336	-0.6892	-3.8680	442	
H	0.8597	-0.3231	-2.8958	441		H	0.5506	-0.4218	-2.8954	440		H	0.4910	-0.7102	-2.9653	446	
H	0.2904	-1.2691	3.2273	446		H	-0.2424	-1.4957	3.1974	444		H	-0.3251	-1.1939	3.2017	448	

448	H	2.5288	0.5415	0.6866	444	H	3.0141	-1.7673	1.5830	460
466	H	2.8892	0.1142	1.4944	448	H	3.0278	-2.4574	-0.7177	473
503					464					492
515					473					501
517					498					505
533					518					527
536					524					534
570					532					546
573					553					575
651					575					576
678					577					668
711					597					682
720					663					684
725					684					707
762					713					719
874					725					721
876					728					727
881					748					745
899					857					875
911					874					882
925					883					893
945					901					902
945					910					912
947					915					932
948					937					944
950					945					946
951					947					948
952					948					949
953					949					949
958					950					951
2162					951					951

Reaction 25

Reactant						Transition State						Product					
Silylene												Silane					
Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency		Atomic	Coordinates (Angtroms)			Frequency	
Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}		Symbol	X	Y	Z	cm^{-1}	
Si	-0.0084	-0.0160	-0.0185	19	2049	Si	0.0820	0.3284	0.2668	-1099	948	Si	-0.4153	0.3452	-0.0265	21	948
Si	-0.0067	-0.0374	2.3563	28	2186	H	-1.2402	0.5947	1.0503	19	953	H	0.2232	0.6070	1.2931	24	949
H	1.4028	-0.0836	2.8451	58	2200	H	-0.1181	1.2437	-0.9044	25	959	H	0.2794	1.1680	-1.0559	45	952
H	-0.6779	-1.2812	2.8374	70	2206	H	-1.5723	0.1445	0.1437	46	1021	H	-1.8356	0.7865	0.0471	84	954
Si	1.1341	1.9475	-0.7722	89	2210	Si	-0.1055	-1.9063	-0.4844	85	1675	Si	-0.2941	-1.9454	-0.5570	89	2206
H	2.4718	1.3085	-0.3890	125	2214	H	1.2811	-2.4223	-0.6825	98	2023	H	1.1381	-2.3524	-0.6619	105	2206
H	0.6362	-1.2917	-0.4619	149	2223	H	-0.7948	-2.0663	-1.7976	109	2175	H	-0.9128	-2.1754	-1.8956	120	2209
H	-1.4367	-0.0703	-0.4509	309	2229	Si	-1.1645	-3.2612	1.1287	122	2205	Si	-1.3675	-3.3164	1.0322	301	2212
Si	-1.0704	1.8407	3.3035	354	2243	H	-0.4261	-3.1642	2.4218	307	2207	H	-0.7480	-3.0919	2.3717	321	2217
H	-0.3624	3.0704	2.8333	368	2245	H	-2.5415	-2.7400	1.3812	342	2211	H	-2.7990	-2.9082	1.1460	371	2225
H	-2.4696	1.9291	2.7924	399		Si	-1.3042	-5.5232	0.4794	358	2212	Si	-1.2564	-5.6104	0.5005	379	2227
Si	-1.0947	1.8158	5.6572	416		H	0.0720	-6.0445	0.2317	377	2217	H	0.1757	-6.0147	0.3857	403	2229
H	-1.7694	3.0296	6.1958	428		H	-2.0464	-5.6145	-0.8122	402	2226	H	-1.8812	-5.8304	-0.8369	450	2240
H	-1.8199	0.6141	6.1542	467		Si	-2.3723	-6.8719	2.0868	440	2228	Si	-2.3252	-6.9761	2.0930	471	2241
H	0.2958	1.7755	6.1885	493		H	-2.4344	-8.2903	1.6359	447	2241	H	-2.2296	-8.4131	1.7123	473	2243
				502		H	-1.6355	-6.8216	3.3799	471	2245	H	-1.6963	-6.8023	3.4316	492	2244
				563		H	-3.7626	-6.3935	2.3237	504		H	-3.7655	-6.6145	2.2040	529	
				612						538						570	
				675						580						651	
				688						643						656	
				734						666						715	
				761						701						739	
				784						741						747	
				891						750						797	
				927						802						886	

934	830	893
946	890	931
949	932	932
953	937	937

Supplementary Material (ESI) for PCCP