Supporting Information

Gas Phase Synthesis of the Elusive Trisilicontetrahydride Species (Si_3H_4)

Tao Yang[1], Beni B. Dangi[1†], Aaron M. Thomas[1], Ralf I. Kaiser[1*], Bing-Jian Sun[2], Monika Staś[3], and Agnes H. H. Chang[2*]

[1]Department of Chemistry, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, USA

[2]Department of Chemistry, National Dong Hwa University, Shoufeng, Hualien 974, Taiwan

[3]Department of Physical Chemistry and Molecular Modeling, Opole University, 45-052 Opole, Poland

†Current Address: Department of Chemistry, Florida A&M University, Tallahassee, Florida 32307, USA

*To whom correspondence should be addressed:

Prof. Dr. Ralf I. Kaiser; Email: ralfk@hawaii.edu; Phone: +1-808-956-5731;

Prof. Dr. Agnes H. H. Chang; Email: hhchang@mail.ndhu.edu.tw; Phone: +886-03-863-3596

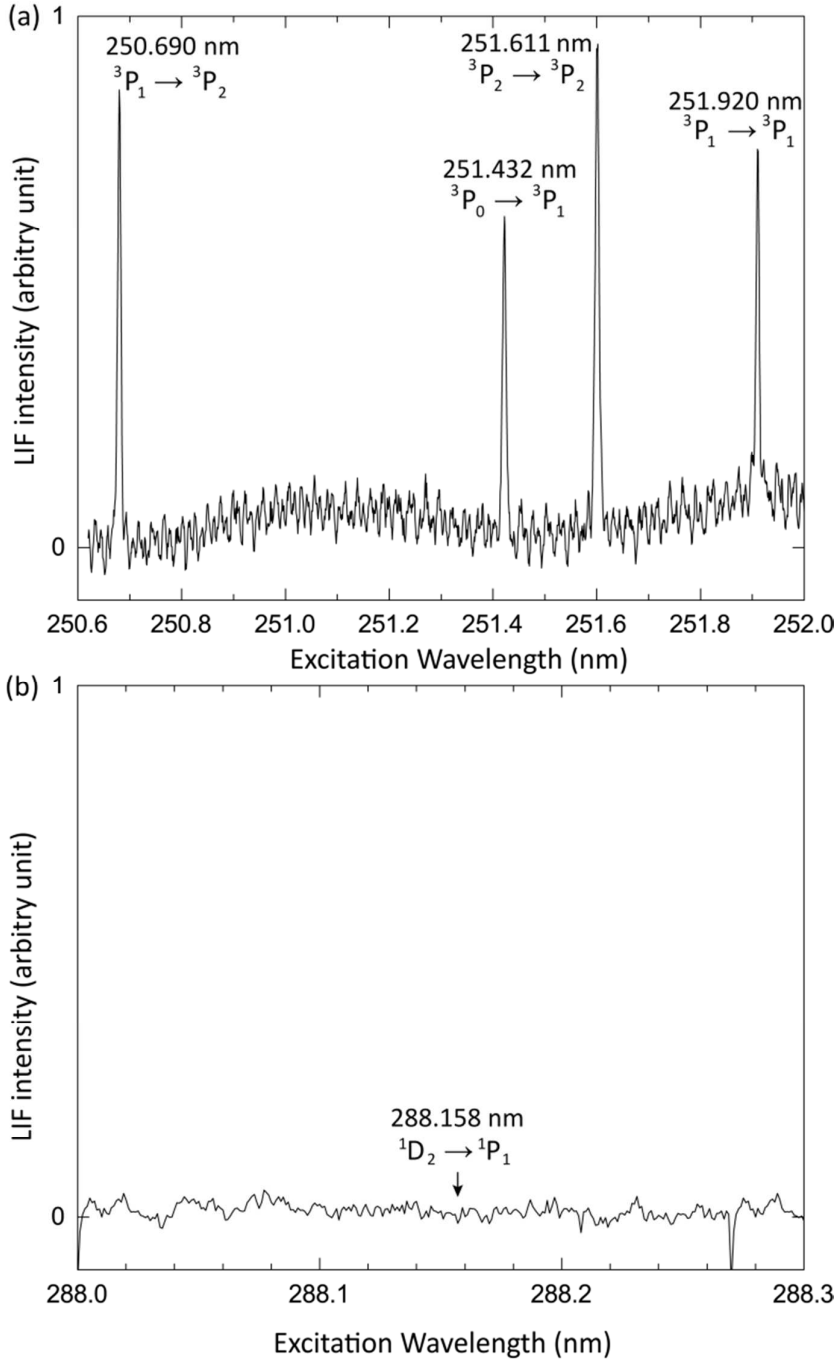
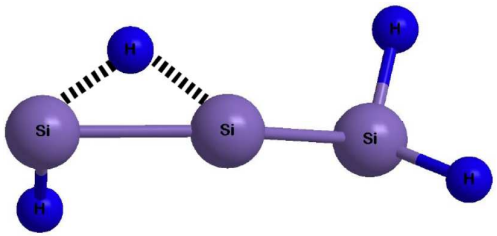
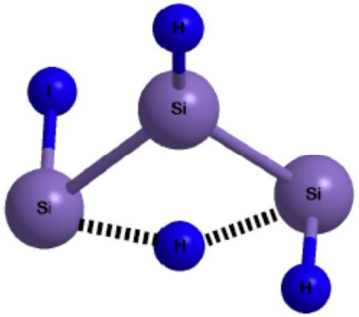
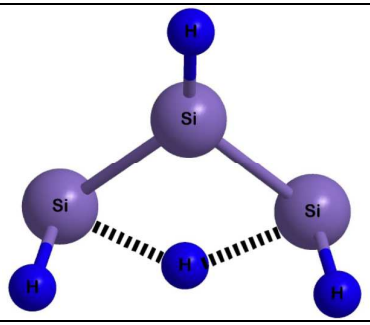
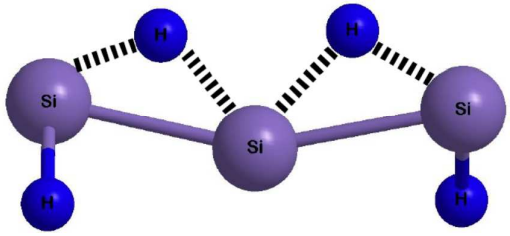
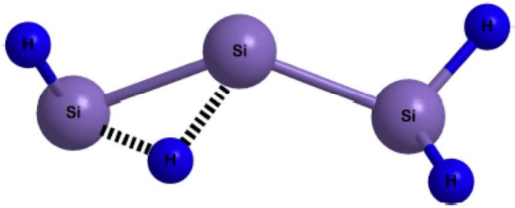
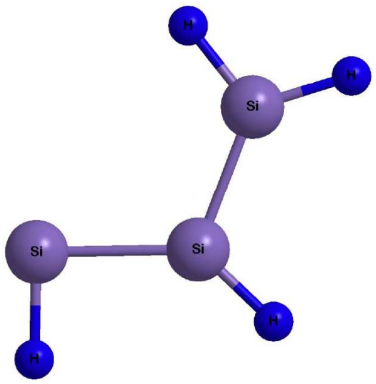
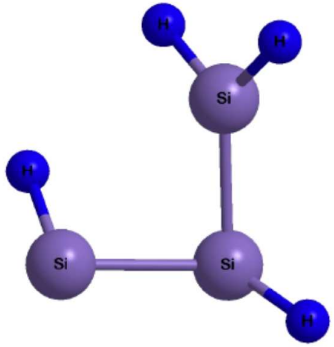


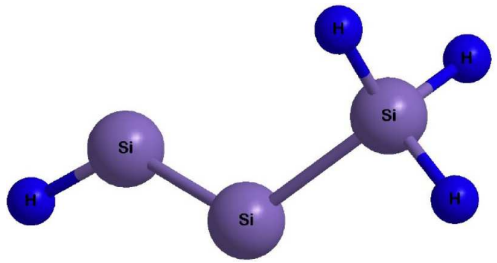
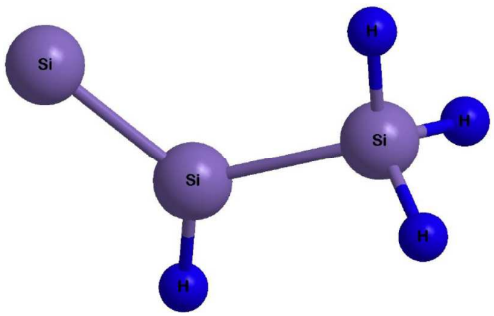
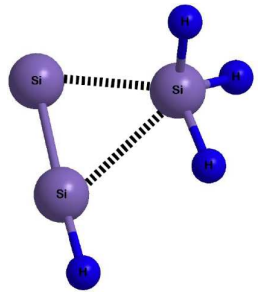
Figure S1: Laser-induced fluorescence (LIF) spectra of the **(a)** ground (^{3}P) and **(b)** excited (^{1}D) states of atomic silicon. The arrow in panel **(b)** indicates the expected position for the noted transition.

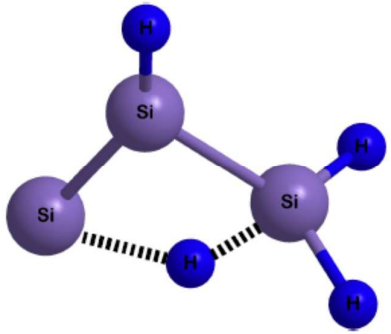
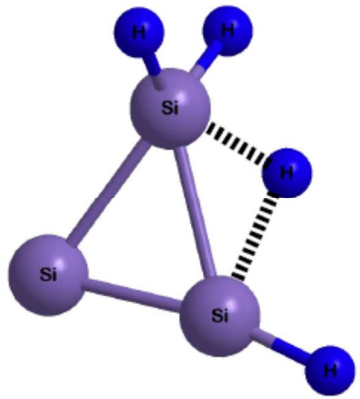
Table S1. Optimized Cartesian coordinates (Å), rotational constants (GHz), and vibrational frequencies (cm^{-1}) of H_2 dissociation products for the Si + Si_2H_6 reaction on the triplet and singlet ground state potential energy surfaces of Si_3H_6.

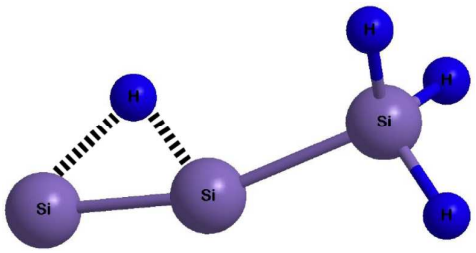
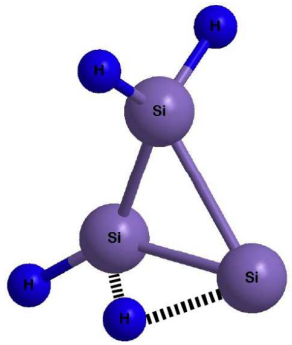
Species	Rotational Constants (GHz)	Vibrational Frequencies (cm^{-1})	Cartesian Coordinates (Å)			
			Atom	X	Y	Z
^{1}p1 	35.95221, 1.76207, 1.72508	99.8349, 137.5634, 296.3462, 341.8833, 356.7685, 486.6791, 522.9825, 571.7120, 820.0694, 920.2613, 962.3431, 1515.0127, 2025.1354, 2163.7173, 2191.9736,	Si	2.087534	0.210060	-0.111344
			Si	-0.040458	-0.428604	0.087341
			H	2.594068	0.845476	1.138734
			H	2.929353	-0.979362	-0.426766
			H	-0.889015	0.752528	0.896996
			Si	-2.247466	0.097755	-0.011790
			H	-1.828952	1.072406	-1.107865
^{1}p2 	7.41974, 3.62621, 2.54571	37.8209, 234.4149, 298.3347, 354.2542, 438.6596, 454.8558, 494.3961, 592.6509, 769.6255, 803.7886, 1139.5322, 1169.9996, 1939.2304, 1953.1074, 2192.1993	Si	0.000000	0.000000	1.127610
			Si	0.000000	1.530865	-0.581662
			Si	0.000000	-1.530865	-0.581662
			H	0.000000	0.000000	2.616895
			H	1.511987	1.341944	-0.359341
			H	0.000000	0.000000	-1.398224
			H	-1.511987	-1.341944	-0.359341
^{1}p2’	7.35742,	235.6270, 290.0509, 307.4725,	Si	-0.065114	-0.586163	1.503820

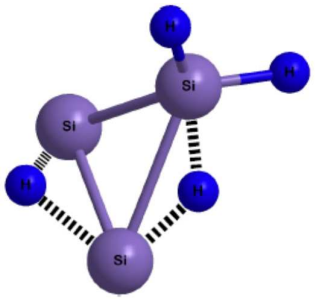
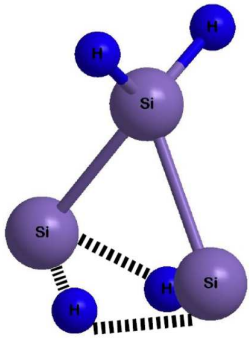
	3.67746, 2.55711	393.9933, 424.0840, 474.4440, 520.5618, 553.6987, 658.4356, 810.6976, 979.7089, 1226.0672, 2024.6013, 2035.8207, 2208.2533,	Si H H H Si H	-0.065114 1.400994 0.121753 -0.188948 -0.065114 1.400994	1.134689 -0.330311 -1.427703 2.615258 -0.586163 -0.330311	0.000000 1.816158 0.000000 0.000000 -1.503820 -1.816158
^{1}p3 	47.02489, 1.75169, 1.73296	113.8690, 127.8459, 326.9217, 399.7268, 445.2804, 500.4744, 626.2395, 838.6766, 881.2835, 1004.5895, 1050.6107, 1498.7959, 1532.6400, 1986.2355, 1986.3948,	Si Si Si H H H H	0.000000 0.000000 0.000000 1.141093 -1.141093 -0.813746 0.813746	0.000000 2.212333 -2.212333 2.100388 -2.100388 -0.943987 0.943987	0.300083 -0.147456 -0.147456 0.872225 0.872225 -0.908425 -0.908425
^{1}p4 	24.62810, 1.89057, 1.81000	94.3074, 170.2807, 359.7335, 385.4882, 404.0254, 484.6987, 532.0373, 592.9751, 770.8712, 933.4243, 1012.2044, 1517.9987, 2023.8538, 2171.6213, 2196.6720,	Si Si H H H Si H	2.018411 -0.050946 2.632789 2.947272 -0.841527 -2.119143 -2.615045	-0.274935 0.574338 -0.606650 0.631440 -0.465257 -0.329295 0.858959	-0.069488 0.03922 1.247655 -0.802609 1.071636 -0.127332 0.689710
^{1}p5	12.94747,	88.3067, 92.0509, 308.2633,	Si	1.794591	-0.371560	-0.000176

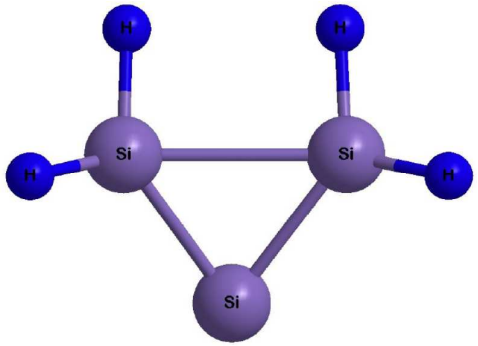
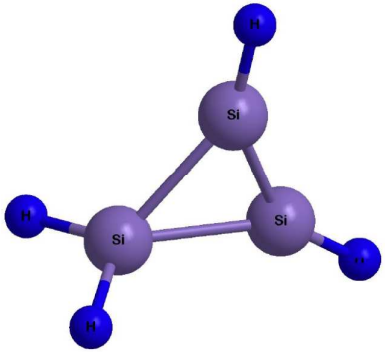
	2.35539, 1.99285	406.7185, 440.9098, 445.5668, 539.6250, 559.0784, 653.4834, 691.2549, 946.6835, 2020.1398, 2181.2244, 2218.8583, 2251.7216,	Si H H H Si H	-0.042648 3.196177 1.740787 0.219740 -1.916813 -2.848528	0.810572 0.113531 -1.850480 2.276106 -0.526368 0.683814	0.000019 -0.000197 -0.000176 0.000025 0.000210 -0.000395
^{1}p5’ 	7.71545, 3.54701, 2.55446	86.2311, 303.0253, 353.3373, 411.3930, 472.0274, 482.5825, 487.8947, 532.9455, 637.4747, 742.7318, 951.1870, 2023.3648, 2162.7860, 2189.0236, 2256.3456	Si Si H H H Si H	1.440562 -0.087544 2.399052 1.658654 0.027845 -1.578165 -0.933504	-0.443928 1.129968 -0.659045 -1.451838 2.160399 -0.582246 -1.502622	-0.035212 0.173924 -1.153036 1.022339 -0.900587 -0.129500 0.902323
^{1}p6	19.34406, 2.00966, 1.86028	32.4230, 59.3025, 151.6915, 366.0476, 423.0768, 495.7646, 541.4676, 618.3912, 875.8427, 942.7074, 944.1299, 2164.1769,	Si Si H Si	-2.026703 0.000000 -3.269528 1.789929	0.206825 0.746145 1.033291 -0.792686	0.000000 0.000000 0.000000 0.000000

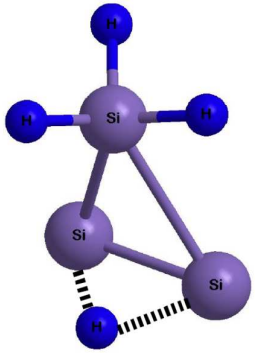
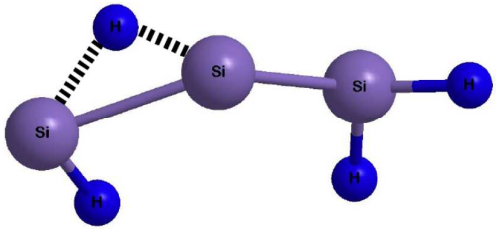
		2207.4758, 2219.8868, 2222.7582,	H	1.774287	-1.646134	1.213188
			H	1.774287	-1.646134	-1.213188
			H	3.035788	0.014991	0.000000
^{1}p7 	14.27980, 2.12734, 1.89210	52.2868, 104.8507, 259.4803, 396.1739, 438.4890, 507.7579, 538.0925, 669.7979, 880.7514, 936.3557, 951.0915, 2182.4224, 2201.6321, 2209.3802, 2218.5594,	Si	0.000000	0.781355	0.000000
			Si	2.122840	0.206764	0.000000
			H	-0.492613	2.186559	0.000000
			Si	-1.657137	-0.876118	0.000000
			H	-0.986951	-2.201192	0.000000
			H	-2.520139	-0.776687	1.205302
			H	-2.520139	-0.776687	-1.205302
^{1}p8 	6.79008, 4.41379, 2.76176	114.1397, 210.9366, 231.6394, 270.4681, 404.5813, 526.1434, 528.8920, 623.9471, 882.3955, 905.7434, 954.7872, 2092.6418, 2183.0610, 2202.6587, 2211.5625,	Si	1.396171	-0.248543	0.000000
			Si	0.000000	1.338514	0.000000
			H	-1.037212	2.406511	0.000000
			Si	-0.998975	-0.997620	0.000000
			H	-1.182252	-1.832236	1.213610
			H	-1.182252	-1.832236	-1.213610
			H	-2.159030	-0.034955	0.000000

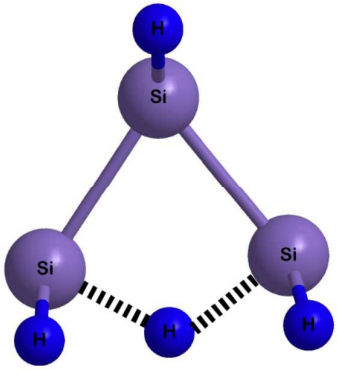
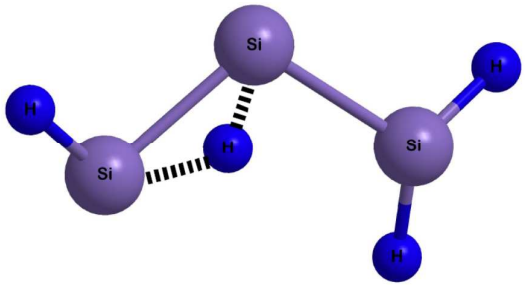
^{1}p9 	7.38492, 4.01801, 2.68362	113.1579, 260.4129, 454.8237, 459.0156, 495.0801, 503.6346, 526.8156, 577.2152, 748.0324, 964.3050, 1096.9153, 1615.5950, 2198.4969, 2206.2541, 2255.5765,	Si Si Si H H H H	1.264413 0.000000 -1.559646 1.941813 1.941813 0.362908 -0.113273	-0.695021 1.170677 -0.378389 -1.228717 -1.228717 2.600594 -1.504905	0.000000 0.000000 0.000000 1.209003 -1.209003 0.000000 0.000000
^{1}p10 	6.54482, 4.96920, 2.91997	77.5454, 309.1159, 346.2695, 419.6003, 424.1319, 524.9873, 529.9134, 690.4204, 726.3457, 975.0501, 1115.9505, 1681.2403, 2186.2862, 2192.1495, 2194.2162	Si Si Si H H H H	1.334127 -0.917143 -0.688057 2.203478 -1.380541 0.768609 2.203474	0.053162 0.903223 -1.250859 0.125950 2.314290 1.557271 0.125118	0.000008 -0.000197 0.000048 -1.203912 0.001793 0.000103 1.203991
^{1}p11	52.17368, 1.68285, 1.66200	31.7353, 108.1988, 113.3766, 330.5477, 500.6604, 504.4852, 650.8059, 868.2300, 933.8024,	Si Si H	-1.796615 0.000000 -1.535405	1.493746 0.359408 -0.215585	0.000000 0.000000 0.000000

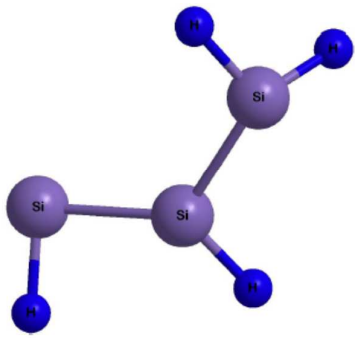
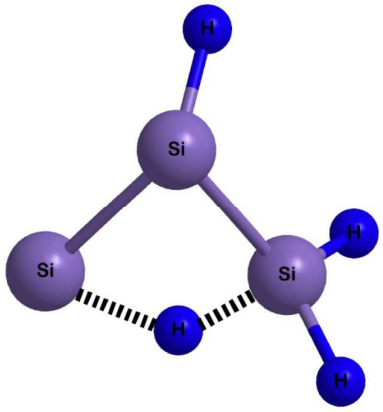
		944.5529, 1035.7436, 1607.2169, 2212.3981, 2228.0678, 2230.7758,	Si H H H	1.510906 2.869885 1.332722 1.332722	-1.450043 -0.855190 -2.286391 -2.286391	0.000000 0.000000 1.211754 -1.211754
^{1}p12 	6.22571, 5.10625, 2.95010	302.1926, 331.7267, 411.5137, 455.5911, 460.7769, 527.2012, 538.0866, 602.4617, 669.0027, 943.1975, 1142.6213, 1547.0703, 2169.2659, 2194.6813, 2231.2085,	Si Si Si H H H H	1.323413 -0.946779 -0.520608 -1.116949 2.280914 2.024513 -1.172841	-0.149087 -1.127275 1.123409 2.452804 -0.259364 -0.225678 0.173581	0.025643 -0.033714 -0.077978 0.232271 1.155859 -1.276823 1.093382
^{1}p13	6.36148, 4.67797, 2.83357	266.5410, 349.1750, 401.5036, 414.4946, 453.9782, 475.4757, 680.1965, 823.5436, 919.5923, 956.7784, 1094.7312, 1449.1253, 1515.9814, 2209.3310, 2234.1823	Si Si Si H H H H	-0.468315 -1.144770 1.337424 -0.956447 0.520941 2.071015 2.223740	1.293518 -0.933042 -0.198161 0.157788 -1.602446 -0.418704 -0.409051	-0.038065 -0.051747 0.000872 1.200702 0.140523 -1.267343 1.171294

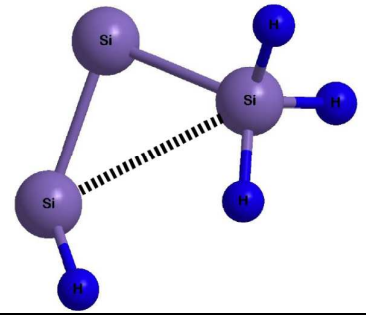
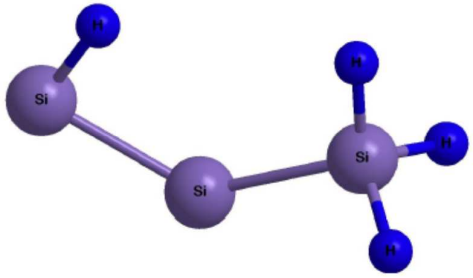
						
^{1}p14 	5.57312, 5.19749, 2.84263	328.0170, 374.9720, 378.3908, 461.7214, 465.1961, 501.8496, 611.2834, 890.2825, 940.0899, 995.9433, 1025.0136, 1385.4045, 1566.5059, 2219.6929, 2240.9772,	Si H H Si H H Si	0.000000 0.000000 0.000000 1.283451 0.000000 0.000000 -1.283451	0.000000 1.236622 -1.236622 0.000000 -0.991866 0.991866 0.000000	1.283048 2.096821 2.096821 -0.702754 -1.239605 -1.239605 -0.702754
^{1}p15	6.76544, 4.48879, 2.78374	184.8303, 350.4442, 396.8931, 411.7319, 440.0536, 446.7866, 496.1474, 553.3749, 580.6515, 951.8819, 969.3108, 2174.4200, 2180.7882, 2188.4696, 2201.8674,	Si Si Si H H H	-0.009533 -0.009533 -0.009533 -0.741784 0.941986 -0.741784	1.346074 -0.503138 -0.503138 -1.797386 -0.581202 -1.797386	0.000000 1.299935 -1.299935 1.245827 2.443591 -1.245827

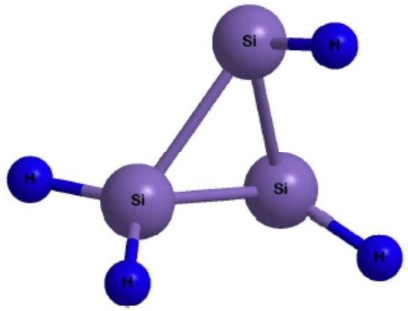
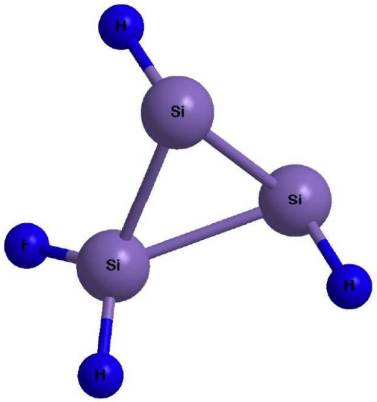
			H	0.941986	-0.581202	-2.443591
^{1}p16 	6.59792, 5.29751, 3.04037	222.4910, 274.6582, 370.3493, 443.3190, 453.7710, 538.1364, 557.5512, 608.6886, 661.3551, 674.5438, 989.9420, 2168.3964, 2171.3113, 2184.8723, 2188.1318,	Si H H Si H Si H	0.000000 -1.196694 1.196694 0.000000 0.000000 0.000000 0.000000	0.000000 0.000000 0.000000 1.058075 2.343350 -1.058075 -2.343350	1.329285 2.216695 2.216695 -0.718369 -1.464534 -0.718369 -1.464534
^{1}p17	6.78757, 4.09171, 2.67437	112.7055, 206.7394, 281.0200, 407.7155, 440.5986, 530.7270, 699.3039, 865.9985, 929.6282, 948.4155, 1118.6696, 1510.0927, 2151.4500, 2207.4017, 2225.9351,	Si Si Si H H	1.443143 -1.146094 -0.632480 2.093764 2.189618	-0.169864 -0.965564 1.197532 0.479083 0.129120	0.011907 -0.045105 -0.044042 -1.154333 1.257025

			H	1.553409	-1.643732	-0.212815
			H	-1.140759	0.166078	1.191468
^{3}p1 	17.37811, 1.94808, 1.77955	101.0534, 156.3882, 263.6684, 330.5645, 393.2718, 447.7222, 458.5306, 545.3384, 843.6365, 917.3222, 1012.2407, 1445.8312, 1979.7060, 2155.0254, 2193.1855,	Si	2.005353	0.283777	0.089638
			Si	-0.081899	-0.772602	-0.064785
			H	2.102892	1.692575	-0.393253
			H	3.103312	-0.514723	-0.523963
			H	-0.929497	-0.001404	1.175887
			Si	-2.137841	0.297202	-0.015031
			H	-1.275287	1.506277	-0.396176
^{3}p2	6.19257, 4.42179, 2.72579	215.6569, 285.0554, 315.6337, 371.5002, 418.7802, 463.2020, 465.7501, 560.5544, 563.4815, 855.9127, 1137.9294, 1341.3478, 2086.2928, 2096.1712, 2162.8604,	Si	-0.075841	-0.593007	1.366256
			Si	-0.075841	1.292481	0.000000
			H	1.317508	-1.143610	1.510317
			H	-0.505173	-1.467698	0.000000
			H	1.055491	2.264382	0.000000
			Si	-0.075841	-0.593007	-1.366256
			H	1.317508	-1.143610	-1.510317

						
^{3}p3 	12.80209, 2.27505, 1.96499	94.1456, 153.4740, 311.6412, 347.1464, 413.2287, 433.4879, 469.8939, 585.4496, 702.1921, 926.9541, 1030.1749, 1480.5832, 2069.6060, 2169.0929, 2204.1868,	Si	1.881850	-0.333837	0.082727
			Si	-0.098174	0.912909	-0.064822
			H	3.073616	0.406845	-0.412040
			H	1.957587	-1.745865	-0.387111
			H	-0.911884	0.066319	1.196760
			Si	-1.863589	-0.516985	-0.068995
			H	-3.000525	0.403472	0.317655
^{3}p4	16.13812, 1.93444, 1.75586	97.5445, 109.1178, 217.2920, 288.9458, 366.3110, 447.1709, 467.0073, 488.8871, 575.5920, 719.5922, 921.1308, 2013.8933, 2157.2852, 2165.7484, 2202.4963,	Si	2.040840	-0.259067	-0.056627
			Si	-0.105207	0.672373	-0.050697
			H	2.798302	-0.146577	1.223135
			H	2.078653	-1.671968	-0.520978
			H	0.033964	2.133461	0.229618

			Si	-2.085331	-0.486451	0.078537
			H	-2.815146	0.709111	-0.528768
^{3}p5 	6.01827, 4.18047, 2.58415	185.3818, 222.4886, 301.7988, 378.4418, 405.9152, 451.5446, 486.2976, 546.6571, 800.4290, 915.8968, 1067.6299, 1618.2045, 2072.3258, 2205.5304, 2227.8368,	Si	-1.321173	-0.449758	-0.003313
			Si	0.204778	1.315248	-0.114739
			Si	1.431931	-0.784459	0.023862
			H	-2.002413	-0.922046	-1.232750
			H	-2.143023	-0.723001	1.201600
			H	-0.051890	2.098671	1.147260
			H	-0.220181	-1.588069	0.202552
^{3}p6	6.79008, 4.41379, 2.76176	114.1397, 210.9366, 231.6394, 270.4681, 404.5813, 526.1434, 528.8920, 623.9471, 882.3955,	Si	0.204155	1.208960	-0.026961
			Si	1.730099	-0.519467	0.037292
			H	1.436607	-1.942402	-0.379720

		905.7434, 954.7872, 2092.6418, 2183.0610, 2202.6587, 2211.5625,	Si H H H	-1.599151 -2.696392 -2.128517 -1.303135	-0.398588 0.099241 -0.431178 -1.798332	0.007677 -0.871353 1.401258 -0.402301
^{3}p7 	18.58207, 1.79406, 1.66771	29.0588, 96.6811, 121.4448, 323.7787, 444.5096, 446.5172, 481.1735, 601.3200, 864.4500, 937.1972, 938.2403, 1976.7135, 2189.5974, 2205.6335, 2206.2207,	Si Si H Si H H H	-2.27645 0.00000 -1.81923 1.90744 2.73175 1.52194 2.73175	0.22292 0.74659 -1.24248 -0.67387 -0.39334 -2.10995 -0.39334	0.00000 0.00000 0.00000 0.00000 1.20517 0.00000 -1.20517
^{3}p8	5.42029, 5.26368, 2.87109	83.4512, 313.1937, 353.3216, 371.5691, 385.5575, 433.0078, 450.8446, 474.8545, 619.0578, 632.4415, 917.1908, 2095.0857, 2105.1226, 2195.3186, 2219.5385,	Si H H Si H Si H	-0.05375 1.01092 -1.40010 -0.05375 1.32331 -0.05375 1.32331	1.30800 2.34371 1.93352 -0.73138 -1.05527 -0.73138 -1.05527	0.00000 0.00000 0.00000 1.20090 1.71529 -1.20090 -1.71529

						
^{3}p9 	5.78141, 5.00120, 2.88871	226.9446, 346.7746, 360.1292, 372.1065, 384.7530, 423.7826, 447.7917, 530.7375, 609.7270, 709.1129, 931.3185, 2093.7062, 2098.8103, 2205.0655, 2229.5194,	Si H H Si H Si H	0.000000 1.202088 -1.202088 0.000000 1.442624 0.000000 -1.442624	0.000000 -0.182313 0.182313 -1.158811 -1.591082 1.158811 1.591082	1.339607 2.189693 2.189693 -0.772132 -0.757102 -0.772132 -0.757102
^{3}p10	6.02641 4.86511 2.87181	316.7591, 362.9432, 372.2480, 393.3172, 445.0177, 456.5151, 481.0983, 498.1896, 549.7999, 937.3567, 942.5348, 2178.6240,	Si Si Si H	0.000000 0.000000 0.000000 1.207709	0.000000 1.223361 -1.223361 1.880585	1.418264 -0.549419 -0.549419 -1.117993

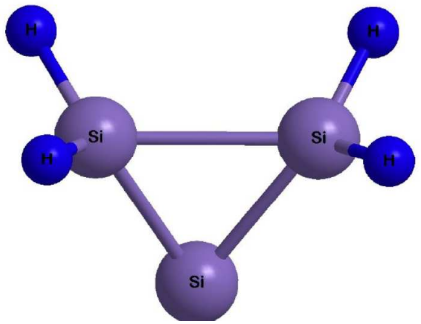
		2182.5675, 2191.7613, 2197.5632,	H	-1.207709	1.880585	-1.117993
			H	1.207709	-1.880585	-1.117993
			H	-1.207709	-1.880585	-1.117993

Table S2. The coupled cluster CCSD(T)/CBS energies with B3LYP/cc-pVTZ zero-point energy corrections of H_2 dissociation products for the Si + Si_2H_6 reaction on the adiabatic triplet and singlet ground state potential energy surfaces of Si_3H_6.

	B3LYP/ cc-pVTZ + E_{zpc} [a]	E_{zpc} [b]	CCSD(T)/ cc-pVDZ [c]	CCSD(T)/ cc-pVTZ [d]	CCSD(T)/ cc-pVQZ [e]	CCSD(T)/ CBS [f]	E(kJ/ mol) [g]	E(kJ/ mol) [h]	E(kJ/ mol) [i]	E(kJ/ mol) [j]	E_{CBS}(kJ/ mol) [k]
Si(^{3}P)	-289.396332	0.000000	-288.915089	-288.933123	-288.937603	-288.940006					
Si_2H_6($^1A_{1g}$)	-582.598242	0.048781	-581.611097	-581.694827	-581.720224	-581.734492					
Si+Si_2H_6	-871.994574	0.048781	-870.526186	-870.627950	-870.657827	-870.674498	0.0	0.0	0.0	0.0	0.0
H	-0.502156	0.000000	-0.499278	-0.499810	-0.499946	-0.500019					
H_2	-1.169930	0.010069	-1.163453	-1.172337	-1.173796	-1.174474					
^{3}p1+H_2	-871.966329	0.040240	-870.474288	-870.584955	-870.616104	-870.633325	74.2	113.8	90.5	87.1	85.7
^{3}p2+H_2	-871.971319	0.040460	-870.478982	-870.591952	-870.624184	-870.642059	61.1	102.1	72.7	66.5	63.3
^{3}p3+H_2	-871.975934	0.040577	-870.483480	-870.594522	-870.626009	-870.643446	48.9	90.6	66.2	62.0	60.0
^{3}p4+H_2	-871.977810	0.040227	-870.485278	-870.594986	-870.626351	-870.643752	44.0	84.9	64.1	60.2	58.3
^{3}p5+H_2	-871.979571	0.041704	-870.491356	-870.603370	-870.634925	-870.652375	39.4	72.9	46.0	41.5	39.5
^{3}p6+H_2	-871.985738	0.041803	-870.498197	-870.607909	-870.639125	-870.656425	23.2	55.2	34.3	30.8	29.1
^{3}p7+H_2	-871.987526	0.041650	-870.500098	-870.608949	-870.639804	-870.656891	18.5	49.8	31.2	28.6	27.5
^{3}p8+H_2	-871.995028	0.041165	-870.504091	-870.617562	-870.650167	-870.668277	-1.2	38.0	7.3	0.1	-3.7
^{3}p9+H_2	-872.000624	0.041896	-870.510920	-870.624522	-870.657168	-870.675301	-15.9	22.0	-9.1	-16.3	-20.2
^{3}p10+H_2	-872.008675	0.043117	-870.520854	-870.635490	-870.668479	-870.686807	-37.0	-0.9	-34.7	-42.8	-47.2
^{1}p1+H_2	-871.991012	0.040624	-870.502120	-870.614282	-870.646200	-870.663890	9.4	41.8	14.5	9.1	6.4

^{1}p2+H_2	-871.991873	0.039396	-870.497925	-870.612780	-870.644863	-870.662570	7.1	49.6	15.2	9.4	6.7
^{1}p2'+H_2	-871.992852	0.040012	-870.499513	-870.613852	-870.646037	-870.663831	4.5	47.0	14.0	7.9	5.0
^{1}p3+H_2	-871.994121	0.040413	-870.501729	-870.616108	-870.648018	-870.665625	1.2	42.2	9.1	3.8	1.3
^{1}p4+H_2	-871.996352	0.041166	-870.507749	-870.619691	-870.651666	-870.669403	-4.7	28.4	1.7	-3.8	-6.6
^{1}p5+H_2	-872.008102	0.041602	-870.519561	-870.631256	-870.663570	-870.681544	-35.5	-1.5	-27.5	-33.9	-37.3
^{1}p5'+H_2	-872.011064	0.042174	-870.523548	-870.637048	-870.669918	-870.688206	-43.3	-10.4	-41.2	-49.1	-53.3
^{1}p6+H_2	-872.004259	0.042567	-870.525172	-870.636185	-870.668422	-870.686367	-25.4	-13.7	-37.9	-44.1	-47.5
^{1}p7+H_2	-872.014401	0.043210	-870.531660	-870.642375	-870.674546	-870.692458	-52.1	-29.0	-52.5	-58.5	-61.8
^{1}p8+H_2	-872.015104	0.042763	-870.530974	-870.646056	-870.678738	-870.696843	-53.9	-28.4	-63.3	-70.7	-74.5
^{1}p9+H_2	-872.016846	0.043046	-870.531676	-870.646842	-870.679819	-870.698120	-58.5	-29.5	-64.7	-72.8	-77.1
^{1}p10+H_2	-872.015225	0.042859	-870.529164	-870.646795	-870.680278	-870.698837	-54.2	-23.4	-65.0	-74.5	-79.5
^{1}p11+H_2	-872.019665	0.042648	-870.535662	-870.648497	-870.680794	-870.698717	-65.9	-41.0	-70.0	-76.4	-79.7
^{1}p12+H_2	-872.018627	0.043163	-870.531178	-870.648994	-870.682629	-870.701284	-63.2	-27.9	-70.0	-79.9	-85.1
^{1}p13+H_2	-872.022355	0.042521	-870.535928	-870.652161	-870.684911	-870.703023	-72.9	-42.0	-80.0	-87.5	-91.3
^{1}p14+H_2	-872.023710	0.042841	-870.537461	-870.653467	-870.685987	-870.703950	-76.5	-45.2	-82.6	-89.5	-92.9
^{1}p15+H_2	-872.024414	0.043165	-870.538254	-870.653512	-870.686582	-870.704944	-78.3	-46.4	-81.9	-90.2	-94.7
^{1}p16+H_2	-872.019927	0.043120	-870.532619	-870.651322	-870.685813	-870.705016	-66.6	-31.8	-76.2	-88.3	-95.0
^{1}p17+H_2	-872.024709	0.043413	-870.540552	-870.655248	-870.687848	-870.705911	-79.1	-51.8	-85.8	-92.9	-96.6

[a] B3LYP/cc-pVTZ energy with zero-point energy correction in hartree

[b] zero-point energy by B3LYP/cc-pVTZ in hartree

[c] CCSD(T)/cc-pVDZ energy in hartree

[d] CCSD(T)/cc-pVTZ energy in hartree

[e] CCSD(T)/cc-pVQZ energy in hartree

[f] CCSD(T)/CBS energy in hartree

[g] relative energy by B3LYP/cc-pVTZ with zero-point energy correction

[h] relative energy by CCSD(T)/cc-pVDZ with B3LYP/cc-pVTZ zero-point energy correction

[j] relative energy by CCSD(T)/cc-pVTZ with B3LYP/cc-pVTZ zero-point energy correction

[i] relative energy by CCSD(T)/cc-pVQZ with B3LYP/cc-pVTZ zero-point energy correction

[k] relative energy by CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point energy correction