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Supporting Information

Gas-Phase Synthesis of 1-Silacyclopenta-2,4-diene

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1. Materials and Method

Experimental: The gas phase reaction between the simplest silicon-containing radical silylidyne (SiH; $X^2\Pi$) and 1,3-butadiene (C_4H_6; X^1A_g) was conducted by exploiting a crossed molecular beam machine at the molecular level under single collision conditions.[1-5] Briefly, a pulsed supersonic beam of silylidyne radicals in their electronic ground state was prepared *in situ* via photolysis (ArF, 193 nm, 30 mJ per pulse) of the disilane (Si_2H_6; 99.998 %; Voltaix) precursor which was seeded at a fraction of 0.5 % in helium (99.9999 %; Gaspro) at a backing pressure of 1,520 Torr. The silylidyne radical beam was then collimated by a skimmer and velocity-selected through a chopper wheel yielding a peak velocity v_p of 1750 ± 13 m s^{-1} and speed ratio S of 19.0 ± 2.9; this beam perpendicularly crossed a supersonic beam of pure 1,3-butadiene gas (C_4H_6; Aldrich) with a peak velocity of 750 ± 15 m s^{-1} and speed ratio of 9.0 ± 0.5 in the scattering chamber, to yield a collision energy of 33.7 ± 1.0 kJ mol^{-1}. The rotational temperature of the silylidyne radical (SiH; $X^2\Pi$) was determined via laser induced fluorescence (LIF) technique to be essentially 40 ± 10 K.[4] To elucidate the position of the atomic hydrogen loss, we also carried out reactions of the silylidyne radical (SiH; $X^2\Pi$) with D6-1,3-butadiene (C_4D_6; CDN) and D2-1,3-butadiene ($C_4H_4D_2$; CDN) along with the reaction of the D1-silylidyne radical (SiD; $X^2\Pi$) generated via laser ablation of silicon and seeding the ablated products in deuterium gas[6] with 1,3-butadiene (C_4H_6). The reaction products were monitored by a rotatable quadrupole mass spectrometer after electron impact ionization of the neutral products at 80 eV in an ultra-high vacuum chamber system held at a pressure of a few 10^{-12} torr. The velocity distributions of the products were recorded exploiting the angular-resolved time-of-flight (TOF) approach, i.e. collecting the arrival time of the ionized products for distinct mass-to-charge ratios (*m/z*) at different scattering angles in the laboratory reference frame.

Theoretical: The electronic structure calculations of the reaction of silylidyne (SiH; $X^2\Pi$) with 1,3-butadiene (C_4H_6; X^1A_g) was conducted on the doublet SiC_4H_7 potential energy surface (PES). Multiple singlet products as a result of atomic hydrogen loss are located. The optimized geometries and harmonic frequencies of intermediates, transition states along the reaction paths, and dissociation products are obtained at the level of the hybrid density functional theory, B3LYP[7-10]/cc-pVTZ; their energies are refined further by the coupled cluster[11-14] CCSD(T)/cc-

pVTZ with B3LYP/cc-pVTZ zero-point energy corrections (Tables S1&S2). The energies thus computed are expected to have an accuracy of 8 kJ mol^{-1}.[15] The GAUSSIAN09 program[16] is facilitated in the calculations.

2. Results for Reactions involving (Partially-)Deuterated Reactants

First, involving indirect reaction dynamics, the reaction of the D1-silylidyne radical with 1,3-butadiene leads to a SiC_4H_6D (84 amu) intermediate, which can decompose via atomic hydrogen and/or deuterium loss to SiC_4H_5D (83 amu) and/or SiC_4H_6 (82 amu). In our experiments, we observed signal at both mass-to-charge ratios of *m/z* = 83 *and* 82. It should be noted that signal at *m/z* = 82 can also originate from $SiC_4H_4D^+$ formed via dissociative electron impact ionization of the SiC_4H_5D product (83 amu) (Figure S1.II). This has been verified for the SiH-C_4H_6 system depicting that – corrected for naturally occurring silicon and carbon isotopes – the parent product (SiC_4H_6; 82 amu) undergoes also dissociative electron impact ionization to *m/z* = 81 ($SiC_4H_5^+$) yielding signal at *m/z* = 82 and 81 at a ratio of 2.7 ± 0.3 : 1 (Figure S1.I; Figure S2.I). Considering that for the SiD-C_4H_6 system, signal at *m/z* = 83 and 82 was recorded to depict a ratio of 3.3 ± 0.3 : 1, we may conclude that the (majority of) signal at *m/z* = 82 originates from dissociative electron impact ionization (Figure S1.II; Figure S2.II); further, we can state that signal at *m/z* = 83 presents the evidence of a hydrogen atom elimination channel from the 1,3-butadiene reactant. Second, the SiH-C_4D_6 system reveals signal at *m/z* = 88 ($SiC_4D_6^+$) and *m/z* = 87 ($SiC_4HD_5^+$) (Figure S1.III). Here, dissociative electron impact ionization of SiC_4D_6 cannot lead to *m/z* = 87. Considering the branching ratios of signal at *m/z* = 87 and 88 of 5.0 ± 0.1 : 1, the isotopic contributions from $^{29}SiC_4HD_5^+$ and $Si^{13}CC_3HD_5^+$ to *m/z* = 88, as well as the distinct recoil circles for a potential hydrogen atom loss versus deuterium atom loss, signal at *m/z* = 88 originates from isotopically-substituted $SiC_4D_6^+$, and signal at *m/z* = 87 originates from an atomic deuterium loss (Figure S2.III). Finally, having established that the hydrogen atom is emitted from the 1,3-butadiene reactant, but not from the silylidyne radical, we are probing now if atomic hydrogen is ejected from the terminal (C1/C4) and/or from the central (C3/C4) carbon atoms. This is done by conducting the reaction of the silylidyne radical (SiH; $X^2\Pi$; 29 amu) with D2-1,3-butadiene ($C_4H_4D_2$; 56 amu). Once again, the $SiC_4H_5D_2$ (85 amu) reaction intermediate can lose a hydrogen and/or deuterium atom forming $SiC_4H_4D_2$ (84 amu) and/or SiC_4H_5D (83 amu) respectively; signal at *m/z* = 83 can also be obtained from dissociative electron impact

ionization of $SiC_4H_4D_2$ (84 amu) (Figure S2.IV). Considering the branching ratio of both channels of 2.9 ± 0.3 : 1, we can conclude that most likely only the atomic hydrogen elimination pathway is open (Figure S1.IV).

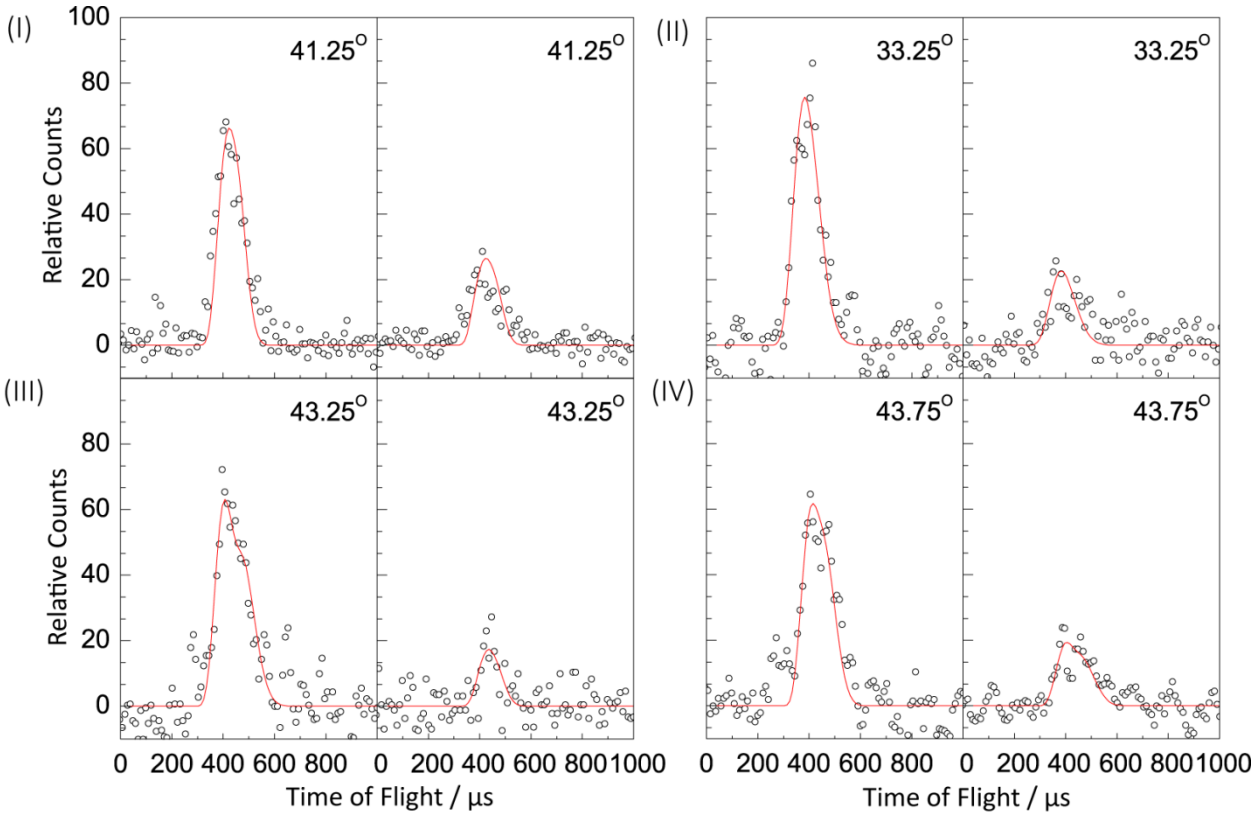


Figure S1. The center-of-mass TOF data for the reaction of the silylidyne radical (SiH; $X^2\Pi$) with 1,3-butadiene ($H_2CCHCHCH_2$; X^1A_g) at *m/z* of 82 ($SiC_4H_6^+$,(I) left) and 81 ($SiC_4H_5^+$, (I) right), D1-silylidyne radical (SiD; $X^2\Pi$) with 1,3-butadiene at *m/z* of 83 ($SiC_4H_5D^+$, (II) left) and 82 ($SiC_4H_6^+/SiC_4H_4D^+$, (II) right), silylidyne radical with D6-1,3-butadiene ($D_2CCDCDCD_2$; X^1A_g) at *m/z* of 87 ($SiC_4HD_5^+$, (III) left) and 88 ($SiC_4D_6^+/^{29}SiC_4HD_5^+/Si^{13}CC_3HD_5^+$, (III) right), and silylidyne radical with D2-1,3-butadiene ($H_2CCDCDCH_2$; X^1A_g) at *m/z* of 84 ($SiC_4H_4D_2^+$, (IV) left) and 83 ($SiC_4H_5D^+/SiC_4H_3D_2^+$, (IV) right), respectively. The circles represent the experimental data, while the red lines represent the fits obtained from the forward-convolution routine. The branching ratios for the two channels at the respective system are: 2.7 ± 0.3 : 1, 3.3 ± 0.3: 1, 5.0 ± 0.1 : 1 and 2.9 ± 0.3 : 1.

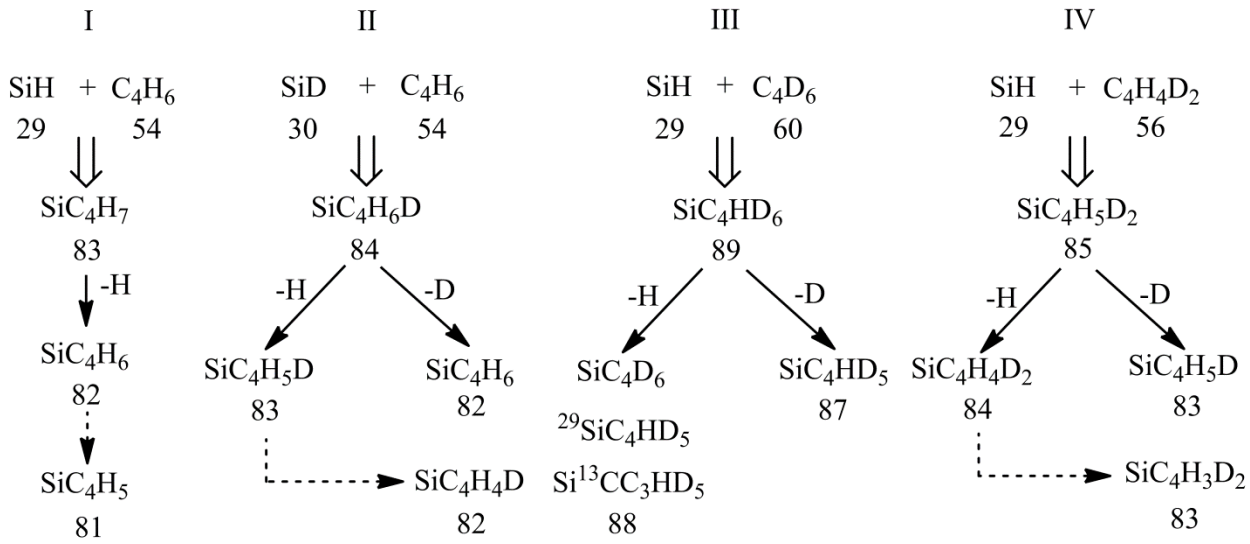


Figure S2. Reaction schemes of silylidyne with 1,3-butadiene (I), D1-silylidyne with 1,3-butadiene (II), silylidyne with D6-1,3-butadiene (III), and silylidyne with D2-1,3-butadiene (IV), with numbers denoting the mass-to-charge ratios.

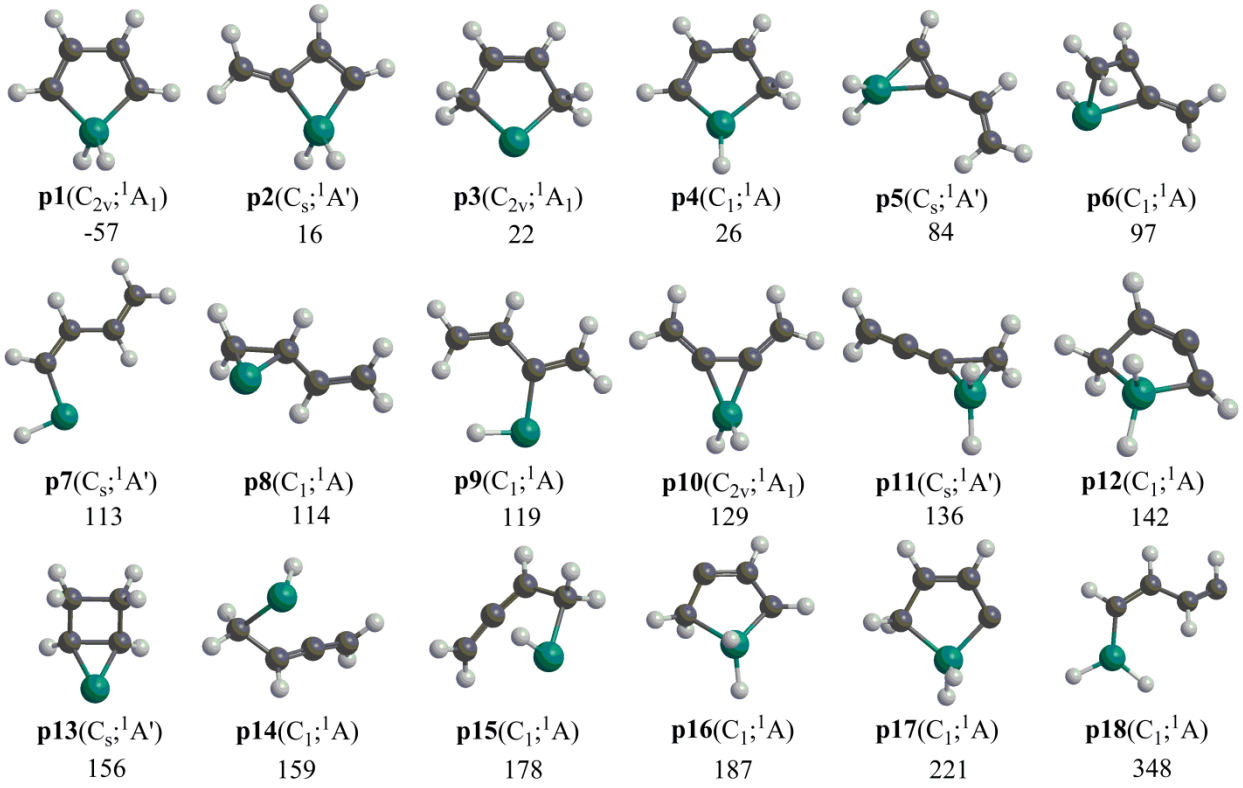


Figure S3. Overview of the SiC_4H_6 isomers with the point groups and symmetries of the electronic wave functions are included. The energetics are presented with respect to the initial reactant system and given in kJ mol^{-1}. Carbon: black, hydrogen: light grey, silicon: dark green.

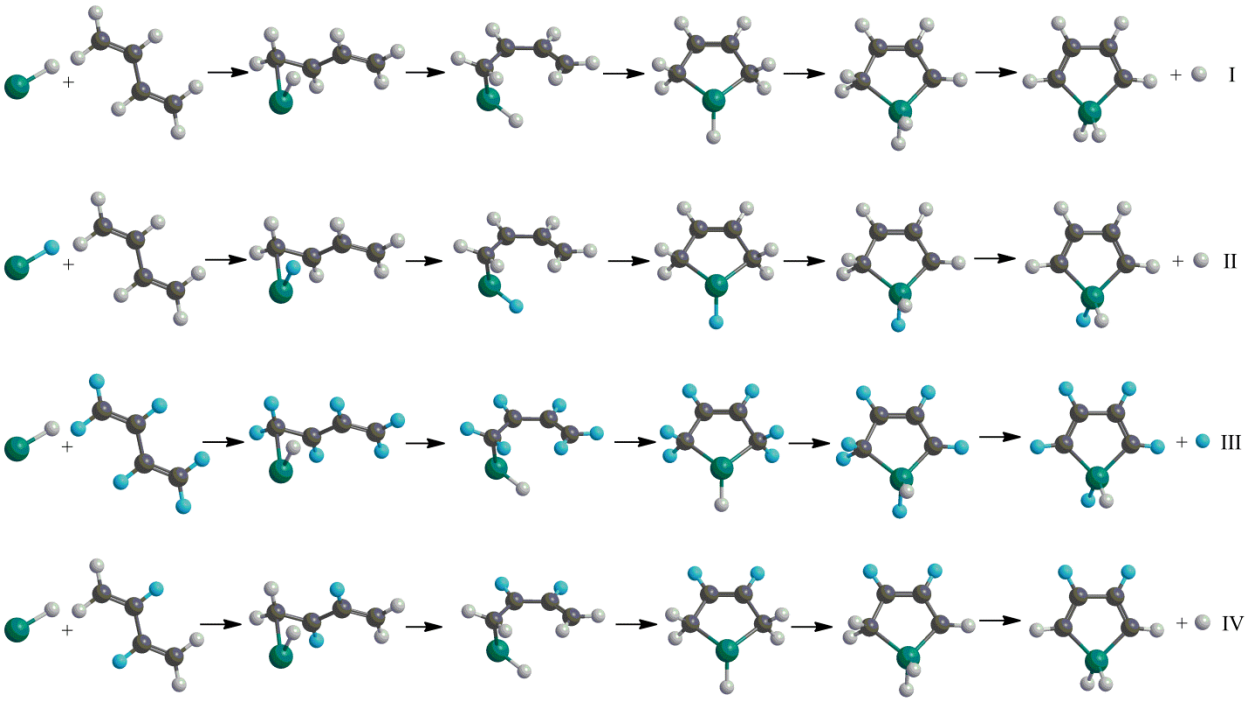


Figure S4. Reaction pathways leading from silylidyne (SiH) with 1,3-butadiene (C_4H_6) (I), D1-silylidyne (SiD) with 1,3-butadiene (C_4H_6) (II), silylidyne (SiH) with D6-1,3-butadiene (C_4D_6) (III), and silylidyne (SiH) with D2-1,3-butadiene ($C_4H_4D_2$) to **p1**(silole; c-SiC_4H_6) plus hydrogen (H), D1-**p1** (c-SiC_4H_5D) plus hydrogen, D5-**p1**(c-SiC_4HD_5) plus deuterium (D) and D2-**p1**(c-$SiC_4H_4D_2$) plus hydrogen, respectively. Carbon: black, hydrogen: light grey, deuterium: light blue, silicon: dark green.

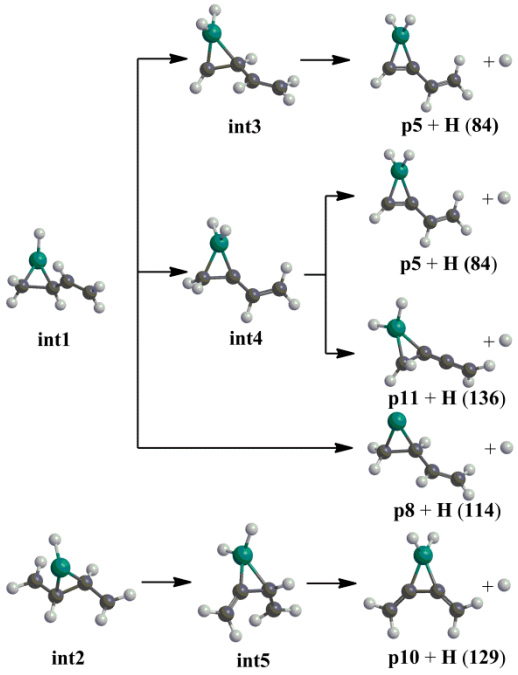


Figure S5. The possible additions of the silylidyne radical to the C1-C2 and C2-C3 bonds of 1,3-butadiene are represented. In principle, these intermediates cannot lose a hydrogen atom to form any product since the formation of the products are overall endoergic and hence not feasible under our experimental conditions. Therefore, these intermediates decompose back to the initial reactants. The energetics are presented in parentheses with respect to the initial reactant system and given in kJ mol^{-1}

Table S1. The energies for the B3LYP/cc-pVTZ optimized geometries of collision complexes, intermediates, transition states, and dissociation products for the silylidyne (SiH; $X^2\Pi$) with 1,3-butadiene (C_4H_6; X^1A_g) reaction on the adiabatic doublet ground state potential energy surface of SiC_4H_7.

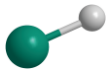
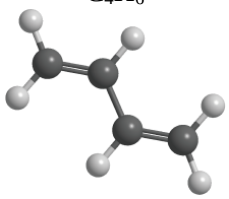
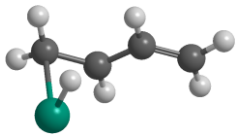
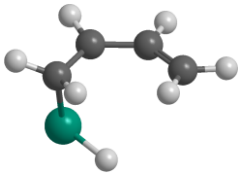
	B3LYP/ cc-pVTZ + E_{zpc}[a]	E_{zpc}	[b]CCSD(T)/ cc-pVTZ	E(kJ mol^{-1})[c]
SiH($C_{\infty v}$;$^2\Pi$)	-290.012583	0.004577	-289.546533	-
trans-1,3-butadiene(C_{2h};^1A_g)	-155.970960	0.084962	-155.695624	-
SiH($C_{\infty v}$;$^2\Pi$) +trans-1,3-tutadiene(C_{2h};^1A_g)	-445.983543	0.089539	-445.242157	0.0
trans[i1](C_1;^2A)	-446.019070	0.092597	-445.281028	-94
cis[i1](C_1;^2A)	-446.015705	0.092627	-445.279349	-90
i2(C_s;$^2A''$)	-446.060132	0.094846	-445.333767	-227
i3(C_1;^2A)	-446.075527	0.091377	-445.341399	-256
TStrans[i1]-cis[i1](C_1;^2A)	-446.001881	0.091847	-445.267502	-60
TScis[i1]-i2(C_1;^2A)	-446.004445	0.090581	-445.266053	-60
TSi2-i3(C_1;^2A)	-446.001146	0.088724	-445.263281	-58
TSi3-p1(C_1;^2A)	-445.994248	0.082294	-445.255863	-55
H	-0.502156	0.000000	-0.499810	-
p1+H(C_{2v};$^1A_1$)	-445.994674	0.081811	-445.256273	-57
p2+H(C_s;$^1A'$)	-445.968971	0.080802	-445.227188	16
p3+H(C_{2v};$^1A_1$)	-445.963444	0.085112	-445.229208	22
p4+H(C_s;$^1A'$)	-445.963438	0.082796	-445.225645	26
p5+H(C_s;$^1A'$)	-445.945764	0.080069	-445.200868	84
p6+H(C_1;^1A)	-445.940004	0.082767	-445.198479	97
p7+H(C_s;$^1A'$)	-445.936512	0.082328	-445.191967	113
p8+H(C_1;^1A)	-445.932493	0.084628	-445.193664	114
p9+H(C_1;^1A)	-445.931367	0.081789	-445.189256	119
p10+H(C_{2v};$^1A_1$)	-445.930952	0.079041	-445.182489	129
p11+H(C_s;$^1A'$)	-445.931003	0.078422	-445.179111	136
p12+H(C_1;^1A)	-445.916393	0.079662	-445.178117	142
p13+H(C_s;$^1A'$)	-445.909434	0.087096	-445.180389	156
p14+H(C_1;^1A)	-445.918717	0.081615	-445.173803	159
p15+H(C_1;^1A)	-445.909848	0.080991	-445.165793	178
p16+H(C_1;^1A)	-445.903960	0.079615	-445.160966	187
p17+H(C_1;^1A)	-445.890090	0.079436	-445.147924	221
p18+H(C_1;^1A)	-445.847528	0.076626	-445.096861	348

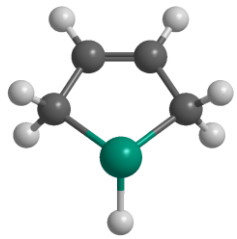
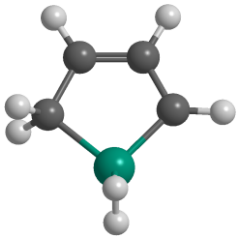
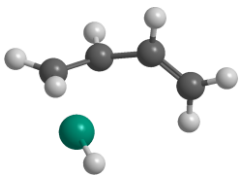
[a] B3LYP/cc-pVTZ energy with zero-point energy correction in hartree.

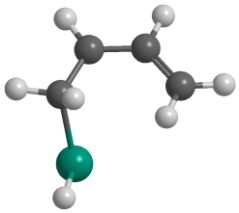
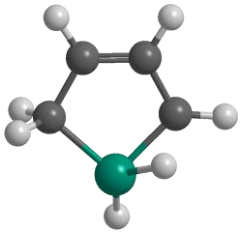
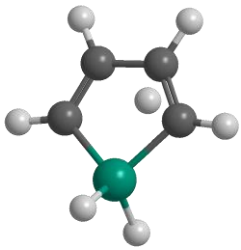
[b] zero-point energy by B3LYP/cc-pVTZ in hartree.

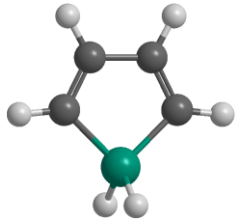
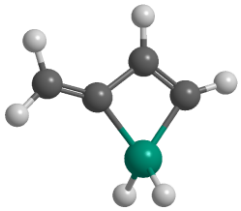
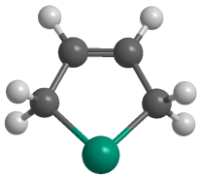
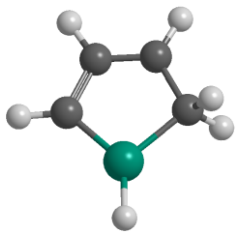
[c] relative energy by CCSD(T)/cc-pVTZ with B3LYP/cc-pVTZ zero-point energy correction.

Table S2. Optimized Cartesian coordinates (Å) together with rotational constants (GHz) and vibrational frequencies (cm^{-1}) of reactants, intermediates, transition states, and dissociation products for the reaction of silylidyne (SiH; $X^2\Pi$) with 1,3-butadiene (C_4H_6; X^1A_g). Carbon: black; hydrogen: light grey; silicon: dark green.

Species	Rotational Constants (GHz)	Vibrational Frequencies (cm^{-1})	Cartesian Coordinates (Å)			
			Atom	X	Y	Z
SiH 	0.0000000 225.422772 225.422772	2094.6449	Si H	0.000000 0.000000	0.000000 0.00000	0.101207 -1.416898
C_4H_6 	42.28315 4.48064 4.05133	168.4841, 301.7245 520.8389, 545.0638 788.7399, 907.0032 963.7576, 969.3731 1003.0370, 1013.1856 1062.4210, 1231.3092 1320.2069, 1321.4944 1422.3800, 1477.5016 1684.9821, 1746.6489 3160.0915, 3164.0904 3169.1439, 3173.5305 3255.3159, 3255.4331	C C H H H C C H H H	1.833441 0.607299 1.989303 2.712953 0.472297 -0.607299 -1.833441 -0.472298 -2.712953 -1.989302	0.110583 -0.402612 1.182597 -0.517213 -1.479608 0.402612 -0.110583 1.479608 0.517212 -1.182597	0.000015 0.000028 -0.000028 0.000045 0.000069 -0.000014 -0.000027 0.000031 -0.000055 -0.000009
trans[i1] 	8.21204 2.39485 2.0624	92.1214, 215.7700 281.1895, 295.9183 405.6031, 408.1723 522.4658, 614.7648 714.5909, 854.7410 863.0640, 890.8896 895.3364, 910.9138 1008.9470, 1023.2652 1201.4422, 1240.6882 1304.4770, 1370.4772 1466.7920, 1500.3196 1570.2092, 2009.4010 3113.7801, 3138.8741 3144.2553, 3152.3952 3198.6679, 3235.8832	C C C C Si H H H H H H H H	-0.975760 0.235836 1.303345 2.457311 -1.564393 -0.991652 -1.542821 0.378764 1.177022 3.250153 2.621444 -1.115805	1.173606 0.631590 0.098748 -0.383153 -0.776748 1.448188 1.825804 0.659338 0.108309 -0.751467 -0.417010 -1.123444	0.150109 -0.381131 0.393861 -0.127772 -0.109845 1.197256 -0.502212 -1.455936 1.471203 0.506395 -1.197104 1.307823
cis[i1] 	7.12537 2.7818 2.52402	110.0733, 163.8991 264.7848, 354.9032 378.7309, 506.8465 576.3546, 608.2172 704.8641, 820.9393 845.3296, 878.2163 883.4382, 901.4849 992.5734, 1054.7574	C C H H H C C H	-0.6816980 0.1141110 -0.2318010 -1.3803390 -0.2100390 1.3278620 2.0432810 1.7113780	1.0557770 0.7641860 0.9655410 1.8777290 1.1837290 0.0146760 -0.4113180 -0.2071550	0.6043390 -0.5563100 1.5826000 0.5028950 -1.5003140 -0.5911830 0.4826450 -1.5805450

		1110.9588, 1217.3446 1293.1036, 1430.3847 1449.4710, 1494.2428 1565.1028, 2013.5685 3118.4060, 3147.6190 3154.5287, 3167.6630 3207.5609, 3243.1200	H H Si H	2.9557540 1.7299190 -1.4777850 -0.7072240	-0.9739600 -0.2136110 -0.6939990 -1.4562150	0.3507510 1.4976890 -0.1040390 0.9665310
i2 	6.04641 4.74469 2.7862	93.1816, 379.0346 445.4480, 514.5450 605.9555, 642.1160 668.6726, 679.6646 774.4494, 832.8739 838.4353, 915.3534 954.7803, 985.4889 1121.4952, 1122.6238 1126.8033, 1192.6771 1235.0211, 1380.1185 1443.9458, 1445.0682 1676.0447, 2148.1627 3015.7680, 3016.1880 3048.5590, 3049.6618 3128.2807, 3152.0394	C C H H H C C H H H Si H	0.015559 0.015559 0.935604 -0.803822 0.008589 0.015559 0.015559 0.008589 -0.803822 0.935604 -0.116627 0.978632	0.007237 1.317145 -0.131007 -0.041985 2.248771 1.317145 0.007237 2.248771 -0.041985 -0.131007 -1.268413 -2.286355	1.418599 0.666694 1.995321 2.139166 1.222712 -0.666694 -1.418599 -1.222712 -2.139166 -1.995321 0.000000 0.000000
i3 	6.42032 4.60362 2.81309	120.2581, 398.2299 475.0673, 510.8223 594.4458, 631.0091 646.0440, 716.8233 725.5697, 737.4537 812.1244, 875.0938 928.9811, 974.9897 978.9187, 1071.5669 1106.8594, 1117.6285 1189.6653, 1264.2429 1404.3063, 1428.6689 1460.8954, 2184.5520 2191.9766, 3019.4247 3042.1582, 3136.8751 3168.9613, 3196.4720	C C H H H C C H H H Si H	-0.106333 -1.340695 -0.036274 2.113939 -2.274821 -1.355157 -0.025946 -2.282869 0.078207 0.079346 1.227105 2.111800	1.371165 0.724211 2.449222 0.091178 1.276617 -0.663765 -1.371643 -1.221998 -2.022288 -2.022947 0.071343 0.091606	0.000450 -0.000087 0.000957 1.195524 -0.000319 -0.000366 0.000500 -0.000666 0.873522 -0.871978 -0.000185 -1.197434
TStrans[i1]-cis[i1] 	6.55586 2.94041 2.24789	-107.9465, 119.5955 204.1077, 315.2314 318.6947, 372.7610 517.0389, 676.8051 699.8564, 766.7980 844.4701, 857.4341 883.6348, 967.4829 1008.0130, 1076.3452 1111.8111, 1237.0993 1323.6389, 1393.3479 1455.4241, 1506.2774 1700.3800, 2023.3971 3088.7260, 3113.0478 3135.8568, 3140.0085	C C H H H C C H H H Si H	-0.880683 0.061950 -0.644693 -1.717689 -0.102890 1.473359 2.038100 2.089357 3.087050 1.480475 -1.389172 -0.899560	1.231934 0.715545 1.302832 1.816737 0.933359 0.444019 -0.727617 1.340963 -0.792569 -1.654278 -0.836700 -1.216538	0.426190 -0.481077 1.477035 0.067256 -1.532760 -0.108685 0.149362 -0.060625 0.405315 0.122444 -0.118966 1.272104

		3221.9352, 3237.1708				
TScis[i1]-i2 	6.62333 2.79972 2.21659	-107.7265, 157.2488 182.7454, 297.2580 374.3784, 516.9179 543.7927, 570.7909 674.1164, 714.0974 791.3602, 807.2798 935.4718, 984.4397 1029.2135, 1092.7252 1120.4444, 1193.5741 1231.9775, 1415.4755 1443.8813, 1464.5359 1531.6438, 1974.2675 2997.9237, 3036.2054 3134.1536, 3142.8540 3174.4132, 3227.3809	C C H H H C C H H H Si H	-0.562195 0.725747 -0.435717 -1.182483 0.907347 1.669057 1.538747 2.555766 2.267228 0.738651 -1.618812 -2.415560	0.912943 1.125591 0.613258 1.816218 2.060972 0.109833 -1.146321 0.310240 -1.920736 -1.398678 -0.475114 -0.841947	0.531127 -0.160353 1.576070 0.540500 -0.673035 -0.267067 0.285255 -0.858415 0.096489 0.970279 -0.349806 0.911618
TSi2-i3 	6.44789 4.69418 2.83229	-1700.2738, 180.3492 418.5068, 448.1473 533.9371, 582.6266 624.8313, 660.2789 722.7576, 740.4092 788.7652, 823.3922 924.3703, 951.7399 1015.3497, 1023.4884 1108.8303, 1130.2165 1205.7762, 1224.8709 1384.2660, 1435.3358 1553.7986, 1756.7253 2150.1614, 2985.2556 3048.2548, 3146.0085 3170.0113, 3207.0006	C C H H H C C H H H Si H	0.025765 -1.292029 0.182766 0.781597 -2.179006 -1.377306 -0.091941 -2.329927 -0.041273 -0.003691 1.252937 2.461483	1.348652 0.766017 2.412492 1.051957 1.387203 -0.585452 -1.385394 -1.097673 -2.080652 -2.001862 -0.032609 -0.077875	-0.105792 -0.032206 -0.202158 1.151985 0.016145 -0.002629 -0.016617 0.048556 0.823616 -0.919766 0.059723 -0.811032
TSi3-p1 	5.918 4.63662 2.8695	-121.6001, 100.7250 118.6764, 251.7569 379.0686, 497.8769 552.0351, 620.4041 678.4768, 709.1756 734.9062, 748.9507 769.4408, 887.3076 934.0774, 960.2032 1002.8255, 1006.3094 1110.9934, 1120.9490 1317.4989, 1371.9727 1525.6423, 1611.1239 2206.4344, 2212.4605 3136.8785, 3151.7599 3200.4257, 3204.6168	C C H H H C C H H H Si H	0.117159 1.304651 0.031309 -2.045085 2.257463 1.283168 0.075913 2.219743 -0.041852 -0.128289 -1.205059 -2.107811	1.388157 0.763727 2.455830 0.226000 1.277724 -0.703655 -1.295166 -1.245376 -2.356680 -2.196847 0.069569 -0.052993	0.121748 0.046812 0.260630 -1.274286 0.116385 -0.141879 -0.207606 -0.219568 -0.365528 2.258373 -0.057583 1.115716
p1	6.72608 4.92948 2.94122	249.9550, 378.5955 498.3080, 549.4659 620.7121, 680.6415 711.1215, 734.7928 749.9538, 768.5653	Si H H C C	0.0000000 1.2028530 -1.2028530 0.0000000 0.0000000	0.0000000 0.0000000 0.0000000 1.3523590 0.7410750	1.206241 2.079863 2.079863 -0.093523 -1.289436

		889.4956, 933.0110 959.9350, 1005.5058 1006.8724, 1110.8679 1121.6818, 1317.6713 1371.3645, 1538.9667 1617.8977, 2203.6083 2205.7491, 3134.8229 3149.7923, 3200.1407 3201.5096	C C H H H H	0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000	-0.7410750 -1.3523590 2.4275580 1.2734950 -1.2734950 -2.4275580	-1.289436 -0.093523 0.008944 -2.23475 -2.23475 0.008944
p2 	7.16186 3.96227 2.62813	200.4765, 296.7767 339.4063, 571.3406 593.9155, 607.1588 667.5104, 698.1981 765.8504, 801.3698 823.0006, 925.5367 937.4912, 976.4309 1008.4928, 1056.6814 1182.8368, 1302.2882 1454.6263, 1537.8742 1696.7855, 2199.0322 2202.6764, 3102.4234 3112.2933, 3196.3808 3211.3200	C C C C Si H H H H H H	0.9720430 1.2754390 0.0000000 -0.2273170 -0.8642330 -1.6558900 -1.6558900 1.6698590 2.264674 -1.230025 0.585545	-1.2393790 0.0789090 0.8215670 2.1322320 -0.8667730 -1.2431430 -1.2431430 -2.0629450 0.533374 2.539072 2.851636	0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 1.201231 -1.201231 0.0000000 0.0000000 0.0000000 0.0000000
p3 	6.51037 4.65028 2.80347	108.8898, 315.6348 476.7802, 521.7044 551.3443, 573.3125 636.5362, 749.1723 771.0199, 931.3003 950.7643, 977.3300 1104.7887, 1107.1333 1114.1062, 1174.2404 1219.8048, 1373.6063 1407.3637, 1409.2491 1676.4142, 2976.1259 2978.2451, 2988.4487 2991.6453, 3125.2383 3149.7427	C H H C C C Si H H H H	0.0000000 -0.86514 0.865140 0.000000 0.000000 0.000000 0.000000 0.865140 -0.865140 0.000000 0.000000	1.359716 2.024438 2.024438 0.665758 -0.665758 -1.359716 0.000000 -2.024438 -2.024438 -1.235793 1.235793	0.018683 0.149948 0.149948 -1.316555 -1.316555 0.018683 1.389624 0.149948 0.149948 -2.240025 -2.240025
p4 	6.80791 5.06298 2.95926	38.8662, 356.7268 462.0132, 497.8349 621.1733, 657.0969 679.4213, 721.8537 777.1950, 808.7911 929.9219, 954.2428 969.8317, 1007.9254 1066.0981, 1107.4314 1186.5166, 1245.3191 1383.5196, 1399.7079 1580.5259, 2266.2445 3008.1632, 3056.6008 3148.8165, 3184.0538	Si C C C C H H H H H H	-1.204059 0.132695 1.3782 1.20013 -0.159044 -2.657607 0.105931 0.0474 2.353295 2.045456 -0.349539	-0.033655 -1.359643 -0.516566 0.82344 1.346956 -0.200281 -2.094607 -1.928295 -0.980087 1.501733 2.407585	-0.041542 0.023891 -0.004861 0.000496 0.031298 0.147061 -0.784714 0.958204 -0.06487 -0.026836 0.0478

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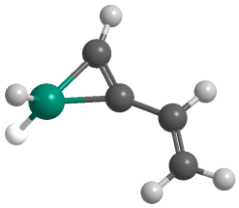
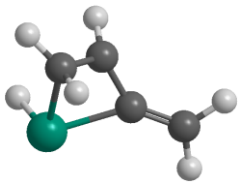
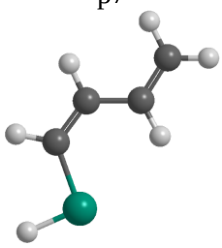
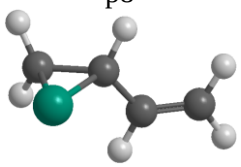
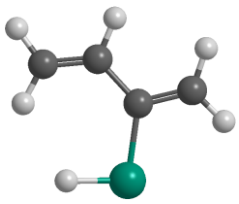
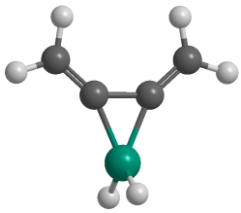
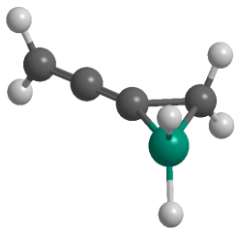
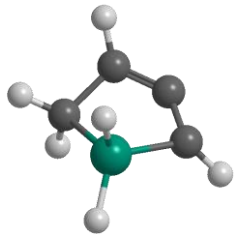
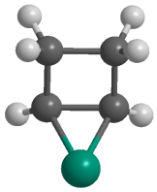
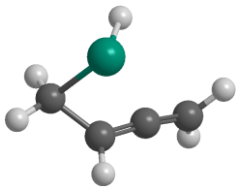
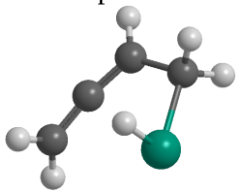
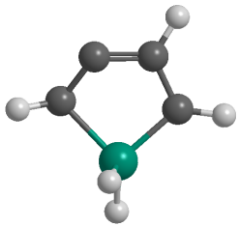
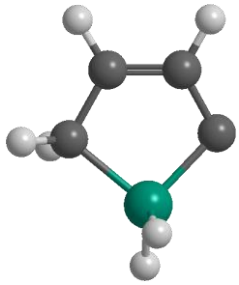
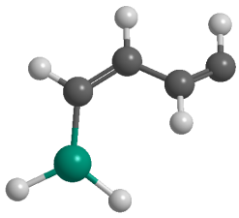
p5 	10.2059 2.52 2.07082	126.8913, 174.5741 271.8176, 513.2854 569.3809, 570.0527 626.6477, 645.5388 712.5170, 765.5289 837.0546, 950.6247 972.6289, 990.2324 1024.8457, 1034.8808 1202.8754, 1321.6381 1436.5015, 1609.6116 1683.8784, 2220.3241 2227.7982, 3114.3755 3140.5780, 3175.6396 3226.3748	Si H H C C C C H H H H	-1.264349 -1.580303 -1.580303 -1.242143 0.0000000 1.351996 2.438578 -1.680688 1.461748 2.355942 3.43391	-0.951397 -1.726554 -1.726554 0.865083 0.370486 0.883796 0.111755 1.853821 1.965419 -0.967561 0.534268	0.000000 1.221854 -1.221854 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
p6 	7.35531 3.66672 2.72728	203.5266, 287.2662 347.9368, 452.7971 495.7165, 574.6169 675.1722, 686.5215 746.2101, 834.6027 891.4905, 911.6894 926.8577, 970.2440 1068.4269, 1105.6899 1201.8338, 1349.6133 1470.1591, 1493.5215 1760.1707, 2071.1804 3121.4231, 3123.5866 3149.7807, 3204.6212 3205.9414	Si H C C C C H H H H H	0.746868 1.068062 1.322318 0.142660 -0.887451 -2.193830 1.226451 2.237886 0.212358 -2.805867 -2.697224	-1.020752 -1.202925 0.920027 0.968035 0.072888 0.016070 1.035266 1.320003 1.287692 0.910951 -0.92258	-0.04852 1.416951 -0.376985 0.426801 0.04601 -0.147276 -1.449213 0.038607 1.460331 -0.144787 -0.333902
p7 	12.2282 1.93027 1.66711	123.0148, 162.4236 193.1380, 264.5570 332.1455, 572.2760 619.5817, 666.9694 831.7428, 855.6793 940.3851, 968.9602 1022.0658, 1066.3816 1123.9372, 1265.4863 1323.5724, 1376.7736 1448.1847, 1571.0135 1674.6499, 2011.2260 3084.8001, 3124.4508 3135.1246, 3155.3299 3224.1359	Si H C C C C H H H H H	-1.282649 -2.810386 -1.167166 0.000000 1.338697 2.434719 2.367952 3.427028 1.435985 -0.033626 -2.067368	-1.565135 -1.591398 0.315827 1.009016 0.456333 1.220704 2.302085 0.791818 -0.623172 2.098016 0.923260	0.0000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
p8 	10.45 2.40306 2.14839	106.6712, 143.0912 271.1033, 415.5018 490.4291, 548.1239 623.6518, 685.6474 834.8911, 870.1573 903.5256, 955.6653	C H H Si C C	-1.065735 -0.935039 -1.539585 -1.547499 0.067707 1.281741	1.10508 1.587893 1.767729 -0.730443 0.237263 0.067706	-0.058939 -1.023889 0.658192 -0.058292 0.438052 -0.370426

		991.2267, 1029.8514 1102.5731, 1204.7947 1299.6956, 1337.1126 1414.2938, 1462.3840 1673.8499, 3081.3603 3094.0672, 3104.4315 3134.3836, 3150.4981 3218.3254	C H H H H	2.500615 0.241657 1.155531 3.337903 2.698547	-0.224297 0.254873 0.195809 -0.340292 -0.354326	0.084884 1.510725 -1.443519 -0.588628 1.141777
p9 	5.73245 3.22974 2.06825	67.4795, 118.4551 231.7387, 321.0415 339.8074, 489.6372 585.5461, 623.7219 796.6197, 823.2511 926.7456, 968.0184 995.4102, 1031.0695 1066.0706, 1266.9229 1339.9636, 1409.8213 1461.3217, 1597.2404 1682.2472, 2012.5284 3091.6501, 3096.4122 3144.5409, 3186.4211 3227.4007	Si C C C C H H H H H H	1.42286 0.699529 0.122453 -1.344865 -2.083817 1.77465 0.116966 0.492479 -1.861521 -1.638675 -3.163744	-0.904743 1.706012 0.484313 0.398613 -0.709056 1.828812 2.620883 -2.069605 1.355854 -1.693338 -0.655491	-0.014878 0.005425 -0.01959 0.015131 -0.0244 -0.045711 0.083474 0.324906 0.063034 -0.071671 -0.005137
p10 	4.68427 4.40693 2.33492	169.4284, 217.1503 238.9653, 342.8310 458.4898, 614.5151 637.5975, 646.7044 682.8785, 702.4225 784.3213, 793.6733 942.1139, 951.2897 952.9089, 1105.4900 1114.1288, 1438.5308 1468.1746, 1665.9245 1704.6054, 2226.0836 2245.0444, 3104.5941 3106.2754, 3190.1097 3190.5603	Si H H C C C C H H H H	0.0000000 1.232406 -1.232406 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000	0.0000000 0.0000000 0.0000000 0.730838 -0.730838 1.729209 -1.729209 1.549697 2.764412 -1.549697 -2.764412	1.396155 2.214451 2.214451 -0.299984 -0.299984 -1.179187 -1.179187 -2.250122 -0.862384 -2.250122 -0.862384
p11 	12.1657 2.18046 1.94092	124.7992, 160.5480 370.2505, 468.7775 483.7297, 510.0919 575.6904, 637.5814 652.8713, 666.1732 797.5734, 829.7088 840.5864, 946.6436 1006.1768, 1012.2411 1027.6205, 1303.9864 1417.2384, 1480.4459 2052.3944, 2241.3068 2264.8935, 3080.6206 3124.0505, 3151.7688 3195.6900	Si H H C C C C H H H H	0.256191 0.030238 0.030238 1.475214 0.0000000 -0.712317 -1.455536 2.029029 2.029029 -1.774684 -1.774684	-1.613909 -2.385035 -2.385035 -0.196102 0.19795 1.269184 2.341994 0.038088 0.038088 2.805232 2.805232	0.000000 1.238882 -1.238882 0.0000000 0.0000000 0.0000000 0.0000000 0.904191 -0.904191 0.925447 -0.925447

p12 	6.26974 5.19509 3.22076	192.9261, 321.2203 404.5774, 505.5147 544.9538, 614.0923 643.5462, 695.6809 713.1477, 781.7753 845.8462, 883.9859 922.4054, 952.9568 1088.7291, 1104.3689 1135.1002, 1193.2589 1365.9078, 1455.7385 1761.1847, 2156.712 2201.5682, 3042.9192 3094.0353, 3165.1139 3180.248	C C C C H H H Si H H H	0.389056 -0.878945 -1.459622 -0.618962 -2.219843 -0.852112 -0.689128 1.059396 2.300993 1.28639 0.752991	1.409601 1.105935 -0.072326 -1.18028 -0.288626 -2.16962 -1.223129 -0.339152 -0.695249 -0.64173 2.188909	-0.17589 0.047135 0.235028 -0.4051 0.972936 -0.01085 -1.49329 0.154555 -0.59947 1.592379 -0.83251
p13 	8.63831 3.75018 3.26135	130.9042, 202.1760 525.5380, 565.6999 680.5674, 784.3580 849.1606, 893.3645 912.1812, 931.7088 976.7927, 1002.7673 1074.9797, 1076.9321 1207.6294, 1209.4170 1219.5965, 1271.4942 1289.0370, 1496.6060 1515.1365, 3020.4597 3029.4054, 3061.8118 3081.0984, 3105.0273 3116.6773	Si C C C C H H H H H H	-1.079746 0.455571 0.455571 0.455571 0.455571 1.106876 1.106876 1.370862 -0.386368 1.370862 -0.386368	-1.119083 -0.323621 1.218954 1.218954 -0.323621 -0.888555 -0.888555 1.637574 1.712565 1.637574 1.712565	0.0000000 0.778493 0.777788 -0.777788 -0.778493 1.437762 -1.437762 1.195335 1.268002 -1.195335 -1.268002
p14 	7.71031 2.8723 2.30742	103.0840, 207.6943 256.5679, 356.2726 477.7269, 554.4234 598.4342, 639.2484 714.7666, 881.4020 888.1870, 915.5522 931.5113, 991.0898 1011.1139, 1119.4428 1147.5168, 1359.1192 1463.8021, 1470.9785 1980.9549, 2023.2943 3111.0584, 3117.6373 3120.2741, 3186.0826 3197.5457	Si C C C C H H H H H H	-1.275929 -1.092286 0.112297 1.198802 2.348643 2.523099 3.174706 0.031553 -1.813164 -0.891791 -0.566134	-0.868678 1.01093 0.893745 0.190719 -0.343196 -1.408276 0.274149 1.248361 1.714691 1.164871 -1.345492	-0.133473 0.434417 -0.428551 -0.133728 0.147329 0.069978 0.483708 -1.45247 0.035376 1.487249 1.127984
p15 	5.63386 4.03749 2.47921	45.0672, 111.3013 304.6455, 350.3037 482.4784, 526.3371 540.5321, 667.5261 683.1891, 884.4186 889.6702, 911.7949 948.5455, 1034.369	C C H C C H H	-1.91377 -1.13456 -2.26902 -0.18748 1.212557 -0.40435 1.751635	-0.53532 0.519619 -1.00022 1.416439 0.861705 2.480411 1.231242	-0.02033 0.010183 0.89206 0.019734 -0.0081 0.034228 -0.88361

		1098.8122, 1119.5378 1155.3778, 1333.624 1448.472, 1482.9621 2005.9993, 2010.2948 3023.791, 3063.3998 3115.976, 3120.7448 3191.5607	H Si H H	1.770548 0.916963 0.731597 -2.27839	1.164232 -1.09017 -1.2492 -0.93877	0.880606 -0.09885 1.409229 -0.95752
p16 	6.51026 5.04136 3.1059	199.9778, 409.5386 460.7861, 487.1845 523.3076, 606.0262 651.2749, 709.3619 773.4042, 804.5717 838.597, 938.444 975.212, 983.8389 1008.1616, 1091.2852 1126.2303, 1247.4534 1363.5492, 1415.7742 1473.3144, 2204.6278 2225.4259, 2996.0661 3119.6267, 3137.0678 3177.047	C C C C H H Si H H H H	0.445027 1.472573 1.074683 -0.14048 -0.60872 -0.11985 -1.1158 -2.25662 -1.63497 0.610822 2.51975	-1.26396 -0.35966 0.937252 1.390723 2.290413 1.385635 -0.29342 -0.58885 -0.22967 -2.33235 -0.64349	-0.13935 -0.03885 0.380263 -0.24588 0.142965 -1.34304 0.077136 -0.8282 1.464154 -0.18292 -0.06993
p17 	6.76591 4.71554 2.97776	146.3583, 288.0116 389.2218, 534.368 561.5778, 619.8191 669.2299, 714.8677 761.5697, 822.5518 848.7595, 926.765 953.2528, 983.0294 1091.2401, 1125.6741 1199.2677, 1230.9767 1397.9165, 1434.3681 1479.5792, 2195.8999 2224.3907, 3011.8093 3056.3646, 3089.9223 3111.6854	C C C C H H H Si H H H	0.106152 1.300169 1.321057 0.040463 2.263671 0.005395 -0.08469 -1.20945 -2.34292 -1.74668 2.23041	-1.41976 -0.79108 0.590979 1.334943 1.135361 2.224903 1.690448 -0.121 -0.03822 -0.27121 -1.33784	-0.29909 0.09974 0.063349 -0.10298 0.07624 0.528419 -1.1319 0.08083 -0.87246 1.460283 0.241736
p18 	10.86250 2.18889 1.90286	82.13, 132.0869 250.3713, 332.4019 389.657, 421.0322 527.0927, 640.8592 730.3353, 800.7886 826.5569, 854.3018 916.2411, 945.9996 995.4333, 1069.5273 1225.5092, 1272.9582 1357.3709, 1434.0794 1475.8103, 2272.4618 2304.6853, 3030.7356 3054.8518, 3135.9319 3155.8398	C C C C Si H H H H H H	-0.61186 0.777481 1.456935 2.506153 -1.75804 -1.37532 -1.01833 1.391144 0.937845 3.108897 -3.20392	0.937892 0.828227 -0.37684 -0.62337 -0.38546 -1.79181 1.938931 1.694003 -1.15104 0.213575 -0.10272	-0.02143 0.133238 0.444598 -0.36259 -0.0645 -0.26168 -0.12467 -0.08882 1.015488 -0.72892 -0.07134

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