Formation of the Elusive Silylenemethyl Radical ($HCSiH_2$; X^2B_2) via the Unimolecular Decomposition of Triplet Silaethylene (H_2CSiH_2; a^3A')

Chao He,[a] Aaron M. Thomas,[a] Beni B. Dangi,[a,b] Tao Yang,[a,c] Ralf I. Kaiser [a]*

[a] *Department of Chemistry, University of Hawai'i at Manoa, Honolulu, HI 96822, USA*

[b] *Present Address: Department of Chemistry, Florida Agricultural and Mechanical University, Tallahassee, FL 32307, USA*

[c] *Present Address: State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai, 200062, China*

Huan-Cheng Lee, Bing-Jian Sun, Agnes H. H. Chang*

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

*E−mail: ralfk@hawaii.edu, hhchang@gms.ndhu.edu.tw

The comparison of CM functions between our study and Lu. et al.

It is very important to perform the comparison of CM functions between our study and Lu. *et al.* (Figure S1-S3).[1] First, the comparison for atomic hydrogen loss product channel (m/z = 43) is conducted. Considering the center-of-mass translational energy distributions, Lu. *et al.* reveals a maximum translational energy of 146 kJ mol^{-1} (no error limits are given by the authors), whereas 105 ± 15 kJ mol^{-1} is derived as the maximum translational energy in the present study. Both studies revealed a similar most probable relative translational energy, which are 25 kJ mol^{-1} (Lu. *et al.*) and 22 ± 3 kJ mol^{-1} (this study). Lu. *et al.* featured a slight "sideway scattering" of the CM angular distribution $T(\theta)$ compared with a much obvious "sideway scattering" in the present study (Figure S2). Further, the CM functions from Lu *et al.* were adapted to fit our experimental data at m/z = 43. The resulting TOFs (figure S1) are faster compared to our study, especially at high laboratory angles, whereas the resulting laboratory angular distribution (figure S1) cannot fit well at low laboratory angles. Second, the molecular hydrogen loss product channel is predicted in the investigation of Lu. *et al.,* whereas it is absent in our study. Therefore, we adapted CM functions of molecular hydrogen loss product channel to fit our experimental data (m/z = 42) (Figure S3). Considering the center-of-mass translational energy distributions of molecular hydrogen loss product, Lu. *et al.* reveals a maximum translational energy of 243 kJ mol^{-1} along with the most probable relative translational energy of 58.6 kJ mol^{-1}. The corresponding $T(\theta)$ depicts non-zero intensity over the complete scattering range from 0° to 180° and featured with the forward−backward symmetry. The resulting TOFs (figure S3) and laboratory angular distribution (figure S3) cannot fit our experimental data well.

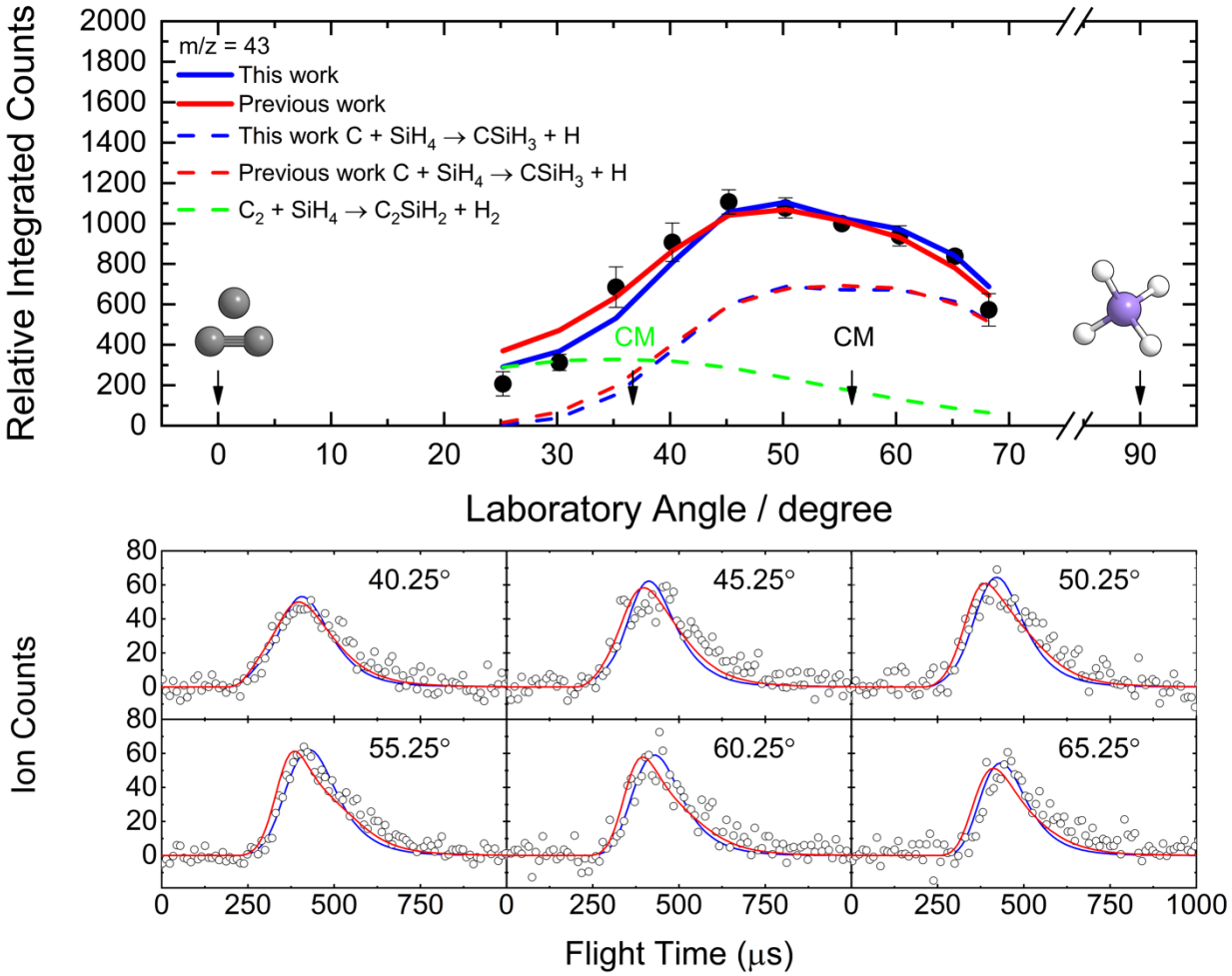


Figure S1. Laboratory angular distribution (top) and TOF spectra (bottom) recorded at $m/z = 43$ for the reaction of atomic carbon and dicarbon with silane. The data were fit with two channels (i) ^{12}C (12 amu) + $^{28}SiH_4$ (32 amu) → $^{12}C^{28}SiH_3$ (43 amu) + H (1 amu) (dash blue/red), (ii) dissociative electron impact ionization of the m/z = 55 ($^{12}C_2{}^{29}SiH_2^+$) formed in the reaction $^{12}C_2$ (24 amu) + $^{29}SiH_4$ (33 amu) → $^{12}C_2{}^{29}SiH_2$ (55 amu) + H_2 (2 amu) (dash green). The black circles depict the experimental data, and error bars the 1s standard deviation. The solid colored lines (blue/red) corresponding to the total fit. The solid red lines define the best fits in this work, while the solid blue lines define the best fits in previous work (J. Chem. Phys. 129, 164304 (2008)). Colors of the atoms: silicon, purple; carbon, gray; and hydrogen, white.

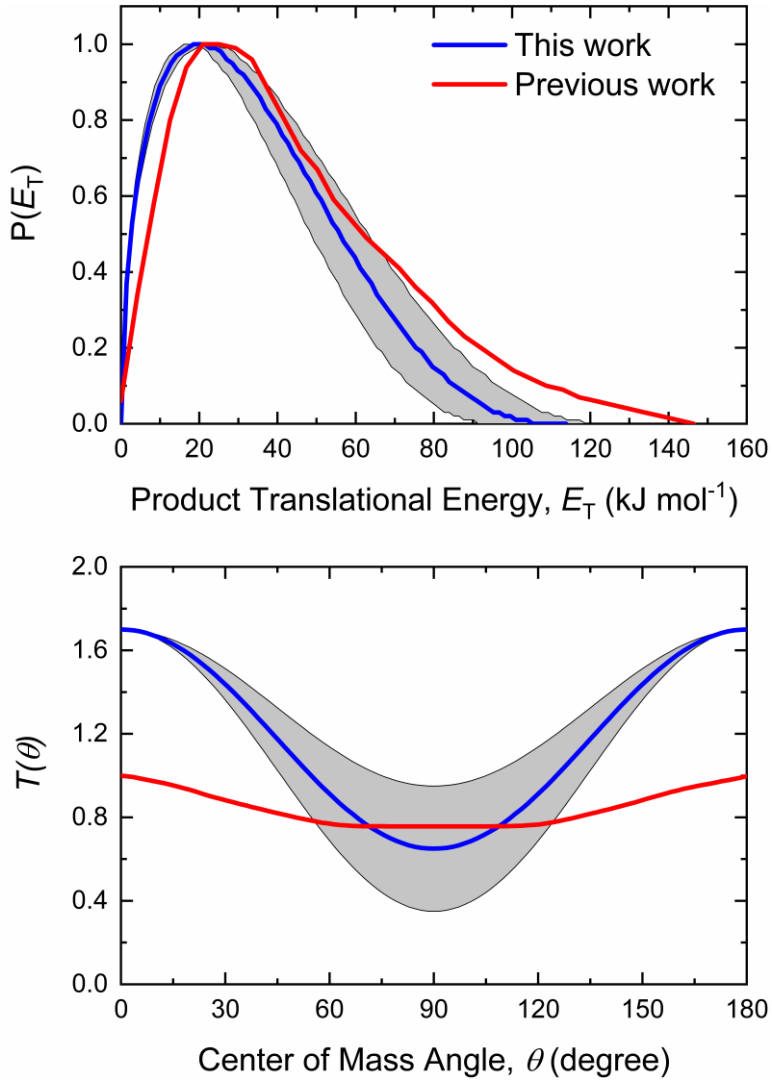


Figure S2. CM translational energy flux distribution (top), and CM angular flux distribution (bottom) for the reaction of atomic carbon with silane leading to atomic hydrogen loss product(s). The blue solid lines define the best fits in this work with shaded areas indicate the acceptable upper and lower error limits. The red solid lines define the best fits in previous work (J. Chem. Phys. 129, 164304 (2008)).

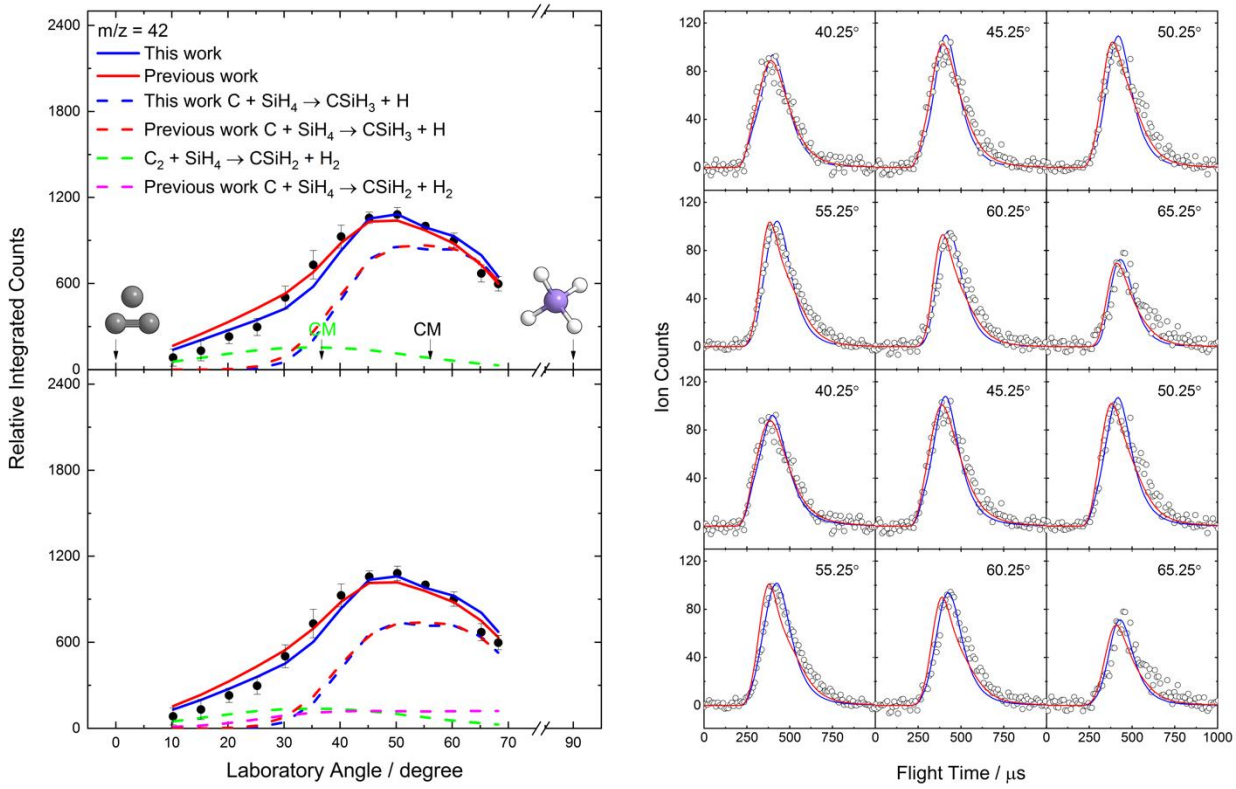


Figure S3. Laboratory angular distribution (left) and TOF spectra (right) recorded at $m/z = 42$ for the reaction of atomic carbon and dicarbon with silane. The data were fit with two channels (top), and with three channels (bottom): (i) ^{12}C (12 amu) + $^{28}SiH_4$ (32 amu) → $^{12}C^{28}SiH_3$ (43 amu) + H (1 amu) (dash blue/red), (ii) dissociative electron impact ionization of the m/z = 55 ($^{12}C_2{}^{29}SiH_2^+$) formed in the reaction $^{12}C_2$ (24 amu) + $^{29}SiH_4$ (33 amu) → $^{12}C_2{}^{29}SiH_2$ (55 amu) + H_2 (2 amu) (dash green) with CM functions derived from A. Rettig et al. (J. Phys. Chem Lett. 12, 10768-10776 (2021)), and iii) ^{12}C (12 amu) + $^{28}SiH_4$ (32 amu) → $^{12}C^{28}SiH_2$ (43 amu) + H_2 (1 amu) (dash magenta) with CM functions stemmed from Lu et al. (J. Chem. Phys. 129, 164304 (2008)). The black circles depict the experimental data, colored lines the fits (red corresponding to the total fit), and error bars the 1s standard deviation. The blue solid lines define the best fits in this work, whereas the red solid lines define the best fits in previous work (J. Chem. Phys. 129, 164304 (2008)). Colors of the atoms: silicon, purple; carbon, gray; and hydrogen, white.

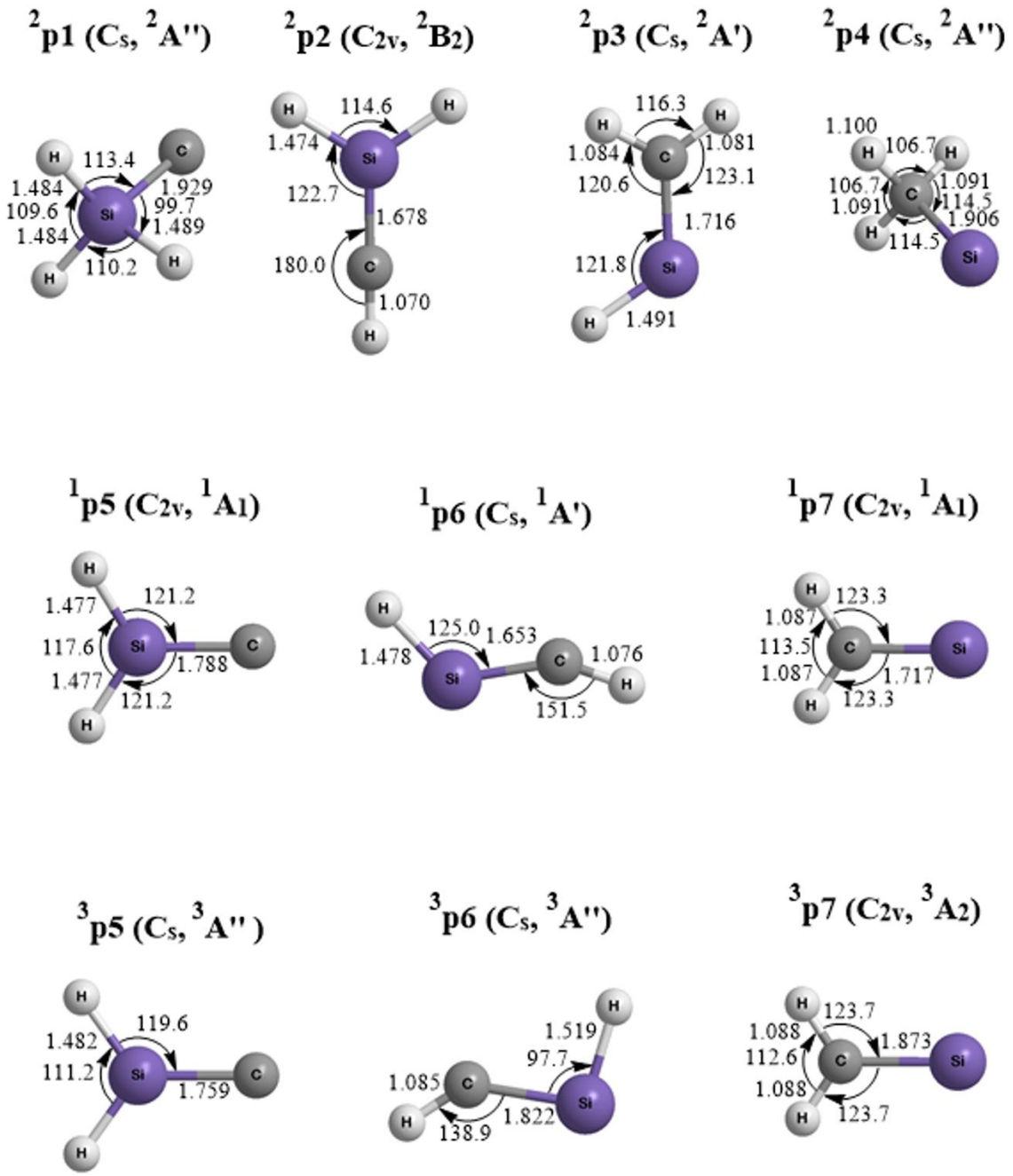


Figure S4. CCSD/cc-pVTZ optimized geometries of $CSiH_3$ and $CSiH_2$ isomers along with their bond lengths (angstroms), bond angles, and ground state symmetry.

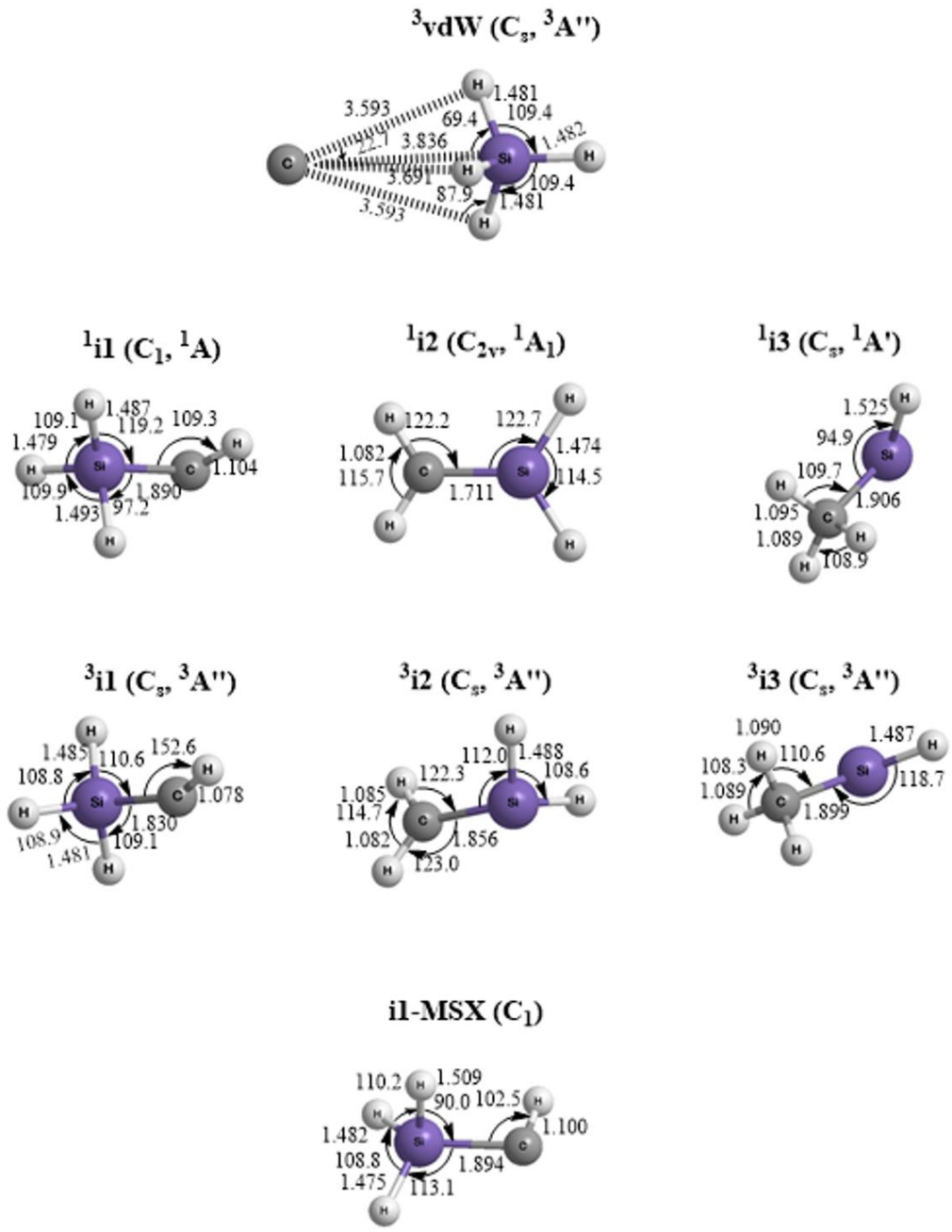


Figure S5. CCSD/cc-pVTZ optimized structures of singlet and triplet intermediates, CPMCSCF/TZVPP optimized minimum-energy crossing point, including electronic states and point groups. The bond angles are in degrees and bond lengths are in angstrom.

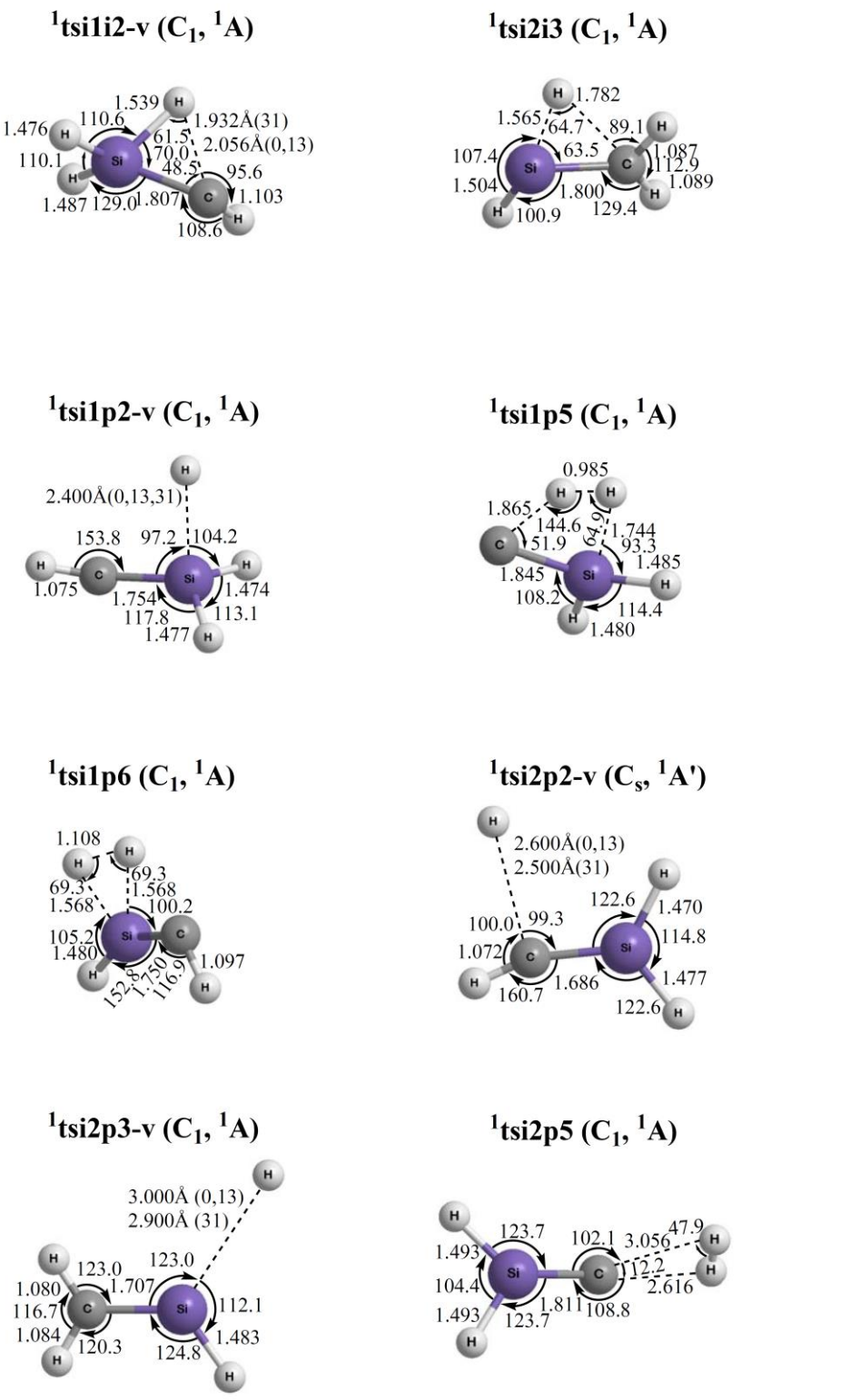
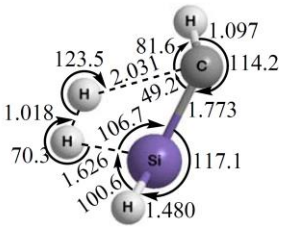
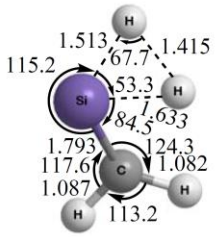


Figure S6. The CCSD/cc-pVTZ optimized geometries of the transition states for the C(^3P) + SiH_4 (X^1A_1) reaction on the adiabatic singlet and triplet ground state potential energy surfaces.

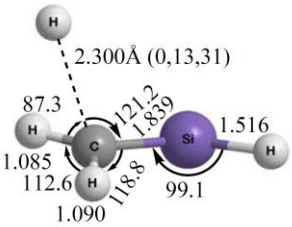
^{1}tsi2p6 (C_1, ^{1}A)



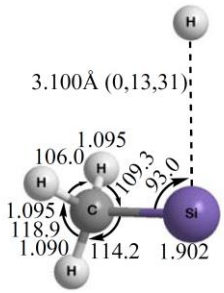
^{1}tsi2p7 (C_1, ^{1}A)



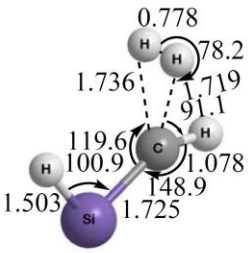
^{1}tsi3p3-v (C_1, ^{1}A)



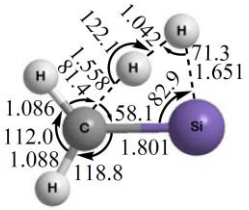
^{1}tsi3p4-v (C_1, ^{1}A)



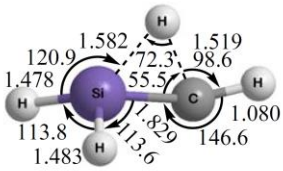
^{1}tsi3p6 (C_1, ^{1}A)



^{1}tsi3p7 (C_1, ^{1}A)



^{3}tsi1i2 (C_1, ^{3}A)



^{3}tsi2i3 (C_1, ^{3}A)

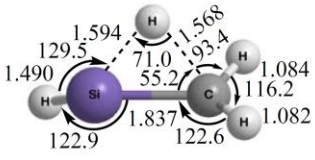
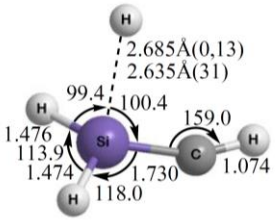
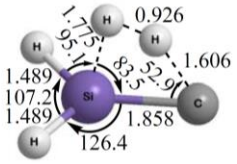


Figure S6 (continued)

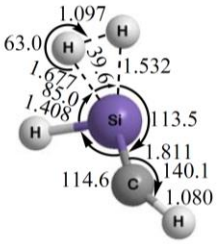
^{3}tsi1p2-v (C_1, ^{3}A)



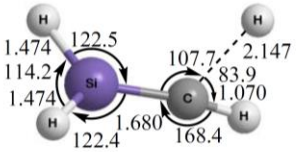
^{3}tsi1p5 (C_1, ^{3}A)



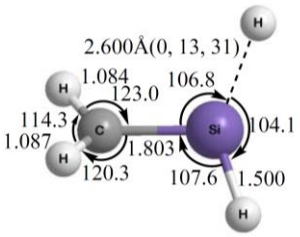
^{3}tsi1p6 (C_1, ^{3}A)



^{3}tsi2p2 (C_1, ^{3}A)



^{3}tsi2p3-v (C_1, ^{3}A)



^{3}tsi2p5' (C_1, ^{3}A)

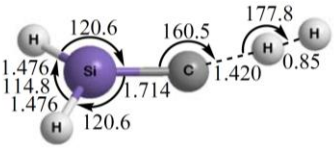
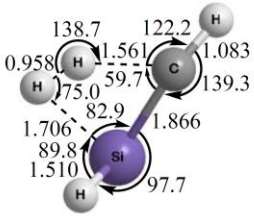
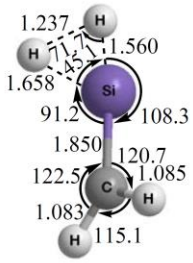


Figure S6 (continued)

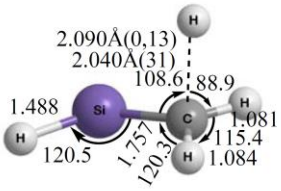
^{3}tsi2p6 (C_1, ^{3}A)



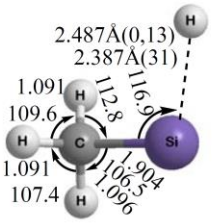
^{3}tsi2p7 (C_1, ^{3}A)



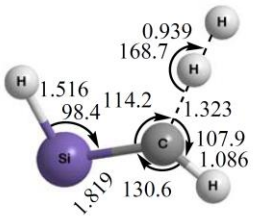
^{3}tsi3p3-v (C_1, ^{3}A)



^{3}tsi3p4-v (C_1, ^{3}A)



^{3}tsi3p6 (C_1, ^{3}A)



^{3}tsi3p7 (C_1, ^{3}A)

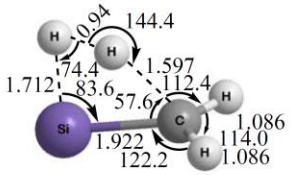


Figure S6 (continued)

Table S1. CCSD(T)/CBS energies with CCSD/cc-pVTZ zero-point energy corrections of CCSD/cc-pVTZ optimized reactants, intermediates, transition states, H, and H_2 dissociation products on the adiabatic triplet and singlet ground state potential energy surfaces of $CSiH_4$.

	CCSD/ cc-pVTZ + E_{zpc} [a]	E_{zpc} [b]	CCSD(T)/ cc-pVDZ	CCSD(T)/ cc-pVTZ	CCSD(T)/ cc-pVQZ	CCSD(T)/ CBS	E(kJ/mol)[c]
C(^{3}P)	-37.778726	0.000000	-37.760377	-37.780762	-37.786540	-37.789739	
SiH_4 (T_d, $^1A_1$)	-291.401964	0.031561	-291.392685	-291.437349	-291.450714	-291.458201	
C + SiH_4	-329.180690	0.031561	-329.153062	-329.218111	-329.237253	-329.247940	0.0
H	-0.499810	0.000000	-0.499278	-0.499810	-0.499946	-0.500019	
H_2 ($D_{\infty h}$, $^1\Sigma_g^+$)	-1.169930	0.010045	-1.163453	-1.172337	-1.173796	-1.174474	
^{1}vdW (C_{3v}, $^1A_1$)	-329.124899	0.032006	-329.095746	-329.165816	-329.186692	-329.198377	131.3
^{3}vdW (C_s, $^3A''$)	-329.180839	0.032073	-329.153850	-329.218898	-329.238124	-329.248867	-1.1
^{1}i1 (C_1, ^1A)	-329.271471	0.035071	-329.237552	-329.317118	-329.340722	-329.353921	-269.0
^{3}i1 (C_s, $^3A''$)	-329.304036	0.035402	-329.269957	-329.347670	-329.370437	-329.383136	-344.9
^{1}i2 (C_{2v}, $^1A_1$)	-329.372317	0.040305	-329.345912	-329.427159	-329.450979	-329.464267	-545.0
^{3}i2 (C_s, $^3A''$)	-329.320357	0.038472	-329.289432	-329.368262	-329.390558	-329.402898	-388.7
^{1}i3 (C_s, $^1A'$)	-329.371477	0.042135	-329.345342	-329.425318	-329.446929	-329.458765	-525.8
^{3}i3 (C_s, $^3A''$)	-329.335244	0.042935	-329.311579	-329.389060	-329.410252	-329.421892	-426.8
^{1}i1-MSX (C_1, ^1A)		0.037132	-329.236874	-329.316340	-329.339881	-329.353041	-261.3
^{2}p1 (C_s, $^2A''$)	-328.629809	0.025179	-328.593024	-328.663947	-328.685423	-328.697484	
^{2}p2 (C_{2v}, $^2B_2$)	-328.705545	0.026603	-328.669179	-328.744582	-328.767401	-328.780214	
^{2}p3 (C_s, $^2A'$)	-328.732179	0.030882	-328.702208	-328.776826	-328.798544	-328.810640	
^{2}p4 (C_s, $^2A''$)	-328.755451	0.034586	-328.727779	-328.801164	-328.820674	-328.831318	
^{2}p1+H	-329.129619	0.025179	-329.092303	-329.163757	-329.185368	-329.197503	115.7
^{2}p2+H	-329.205355	0.026603	-329.168458	-329.244392	-329.267346	-329.280233	-97.8

^{2}p3+H	-329.231989	0.030882	-329.201486	-329.276636	-329.298490	-329.310659	-166.5
^{2}p4+H	-329.255261	0.034586	-329.227057	-329.300974	-329.320619	-329.331337	-211.0
^{1}p5 (C_{2v}, $^1A_1$)	-328.031342	0.016006	-327.995423	-328.061776	-328.082390	-328.094028	
^{3}p5' (C_s, ^{3}A'')	-328.027710	0.016540	-327.993785	-328.058133	-328.077915	-328.089059	
^{1}p6 (C_s, ^{1}A')	-328.103091	0.019254	-328.075778	-328.143846	-328.164505	-328.176113	
^{3}p6 (C_s, ^{3}A'')	-328.073835	0.018028	-328.035546	-328.102023	-328.121096	-328.131685	
^{1}p7 (C_{2v}, $^1A_1$)	-328.164733	0.022130	-328.131141	-328.201282	-328.221352	-328.232489	
^{3}p7 (C_{2v}, $^3A_2$)	-328.109953	0.022398	-328.075284	-328.142045	-328.160111	-328.170009	
^{1}p5 + H_2	-329.201272	0.026051	-329.158876	-329.234113	-329.256186	-329.268501	-68.4
^{3}p5' + H_2	-329.197640	0.026585	-329.157238	-329.230470	-329.251711	-329.263533	-54.0
^{1}p6 + H_2	-329.273021	0.029299	-329.239231	-329.316182	-329.338301	-329.350587	-275.4
^{3}p6 + H_2	-329.243765	0.028073	-329.198999	-329.274360	-329.294892	-329.306159	-162.0
^{1}p7 + H_2	-329.334663	0.032175	-329.294595	-329.373618	-329.395148	-329.406963	-415.9
^{3}p7 + H_2	-329.279883	0.032443	-329.238737	-329.314382	-329.333907	-329.344483	-251.2
^{1}tsi1i2-v (C_1, ^{1}A)[d]	-329.270942	0.034253	-329.236765	-329.317107	-329.341105	-329.354543	-272.8
	-329.271583	0.034319	-329.237583	-329.318399	-329.342533	-329.356048	-276.6
^{3}tsi1i2 (C_1, ^{3}A)	-329.236515	0.032258	-329.199373	-329.280388	-329.303925	-329.317029	-179.6
^{1}tsi2i3 (C_1, ^{1}A)	-329.310894	0.038513	-329.215929	-329.297801	-329.321088	-329.333993	-207.7
^{3}tsi2i3 (C_1, ^{3}A)	-329.256678	0.036297	-329.224066	-329.305752	-329.328604	-329.341222	-232.5
^{2}tsp2p3 (C_1, ^{2}A)	-328.660118	0.025347	-328.627192	-328.701575	-328.723703	-328.736084	
^{2}tsp3p4 (C_1, ^{2}A)	-328.699310	0.029334	-328.668305	-328.743392	-328.764197	-328.775658	
^{3}tsp5p6 (C_1, ^{3}A)	-327.997986	0.014125	-327.962453	-328.027030	-328.046457	-328.057352	
^{3}tsp6p7 (C_1, ^{3}A)	-328.031171	0.015969	-327.992380	-328.060262	-328.079364	-328.089924	

^{1}tsi1p2-v (C_1, ^{1}A)^{d}	-329.211826	0.028446	-329.176293	-329.253562	-329.276565	-329.289439	-117.1
	-329.211826	0.028446	-329.176293	-329.253562	-329.276565	-329.289439	-117.1
^{3}tsi1p2-v (C_1, ^{3}A)^{d}	-329.210701	0.027905	-329.167654	-329.243974	-329.267002	-329.279925	-93.6
	-329.212314	0.028165	-329.168151	-329.244432	-329.267389	-329.280266	-93.8
^{1}tsi1p5 (C_1, ^{1}A)	-329.124257	0.030093	-329.086322	-329.169689	-329.194465	-329.208326	100.2
^{1}tsi1p6 (C_1, ^{1}A)	-329.211107	0.032372	-329.180719	-329.262162	-329.286158	-329.299559	-133.4
^{3}tsi1p6 (C_1, ^{3}A)	-329.209363	0.031753	-329.174841	-329.253416	-329.276288	-329.289026	-107.4
^{1}tsi2p2-v (C_1, ^{1}A)^{d}	-329.209596	0.028615	-329.187288	-329.263651	-329.286971	-329.300091	-144.7
	-329.211694	0.029031	-329.189397	-329.266072	-329.289498	-329.302678	-150.4
^{3}tsi2p2 (C^{1}, ^{3}A)	-329.200213	0.028606	-329.165624	-329.243834	-329.267321	-329.280490	-93.2
^{1}tsi2p3-v (C_1, ^{1}A)^{d}	-329.239980	0.032313	-329.217881	-329.294826	-329.317550	-329.330245	-214.1
	-329.243360	0.032630	-329.221547	-329.298902	-329.321745	-329.334507	-224.5
^{3}tsi2p3-v (C_1, ^{1}A)^{d}	-329.238457	0.032004	-329.205937	-329.282357	-329.304132	-329.316204	-178.1
	-329.238457	0.032004	-329.205937	-329.282357	-329.304132	-329.316204	-178.1
^{1}tsi2p5 (C_1, ^{1}A)	-329.104834	0.027368	-329.152932	-329.227567	-329.249339	-329.261470	-46.5
^{3}tsi2p5 (C_1, ^{3}A)	-329.180163	0.025866	-329.144270	-329.219016	-329.241425	-329.253983	-30.8
^{1}tsi2p6 (C_1, ^{1}A)	-329.207660	0.032246	-329.174892	-329.258284	-329.282783	-329.296455	-125.6
^{3}tsi2p6 (C_1, ^{3}A)	-329.210468	0.031945	-329.176287	-329.255395	-329.277614	-329.289893	-109.1
^{1}tsi2p7 (C_1, ^{1}A)	-329.264172	0.035636	-329.240719	-329.320618	-329.343323	-329.355903	-272.8
^{3}tsi2p7 (C_1, ^{3}A)	-329.241842	0.033464	-329.207904	-329.288000	-329.310337	-329.322660	-191.2
^{1}tsi3p3-v (C_1, ^{3}A)^{d}	-329.236685	0.032014	-329.206191	-329.282001	-329.303349	-329.315153	-175.3
	-329.236685	0.032014	-329.206191	-329.282001	-329.303349	-329.315153	-175.3
^{3}tsi3p3-v (C_1, ^{3}A)^{d}	-329.233507	0.033083	-329.211493	-329.286200	-329.308324	-329.320691	-187.0
	-329.234874	0.033358	-329.210619	-329.288584	-329.310815	-329.323141	-192.7
^{1}tsi3p4-v (C_1, ^{3}A)^{d}	-329.258843	0.040381	-329.242270	-329.317964	-329.338618	-329.349956	-244.7
	-329.258843	0.040381	-329.242270	-329.317964	-329.338618	-329.349956	-244.7
^{3}tsi3p4-v (C_1, ^{3}A)^{d}	-329.262756	0.036714	-329.262512	-329.340329	-329.361391	-329.372931	-314.6

	-329.267107	0.037181	-329.269817	-329.348082	-329.369154	-329.380685	-333.8
^{1}tsi3p6 (C_1, ^{1}A)	-329.243690	0.033324	-329.215191	-329.294464	-329.317126	-329.329698	-210.0
^{3}tsi3p6 (C_1, ^{3}A)	-329.212129	0.027878	-329.177838	-329.252864	-329.274002	-329.285691	-108.8
^{1}tsi3p7 (C_1, ^{1}A)	-329.291513	0.038431	-329.265476	-329.347517	-329.370155	-329.382615	-335.6
^{3}tsi3p7 (C^{1}, ^{3}A)	-329.246554	0.035805	-329.216002	-329.295834	-329.317175	-329.328833	-201.2

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

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

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

[d] the variational transition states found at collision energies, 13.0, and 31.0 kJ/mol, respectively.

Table S2. CCSD/cc-pVTZ optimized Cartesian coordinates of intermediates, transition states, products and CPMCSCF/TZVPP optimized minimum-energy crossing point on the triplet and singlet $CSiH_4$ potential energy surfaces.

Atom	X	Y	Z	Atom	X	Y	Z
^{1}vdW				**^{3}vdW**			
Si	0.000000	0.000000	0.948637	Si	0.000046	0.958733	0.000000
H	0.000000	1.399923	0.465823	H	-0.066515	2.439404	0.000000
H	-1.212369	-0.699962	0.465823	H	1.418013	0.530457	0.000000
H	1.212369	-0.699962	0.465823	H	-0.676210	0.436954	1.210401
H	0.000000	0.000000	2.432122	H	-0.676210	0.436954	-1.210401
C	0.000000	0.000000	-2.851752	C	0.000046	-2.877671	0.000000
^{1}i1				**^{1}i2**			
Si	-0.507614	0.010203	-0.004813	Si	0.000000	0.000000	0.551868
H	1.837419	0.827291	-0.037361	H	0.000000	1.240085	1.349331
H	-1.17151	-1.193859	-0.551012	C	0.000000	0.000000	-1.159191
H	-1.128475	1.221539	-0.602451	H	0.000000	-0.915624	-1.734835
C	1.372709	-0.17431	-0.036897	H	0.000000	0.915624	-1.734835
H	-0.667094	0.048049	1.479592	H	0.000000	-1.240085	1.349331
^{1}i3				**^{3}i1**			
Si	0.067372	-0.758358	0.000000	Si	-0.019840	-0.509918	0.000000
H	-1.452055	-0.887920	0.000000	H	0.669965	-1.031553	1.207242
C	0.067372	1.147816	0.000000	H	-1.419863	-0.993685	0.000000
H	-0.480195	1.517424	0.873086	H	0.669965	-1.031553	-1.207242
H	1.065014	1.583191	0.000000	C	-0.019840	1.319883	0.000000
H	-0.480195	1.517424	-0.873086	H	0.476739	2.276344	0.000000
^{3}i2				**^{3}i3**			
Si	0.055972	-0.621080	0.000000	Si	0.053479	-0.729543	0.000000
H	-0.611163	-1.177708	1.208559	H	-1.250191	-1.445095	0.000000
C	0.055972	1.235249	0.000000	C	0.053479	1.169162	0.000000
H	0.963899	1.824105	0.000000	H	-0.448892	1.552957	0.887981
H	-0.861017	1.814930	0.000000	H	1.078391	1.537818	0.000000
H	-0.611163	-1.177708	-1.208559	H	-0.448892	1.552957	-0.887981
i1-MSX				**SiH_4**			
Si	-0.507548	0.006898	-0.006031	Si	0.000000	0.000000	0.000000
H	-1.198234	1.185265	-0.581865	H	0.855367	0.855367	0.855367
H	-1.218069	-1.214088	-0.428909	H	-0.855367	-0.855367	0.855367
H	-0.456636	0.116055	1.497698	H	-0.855367	0.855367	-0.855367
C	1.376823	-0.175588	-0.055127	H	0.855367	-0.855367	-0.855367

H	1.717677	0.869726	-0.071724				
^{2}p1				**^{2}p2**			
Si	0.009933	-0.440872	0.000000	Si	0.000000	0.000000	0.487999
H	-1.458432	-0.690087	0.000000	H	0.000000	1.240409	1.285009
H	0.629885	-1.031885	1.211340	H	0.000000	-1.240409	1.285009
H	0.629885	-1.031885	-1.211340	C	0.000000	0.000000	-1.190247
C	0.009933	1.487677	0.000000	H	0.000000	0.000000	-2.260521
^{2}p3				**^{2}p4**			
Si	0.056306	-0.612445	0.000000	H	1.057638	1.382393	0.000000
H	-1.210531	-1.398595	0.000000	H	-0.448365	1.559608	0.890939
C	0.056306	1.103825	0.000000	H	-0.448365	1.559608	-0.890939
H	-0.87696	1.65585	0.000000	C	-0.008045	1.109443	0.000000
H	0.961369	1.694033	0.000000	Si	-0.008045	-0.797019	0.000000
^{1}p5				**^{1}p6**			
Si	0.000000	0.000000	0.417983	Si	0.031686	-0.530577	0.000000
H	0.000000	1.263419	1.182817	H	-1.179538	-1.377552	0.000000
H	0.000000	-1.263419	1.182817	C	0.031686	1.122912	0.000000
C	0.000000	0.000000	-1.369566	H	0.545823	2.068153	0.000000
^{1}p7							
Si	0.000000	0.000000	0.678703				
C	0.000000	0.000000	-1.038666				
H	0.000000	0.909253	-1.63492				
H	0.000000	-0.909253	-1.63492				
^{3}p5'				**^{3}p6**			
Si	0.036846	-0.413178	0.000000	Si	0.036007	-0.607664	0.000000
H	-0.368461	-1.145791	1.222807	H	-1.469071	-0.812149	0.000000
C	0.036846	1.346013	0.000000	C	0.036007	1.214428	0.000000
H	-0.368461	-1.145791	-1.222807	H	0.748940	2.032876	0.000000
^{3}p7							
Si	0.000000	0.000000	0.735971				
C	0.000000	0.000000	-1.136981				
H	0.000000	0.905146	-1.740857				
H	0.000000	-0.905146	-1.740857				
^{1}tsi1i2-v(31)				**^{1}tsi1i2-v(13)**			
Si	-0.499654	0.010093	-0.017952	Si	-0.502343	0.009794	-0.013327
H	1.756159	0.823962	-0.065342	H	1.77005	0.826287	-0.06649
H	-1.329556	1.205845	-0.320599	H	-1.296592	1.204381	-0.400631
H	0.105382	0.108507	1.39343	H	-0.029783	0.120592	1.432924
C	1.295639	-0.177289	-0.100717	C	1.314246	-0.178442	-0.093399
H	-1.310664	-1.215887	-0.151853	H	-1.296348	-1.217727	-0.218836

^{1}tsi2i3				^{1}tsi1p2-v(13,31)			
Si	0.661559	0.073601	-0.084575	Si	0.483233	-0.075841	0.007825
H	1.069549	-1.279287	0.429688	H	-2.244721	0.291269	0.20501
C	-1.131972	-0.073857	-0.043631	H	1.185276	-0.552491	-1.197312
H	-0.073792	0.815955	1.08094	H	1.126355	-0.513744	1.263685
H	-1.715874	0.832011	-0.182573	C	-1.269312	-0.078012	-0.056955
H	-1.749879	-0.95595	0.117777	H	0.7837	2.304812	-0.039204
^{1}tsi1p5				^{1}tsi1p6			
Si	0.415262	-0.124594	0.007060	Si	0.437786	0.127777	0.000160
H	1.474778	-0.402281	1.009835	H	0.95755	-1.243502	-0.554111
H	0.846745	-0.288295	-1.399122	H	1.618494	1.019331	-0.000967
H	0.689675	1.627838	0.049135	H	0.958003	-1.243587	0.553488
C	-1.428596	-0.091249	0.04515	C	-1.286729	-0.171428	-0.000081
H	-0.253286	1.354555	-0.029584	H	-1.942676	0.707446	-0.000157
^{1}tsi2p2-v(31)				^{1}tsi2p2-v(13)			
Si	0.087867	-0.554611	0.000000	Si	0.093719	-0.554744	0.000000
H	1.331167	-1.351053	0.000000	H	1.334944	-1.354131	0.000000
C	0.087867	1.13101	0.000000	C	0.093719	1.12965	0.000000
H	-2.379545	1.533353	0.000000	H	-2.47458	1.534418	0.000000
H	0.441784	2.142729	0.000000	H	0.412141	2.152872	0.000000
H	-1.150748	-1.346528	0.000000	H	-1.146888	-1.344646	0.000000
^{1}tsi2p3-v(31)				^{1}tsi2p3-v(13)			
Si	0.493978	-0.154522	-0.000060	Si	0.489104	-0.165892	-0.000056
H	2.542401	1.898272	0.000236	H	2.656204	1.908638	0.000242
C	-1.176639	0.197483	0.000054	C	-1.177019	0.217035	0.000036
H	-1.905083	-0.604773	0.000152	H	-1.921861	-0.57027	0.000229
H	-1.5649	1.205257	-0.000134	H	-1.546546	1.231991	-0.000133
H	1.07172	-1.52034	0.000255	H	1.026865	-1.550075	0.000223
^{1}tsi2p5				^{1}tsi2p6			
Si	-0.608438	-0.152886	0.011219	Si	-0.498803	-0.105143	-0.135740
H	-1.596702	-0.084148	1.128669	H	-0.9123	1.459065	0.029568
C	0.92394	0.811053	-0.034024	H	-1.361071	-0.725618	0.894458
H	3.052627	-1.35255	0.318956	H	-0.076738	1.265296	0.577012
H	2.951289	-0.832824	-0.203904	C	1.253686	-0.197414	0.114338
H	-1.432716	-0.456399	-1.19665	H	1.811239	0.657735	-0.286706
^{1}tsi2p7				^{1}tsi3p3-v			
Si	-0.601391	-0.194198	0.042412	Si	0.777825	-0.048861	-0.074048
H	-1.44851	0.858815	-0.637636	H	0.968423	1.338732	0.505022
C	1.170429	0.05102	-0.085588	C	-1.045468	-0.194861	0.112303
H	1.676731	0.97615	0.156812	H	-1.499743	0.082637	1.063285

H	1.80842	-0.823683	0.011375	H	-1.620267	-0.94471	-0.420497
H	-0.639741	1.401364	0.389205	H	-2.46516	1.376567	-0.784964
^{1}tsi3p4-v(13,31)				**^{1}tsi3p6**			
Si	-0.713750	-0.280796	-0.000002	Si	-0.759262	-0.052629	-0.000206
H	-1.48568	2.721557	0.000086	H	-0.832419	1.448272	-0.001622
C	1.15028	0.096963	0.000035	C	0.948608	-0.296409	0.000907
H	1.394743	0.711861	0.871924	H	1.983844	1.019451	0.389985
H	1.785509	-0.789205	0.003961	H	1.78316	-0.978522	-0.003665
H	1.396239	0.705159	-0.876149	H	2.003432	1.026054	-0.387257
^{1}tsi3p7				**^{3}tsi1i2**			
Si	-0.695406	-0.138962	0.015445	Si	0.561785	0.011122	0.056565
H	-0.55281	1.505483	0.05559	H	1.174574	1.26418	-0.448046
C	1.104267	-0.07496	0.028859	H	-0.569212	-0.057921	1.160905
H	1.765705	0.735147	0.32219	H	1.235412	-1.216016	-0.417797
H	1.656028	-0.960745	-0.278472	C	-1.247909	-0.073302	-0.198011
H	0.241157	1.115349	-0.488691	H	-2.218312	0.293862	0.101097
^{3}tsi2i3				**^{3}tsi1p1-v(13,31)**			
Si	-0.659710	-0.101511	-0.014482	Si	0.714445	0.005006	-0.008686
H	0.372402	-0.337769	1.177578	H	1.39842	-1.195622	-0.555278
C	1.165675	0.085115	-0.107327	H	0.769721	-0.016722	1.488929
H	1.813849	-0.701298	-0.472198	H	1.36372	1.240245	-0.519243
H	1.653113	0.916545	0.387814	C	-1.19064	-0.021885	-0.046339
H	-1.597473	1.032982	-0.246491	H	-6.390251	0.033318	-0.014772
^{3}tsi1p2-v(31)				**^{3}tsi1p2-v(13)**			
Si	0.464575	-0.111632	0.005859	Si	0.460843	-0.119692	0.005471
H	1.110227	-0.537926	1.263376	H	1.129286	-0.511671	1.261904
H	1.140869	-0.613237	-1.204285	H	1.156757	-0.579132	-1.210041
H	1.133445	2.436365	-0.045215	H	1.104607	2.486413	-0.03979
C	-1.273377	-0.019548	-0.039521	C	-1.265351	-0.01629	-0.036585
H	-2.248334	0.39493	0.141221	H	-2.250342	0.377819	0.130837
				^{3}tsi1p6			
				Si	-0.475775	-0.141333	-0.136107
				H	-1.227542	1.177904	-0.341231
				H	-1.188976	-0.88935	0.922722
				H	-0.943469	1.225044	0.716846
				C	1.296835	0.077549	0.161189
				H	2.23982	-0.000227	-0.359969
^{3}tsi2p2				**^{3}tsi2p3-v(13,31)**			
Si	0.571513	-0.006019	-0.000140	Si	0.575378	-0.146022	-0.131878
H	1.336276	0.259965	-1.232248	H	1.648222	2.175001	0.339145

C	-1.091698	-0.243112	-0.006066	C	-1.207698	0.057023	0.04416
H	-2.099401	-0.603906	-0.008847	H	-1.858466	0.309186	-0.784788
H	-2.025486	1.689934	0.036271	H	-1.647215	0.222958	1.023963
H	1.33762	0.196948	1.243179	H	1.04835	-1.004977	1.003011
^{3}tsi2p5'				**^{3}tsi2p6**			
Si	-0.651383	-0.000061	-0.056897	Si	-0.608392	-0.149037	-0.116901
H	-1.431343	-1.243951	0.097217	H	-1.027742	0.02265	1.323667
C	1.047275	0.000368	0.173302	C	1.237155	-0.083531	0.149162
H	3.261671	-0.00061	-0.321017	H	2.15285	-0.211372	-0.41445
H	2.437329	-0.000311	-0.116166	H	0.402902	1.234396	0.092166
H	-1.431946	1.243511	0.096718	H	-0.433447	1.542025	-0.259732
^{3}tsi2p7				**^{3}tsi3p3-v(31)**			
Si	-0.616330	-0.209368	-0.038429	Si	-0.701140	-0.049926	-0.103154
H	-0.892514	1.158527	0.857135	H	-1.532477	0.799179	0.791601
C	1.210582	0.080125	0.013655	C	1.047989	-0.148275	0.133924
H	1.85905	-0.423152	0.720002	H	1.483578	0.156807	1.078519
H	1.719049	0.558229	-0.817437	H	1.655491	-0.822823	-0.454193
H	-1.320462	1.156796	-0.303625	H	1.921432	1.455445	-0.775312
^{3}tsi3p3-v(13)				**^{3}tsi3p4-v(31)**			
Si	-0.698105	-0.040226	-0.108057	Si	0.688816	-0.212800	0.000003
H	-1.536331	0.746534	0.836682	H	2.148401	1.675853	-0.000001
C	1.03753	-0.168941	0.132631	C	-1.18273	0.132577	0.00001
H	1.47908	0.107066	1.083275	H	-1.503023	0.673507	-0.890913
H	1.653955	-0.791838	-0.500899	H	-1.689159	-0.838375	-0.000496
H	1.951594	1.51505	-0.702048	H	-1.503263	0.672753	0.89130
^{3}tsi3p4-v(13)				**^{3}tsi3p6**			
Si	0.684824	-0.224489	0.000002	Si	-0.774090	-0.027836	-0.079125
H	2.220228	1.731863	-0.000001	H	-0.899309	1.262668	0.70711
C	-1.183336	0.144978	0.000008	C	1.00783	-0.310052	0.154365
H	-1.507676	0.683854	-0.89102	H	1.760989	0.751517	-0.083191
H	-1.692229	-0.826106	-0.00032	H	1.613086	-1.194766	-0.022411
H	-1.507837	0.683375	0.891263	H	2.315518	1.430601	-0.419943
^{3}tsi3p7							
H	1.769131	-0.148566	0.910730				
H	1.769423	-0.149212	-0.910556				
H	0.261428	1.24596	0.000125				
H	-0.631355	1.554055	-0.00044				
C	1.185524	-0.056893	-0.000022				
Si	-0.734412	-0.154348	0.000019				

Reference:

(1) Lu, I.-C.; Chen, W.-K.; Huang, W.-J.; Lee, S.-H. Dynamics of the Reaction C (^{3}P) + SiH_4: Experiments and Calculations. *J. Chem. Phys.* **2008,** *129*, 164304.