Supporting information for

# Competing $Si_2CH_4$-$H_2$ and $SiCH_2$-$SiH_4$ Channels in the Bimolecular Reaction of Ground State Atomic Carbon ($C(^3P_j)$) with Disilane ($Si_2H_6$, $X^1A_{1g}$) under Single Collision Conditions

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**Figure S1.** Time-of-flight (TOF) spectra recorded at m/z = 74, 73, 72 and 71 for the reaction of ground state atomic carbon ($C(^3P_j)$) with disilane ($Si_2H_6$, $X^1A_{1g}$) at center-of-mass (CM) angle of $56.6^0$.

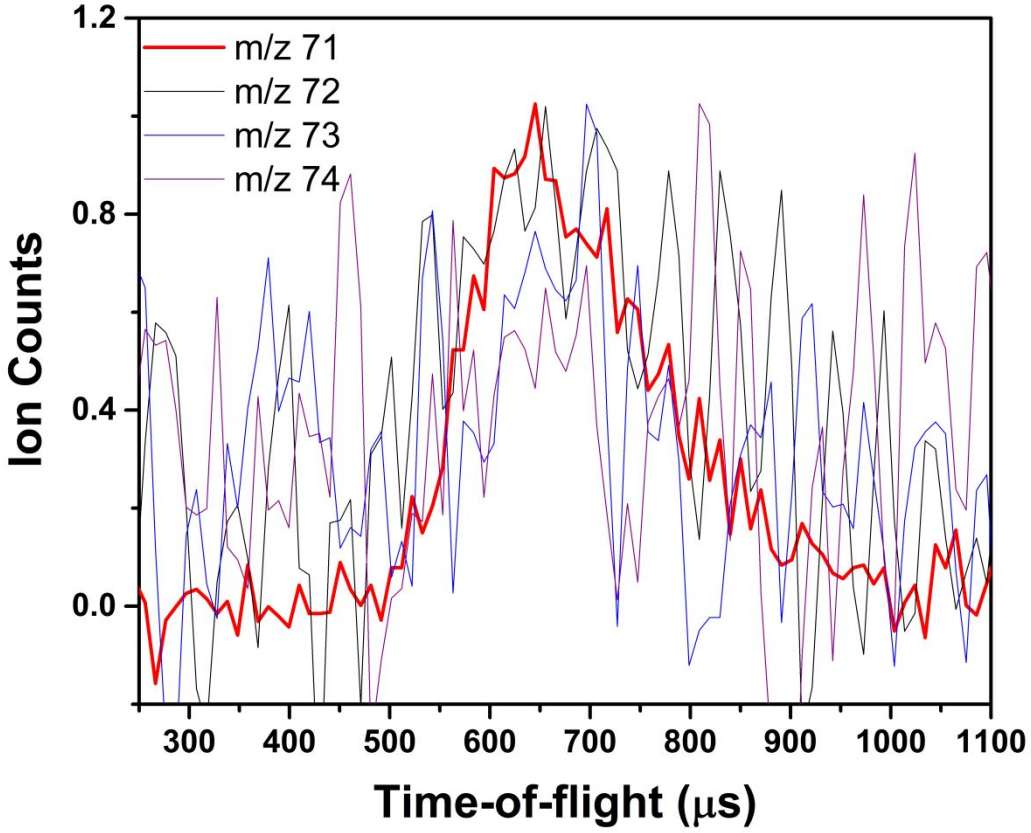


**Figure S2.** TOF spectra recorded at m/z = 71 and 42 for the reaction of ground state atomic carbon ($C(^3P_j)$) with disilane ($Si_2H_6$, $X^1A_{1g}$) at CM angle of $56.6^0$.

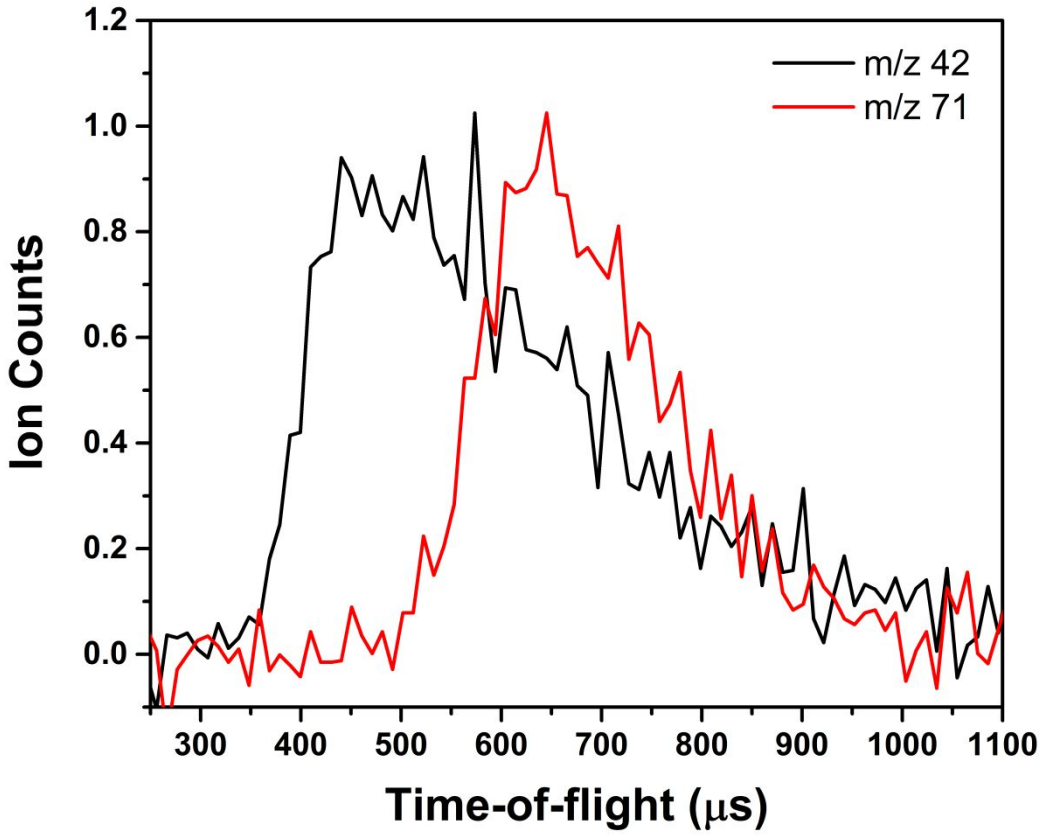
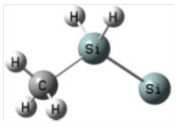
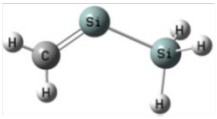


**Figure S3.** B3LYP/cc-pVTZ optimized geometries of doublet $Si_2CH_5$ isomer along with their CCSD(T)/CBS relative energies in kJ $mol^{-1}$ with respect to the separated reactants.

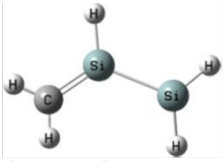


$^2$p1 ($C_1$,$^2$A,-213)

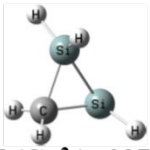
$^2$p2 ($C_1$,$^2$A,-203)



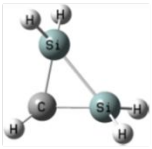
$^2$p3 ($C_s$,$^2$A″,-190)



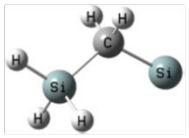
$^2$p4 ($C_1$,$^2$A,-197)



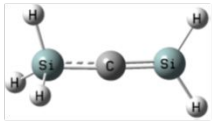
$^2$p5 ($C_1$,$^2$A,-227)



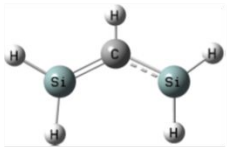
$^2$p6 ($C_s$,$^2$A″,-175)



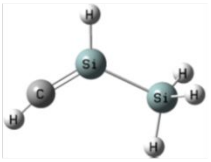
$^2$p7 ($C_s$,$^2$A′,-217)



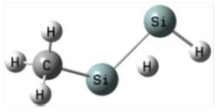
$^2$p8 ($C_s$,$^2$A″,-140)



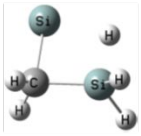
$^2$p9 ($C_1$,$^2$A,-205)



$^2$p10 ($C_s$,$^2$A″,-109)



$^2$p11($C_1$,$^2$A,-197)



$^2$p12 ($C_s$,$^2$A″,-238)

**Table S1.** The H, $H_2$, and $SiH_4$ loss along with dissociative ionization of the primary reaction products from the reaction of ground state atomic carbon ($C(^3P_j)$) with disilane ($Si_2H_6$, $X^1A_{1g}$) considering the natural isotope abundances of silicon [$^{28}Si$ (92.2%), $^{29}Si$ (4.7%), $^{30}Si$ (3.1%)] and carbon [$^{12}C$ (98.9%), $^{13}C$ (1.1%)].

| C + $Si_2H_6$ | | $^{12}C$ (98.9%) | $^{13}C$ (1.1%) | Channel |
|---|---|---|---|---|
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}Si^{28}SiH_5{}^{12}C$ m/z = 73 84.1% | $^{28}Si^{28}SiH_5{}^{13}C$ m/z = 74 0.930% | H loss |
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}Si^{29}SiH_5{}^{12}C/^{29}Si^{28}SiH_5{}^{12}C$ m/z = 74 8.6% | $^{28}Si^{29}SiH_5{}^{13}C/^{29}Si^{28}SiH_5{}^{13}C$ m/z = 75 0.101% | |
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}Si^{30}SiH_5{}^{12}C/^{30}Si^{28}SiH_5{}^{12}C$ m/z = 75 5.6% | $^{28}Si^{30}SiH_5{}^{13}C/^{30}Si^{28}SiH_5{}^{13}C$ m/z = 76 0.063% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}Si^{29}SiH_5{}^{12}C$ m/z = 75 0.2% | $^{29}Si^{29}SiH_5{}^{13}C$ m/z = 76 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}Si^{30}SiH_5{}^{12}C/^{30}Si^{29}SiH_5{}^{12}C$ m/z = 76 0.3% | $^{29}Si^{30}SiH_5{}^{13}C/^{30}Si^{29}SiH_5{}^{13}C$ m/z = 77 0.003% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}Si^{30}SiH_5{}^{12}C$ m/z = 77 0.1% | $^{30}Si^{30}SiH_5{}^{13}C$ m/z = 78 0.001% | |
| | | | | |
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}Si^{28}SiH_4{}^{12}C$ m/z = 72 84.1% | $^{28}Si^{28}SiH_4{}^{13}C$ m/z = 73 0.930% | $H_2$ loss |
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}Si^{29}SiH_4{}^{12}C/^{29}Si^{28}SiH_4{}^{12}C$ m/z = 73 8.6% | $^{28}Si^{29}SiH_4{}^{13}C/^{29}Si^{28}SiH_4{}^{13}C$ m/z = 74 0.101% | |
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}Si^{30}SiH_4{}^{12}C/^{30}Si^{28}SiH_4{}^{12}C$ m/z = 74 5.6% | $^{28}Si^{30}SiH_4{}^{13}C/^{30}Si^{28}SiH_4{}^{13}C$ m/z = 75 0.063% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}Si^{29}SiH_4{}^{12}C$ m/z = 74 0.2% | $^{29}Si^{29}SiH_4{}^{13}C$ m/z = 75 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}Si^{30}SiH_4{}^{12}C/^{30}Si^{29}SiH_4{}^{12}C$ m/z = 75 0.3% | $^{29}Si^{30}SiH_4{}^{13}C/^{30}Si^{29}SiH_4{}^{13}C$ m/z = 76 0.003% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}Si^{30}SiH_4{}^{12}C$ m/z = 76 0.1% | $^{30}Si^{30}SiH_4{}^{13}C$ m/z = 77 0.001% | |
| | | | | |
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}Si^{28}SiH_3{}^{12}C$ m/z = 71 84.1% | $^{28}Si^{28}SiH_3{}^{13}C$ m/z = 72 0.930% | |

| | | | | |
|---|---|---|---|---|
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}Si^{29}SiH_3{}^{12}C/^{29}Si^{28}SiH_3{}^{12}C$ m/z = 72 8.6% | $^{28}Si^{29}SiH_3{}^{13}C/^{29}Si^{28}SiH_3{}^{13}C$ m/z = 73 0.101% | Dissociative ionization |
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}Si^{30}SiH_3{}^{12}C/^{30}Si^{28}SiH_3{}^{12}C$ m/z = 73 5.6% | $^{28}Si^{30}SiH_3{}^{13}C/^{30}Si^{28}SiH_3{}^{13}C$ m/z = 74 0.063% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}Si^{29}SiH_3{}^{12}C$ m/z = 73 0.2% | $^{29}Si^{29}SiH_3{}^{13}C$ m/z = 74 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}Si^{30}SiH_3{}^{12}C/^{30}Si^{29}SiH_3{}^{12}C$ m/z = 74 0.3% | $^{29}Si^{30}SiH_3{}^{13}C/^{30}Si^{29}SiH_3{}^{13}C$ m/z = 75 0.003% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}Si^{30}SiH_3{}^{12}C$ m/z = 75 0.1% | $^{30}Si^{30}SiH_3{}^{13}C$ m/z = 76 0.001% | |
| | | | | |
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}Si^{28}SiH_2{}^{12}C$ m/z = 70 84.1% | $^{28}Si^{28}SiH_2{}^{13}C$ m/z = 71 0.930% | Dissociative ionization |
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}Si^{29}SiH_2{}^{12}C/^{29}Si^{28}SiH_2{}^{12}C$ m/z = 71 8.6% | $^{28}Si^{29}SiH_2{}^{13}C/^{29}Si^{28}SiH_2{}^{13}C$ m/z = 72 0.101% | |
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}Si^{30}SiH_2{}^{12}C/^{30}Si^{28}SiH_2{}^{12}C$ m/z = 72 5.6% | $^{28}Si^{30}SiH_2{}^{13}C/^{30}Si^{28}SiH_2{}^{13}C$ m/z = 73 0.063% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}Si^{29}SiH_2{}^{12}C$ m/z = 72 0.2% | $^{29}Si^{29}SiH_2{}^{13}C$ m/z = 73 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}Si^{30}SiH_2{}^{12}C/^{30}Si^{29}SiH_2{}^{12}C$ m/z = 73 0.3% | $^{29}Si^{30}SiH_2{}^{13}C/^{30}Si^{29}SiH_2{}^{13}C$ m/z = 74 0.003% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}Si^{30}SiH_2{}^{12}C$ m/z = 74 0.1% | $^{30}Si^{30}SiH_2{}^{13}C$ m/z = 75 0.001% | |
| | | | | |
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}Si^{28}SiH^{12}C$ m/z = 69 84.1% | $^{28}Si^{28}SiH^{13}C$ m/z = 70 0.930% | Dissociative ionization |
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}Si^{29}SiH^{12}C/^{29}Si^{28}SiH^{12}C$ m/z = 70 8.6% | $^{28}Si^{29}SiH^{13}C/^{29}Si^{28}SiH^{13}C$ m/z = 71 0.101% | |
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}Si^{30}SiH^{12}C/^{30}Si^{28}SiH^{12}C$ m/z = 71 5.6% | $^{28}Si^{30}SiH^{13}C/^{30}Si^{28}SiH^{13}C$ m/z = 72 0.063% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}Si^{29}SiH^{12}C$ m/z = 71 0.2% | $^{29}Si^{29}SiH^{13}C$ m/z = 72 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}Si^{30}SiH^{12}C/^{30}Si^{29}SiH^{12}C$ m/z = 72 | $^{29}Si^{30}SiH^{13}C/^{30}Si^{29}SiH^{13}C$ m/z = 73 | |

| | | | | |
|---|---|---|---|---|
| | | 0.3% | 0.003% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}Si^{30}SiH^{12}C$ m/z = 73 0.1% | $^{30}Si^{30}SiH^{13}C$ m/z = 74 0.001% | |
| | | | | |
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}SiH_2{}^{12}C$ m/z = 42 84.1% | $^{28}SiH_2{}^{13}C$ m/z = 43 0.93% | $SiH_4$ loss |
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}SiH_2{}^{12}C/^{29}SiH_2{}^{12}C$ m/z = 42/43 8.18%/0.42% | $^{28}SiH_2{}^{13}C/^{29}SiH_2{}^{13}C$ m/z = 43/44 0.1%/0.001% | |
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}SiH_2{}^{12}C/^{30}SiH_2{}^{12}C$ m/z = 42/44 5.42%/ 0.18% | $^{28}SiH_2{}^{13}C/^{30}SiH_2{}^{13}C$ m/z = 43/45 0.06%/0.003% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}SiH_2{}^{12}C$ m/z = 43 0.2% | $^{29}SiH_2{}^{13}C$ m/z = 44 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}SiH_2{}^{12}C/^{30}SiH_2{}^{12}C$ m/z = 43/44 0.18%/0.12% | $^{29}SiH_2{}^{13}C/^{30}SiH_2{}^{13}C$ m/z = 44/45 0.002%/0.001% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}SiH_2{}^{12}C$ m/z = 44 0.1% | $^{30}SiH_2{}^{13}C$ m/z = 45 0.001% | |
| | | | | |
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}SiH^{12}C$ m/z = 41 84.1% | $^{28}SiH^{13}C$ m/z = 42 0.93% | Dissociative ionization |
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}SiH^{12}C/^{29}SiH^{12}C$ m/z = 41/42 8.18%/0.42% | $^{28}SiH^{13}C/^{29}SiH^{13}C$ m/z = 42/43 0.1%/0.001% | |
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}SiH^{12}C/^{30}SiH^{12}C$ m/z = 41/43 5.42%/ 0.18% | $^{28}SiH^{13}C/^{30}SiH^{13}C$ m/z = 42/44 0.06%/0.003% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}SiH^{12}C$ m/z = 42 0.2% | $^{29}SiH^{13}C$ m/z = 43 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}SiH^{12}C/^{30}SiH^{12}C$ m/z = 42/43 0.18%/0.12% | $^{29}SiH^{13}C/^{30}SiH^{13}C$ m/z = 43/44 0.002%/0.001% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}SiH^{12}C$ m/z = 43 0.1% | $^{30}SiH^{13}C$ m/z = 44 0.001% | |
| | | | | |
| $Si_2H_6$ | $^{28}Si^{28}SiH_6$ (85.0%) | $^{28}Si^{12}C$ m/z = 40 84.1% | $^{28}Si^{13}C$ m/z = 41 0.93% | Dissociative ionization |
| | $^{28}Si^{29}SiH_6/^{29}Si^{28}SiH_6$ (8.7%) | $^{28}Si^{12}C/^{29}Si^{12}C$ m/z = 40/41 8.18%/0.42% | $^{28}Si^{13}C/^{29}Si^{13}C$ m/z = 41/42 0.1%/0.001% | |

| | | | | |
|---|---|---|---|---|
| | $^{28}Si^{30}SiH_6/^{30}Si^{28}SiH_6$ (5.7%) | $^{28}Si^{12}C/^{30}Si^{12}C$ m/z = 40/42 5.42%/ 0.18% | $^{28}Si^{13}C/^{30}Si^{13}C$ m/z = 41/43 0.06%/0.003% | |
| | $^{29}Si^{29}SiH_6$ (0.2%) | $^{29}Si^{12}C$ m/z = 41 0.2% | $^{29}Si^{13}C$ m/z = 42 0.002% | |
| | $^{29}Si^{30}SiH_6/^{30}Si^{29}SiH_6$ (0.3%) | $^{29}Si^{12}C/^{30}Si^{12}C$ m/z = 41/42 0.18%/0.12% | $^{29}Si^{13}C/^{30}Si^{13}C$ m/z = 42/43 0.002%/0.001% | |
| | $^{30}Si^{30}SiH_6$ (0.1%) | $^{30}Si^{12}C$ m/z = 42 0.1% | $^{30}Si^{13}C$ m/z = 43 0.001% | |

**Table S2. (a)** B3LYP/cc-pVTZ optimized cartesian coordinates of singlet and triplet $Si_2CH_4$ isomers.

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| **$^1$p1** | | | | **$^1$p2** | | | |
| Si | 1.534991 | 0.930511 | 0.000000 | Si | 0.000000 | 0.000000 | 1.680847 |
| H | 1.949883 | 2.352807 | 0.000000 | H | 0.000000 | 1.229066 | 2.502540 |
| C | 0.000000 | 0.325760 | 0.000000 | H | 0.000000 | -1.229066 | 2.502540 |
| Si | -1.308759 | -0.961070 | 0.000000 | H | 1.229066 | 0.000000 | -2.502540 |
| H | -1.257839 | -1.827031 | 1.205796 | H | -1.229066 | 0.000000 | -2.502540 |
| H | -2.601454 | -0.225476 | 0.000000 | C | 0.000000 | 0.000000 | 0.000000 |
| H | -1.257839 | -1.827031 | -1.205796 | Si | 0.000000 | 0.000000 | -1.680847 |
| **$^1$p3** | | | | **$^1$p4** | | | |
| Si | 0.517363 | -1.032161 | 0.000000 | Si | -1.576711 | 0.224372 | 0.000000 |
| C | -1.076425 | -0.391892 | 0.000000 | C | 0.000000 | 0.876212 | 0.000000 |
| H | -2.135577 | -0.600011 | 0.000000 | Si | 1.220518 | -0.528316 | 0.000000 |
| Si | 0.000000 | 1.128841 | 0.000000 | H | 2.091011 | -0.548658 | 1.204853 |
| H | 0.119191 | 1.996274 | 1.202317 | H | 0.423323 | -1.794898 | 0.000000 |
| H | 0.119191 | 1.996274 | -1.202317 | H | 2.091011 | -0.548658 | -1.204853 |
| H | 1.112659 | -2.394703 | 0.000000 | H | 0.381356 | 1.890154 | 0.000000 |
| **$^1$p5** | | | | **$^1$p6** | | | |
| Si | 0.000000 | 0.681883 | 0.000000 | Si | 0.077910 | -0.195887 | 1.651776 |
| C | 1.359105 | 1.716907 | 0.000000 | Si | 0.077910 | -0.195887 | -1.651776 |
| Si | -0.627539 | -1.470507 | 0.000000 | H | -1.272018 | -0.875677 | -1.417784 |
| H | -1.500920 | -1.696502 | 1.191798 | H | -1.272018 | -0.875677 | 1.417784 |
| H | -1.500920 | -1.696502 | -1.191798 | C | 0.077910 | 0.754942 | 0.000000 |
| H | 1.258976 | 2.794244 | 0.000000 | H | -0.942510 | 1.172052 | 0.000000 |
| H | 2.373786 | 1.338050 | 0.000000 | H | 0.837618 | 1.534483 | 0.000000 |
| **$^1$p7** | | | | **$^1$p8** | | | |
| Si | 0.000000 | 0.380959 | 0.000000 | Si | -0.712913 | -1.126374 | 0.000000 |
| Si | -0.896035 | -1.535435 | 0.000000 | C | 1.094677 | -0.405578 | 0.000000 |
| H | 0.762094 | -1.088552 | 0.000000 | H | 1.679513 | -0.645482 | 0.887727 |
| C | 1.231961 | 1.818861 | 0.000000 | H | 1.679513 | -0.645482 | -0.887727 |
| H | 1.860046 | 1.792037 | 0.889594 | Si | 0.000000 | 1.116374 | 0.000000 |
| H | 1.860046 | 1.792037 | -0.889594 | H | 0.026848 | 1.932221 | -1.235850 |
| H | 0.670538 | 2.753983 | 0.000000 | H | 0.026848 | 1.932221 | 1.235850 |
| **$^1$p9** | | | | **$^1$p10** | | | |
| Si | 0.000000 | 0.583211 | 0.000000 | Si | 1.002196 | -1.333601 | 0.000000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Si | 1.239972 | -1.243201 | 0.000000 | H | 2.477186 | -1.051076 | 0.000000 |
| H | 0.712095 | 1.894339 | 0.000000 | Si | 0.000000 | 0.531943 | 0.000000 |
| C | -1.881250 | 0.799961 | 0.000000 | C | -1.716729 | 1.319247 | 0.000000 |
| H | -2.198978 | 1.355285 | 0.883333 | H | -1.880069 | 1.926325 | 0.889517 |
| H | -2.198978 | 1.355285 | -0.883333 | H | -1.880069 | 1.926325 | -0.889517 |
| H | -2.386246 | -0.164813 | 0.000000 | H | -2.447411 | 0.506165 | 0.000000 |
| **$^3$p1** | | | | **$^3$p2** | | | |
| Si | -0.867409 | 0.431289 | 0.091941 | Si | -0.897449 | -0.713471 | 0.012938 |
| C | -2.036570 | -0.871002 | -0.072349 | C | -1.733923 | 0.852800 | -0.059081 |
| Si | 1.420276 | -0.131070 | -0.016445 | H | -1.990986 | 1.866054 | 0.215229 |
| H | 1.618019 | -1.454100 | 0.618252 | Si | 1.382543 | 0.142346 | 0.000072 |
| H | 1.898762 | -0.159459 | -1.420905 | H | 2.382132 | -0.887610 | 0.396011 |
| H | 2.185290 | 0.903716 | 0.726774 | H | 1.723895 | 0.604132 | -1.372731 |
| H | -1.222789 | 1.732788 | -0.546972 | H | 1.497190 | 1.296369 | 0.933827 |
| **$^3$p3** | | | | **$^3$p4** | | | |
| Si | -1.724764 | 0.818891 | 0.000000 | C | 0.000000 | 0.000000 | 1.214579 |
| H | -1.519983 | 2.334621 | 0.000000 | Si | 0.000000 | 1.185440 | -0.186977 |
| C | 0.000000 | 0.288795 | 0.000000 | H | 1.223973 | 1.957999 | -0.513029 |
| Si | 1.436133 | -0.860773 | 0.000000 | H | -1.223973 | 1.957999 | -0.513029 |
| H | 2.256733 | -0.592052 | 1.210142 | Si | 0.000000 | -1.185440 | -0.186977 |
| H | 1.047348 | -2.296940 | 0.000000 | H | 1.223973 | -1.957999 | -0.513029 |
| H | 2.256733 | -0.592052 | -1.210142 | H | -1.223973 | -1.957999 | -0.513029 |
| **$^3$p5** | | | | **$^3$p6** | | | |
| Si | 1.674555 | 0.425495 | 0.000000 | Si | 1.239106 | -0.257227 | -0.162574 |
| H | 2.450276 | 0.576083 | 1.246212 | C | 0.111436 | 1.108319 | 0.267483 |
| H | 2.450276 | 0.576083 | -1.246212 | H | 0.008487 | 2.091356 | -0.177479 |
| H | -2.435982 | -0.163625 | -1.230119 | Si | -1.140684 | -0.220310 | -0.017648 |
| H | -2.435982 | -0.163625 | 1.230119 | H | -2.152326 | -0.093323 | -1.093619 |
| C | 0.000000 | 0.068682 | 0.000000 | H | -1.670918 | -1.004426 | 1.123518 |
| Si | -1.676597 | -0.513853 | 0.000000 | H | 1.768240 | -0.958000 | 1.065792 |
| **$^3$p7** | | | | **$^3$p8** | | | |
| Si | -1.844650 | 0.287382 | 0.000000 | Si | 0.651869 | -0.663563 | 0.070801 |
| C | 0.000000 | 0.683980 | 0.000000 | C | 1.877779 | 0.613883 | -0.062788 |
| Si | 1.429821 | -0.524662 | 0.000000 | H | -1.711898 | 1.505539 | 0.585742 |
| H | 2.277941 | -0.295345 | 1.202496 | H | -2.574836 | -0.742696 | 0.248586 |
| H | 0.943378 | -1.923654 | 0.000000 | H | 2.887954 | 0.432677 | -0.412594 |
| H | 2.277941 | -0.295345 | -1.202496 | H | 1.744606 | 1.577551 | 0.421779 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.308345 | 1.732390 | 0.000000 | Si | -1.481334 | 0.202394 | -0.104143 |
| **$^3$p9** | | | | **$^3$p10** | | | |
| Si | 0.065572 | -0.344806 | 1.156638 | Si | 0.439148 | -0.704470 | 0.028684 |
| Si | 0.065572 | -0.344806 | -1.156638 | Si | -1.662070 | 0.283683 | 0.046999 |
| H | -1.275339 | -0.537352 | -1.805312 | H | -0.527250 | -0.006580 | -1.207580 |
| H | -1.275339 | -0.537352 | 1.805312 | C | 1.862365 | 0.573641 | 0.015326 |
| C | 0.065572 | 1.189719 | 0.000000 | H | 2.479760 | 0.454223 | -0.878150 |
| H | -0.727939 | 1.930750 | 0.000000 | H | 1.492579 | 1.600144 | 0.049626 |
| H | 1.049182 | 1.660209 | 0.000000 | H | 2.501564 | 0.401340 | 0.884582 |
| **$^3$p11** | | | | **$^3$p12** | | | |
| Si | 0.000000 | 0.772640 | 0.000000 | Si | -0.693549 | -1.161898 | 0.000000 |
| Si | -1.308736 | -1.169168 | 0.000000 | C | 1.079832 | -0.429272 | 0.000000 |
| C | 1.902570 | 0.820232 | 0.000000 | H | 1.693947 | -0.497797 | 0.898791 |
| H | 2.269745 | 1.353022 | 0.880279 | H | 1.693947 | -0.497797 | -0.898791 |
| H | 2.313993 | -0.190591 | 0.000000 | Si | 0.000000 | 1.136304 | 0.000000 |
| H | 2.269745 | 1.353022 | -0.880279 | H | -0.078598 | 1.964770 | -1.224385 |
| H | 0.053398 | -1.885452 | 0.000000 | H | -0.078598 | 1.964770 | 1.224385 |
| **$^3$p13** | | | | | | | |
| Si | 0.000000 | 0.618884 | 0.000000 | | | | |
| Si | 1.248430 | -1.300932 | 0.000000 | | | | |
| H | 0.567630 | 2.005586 | 0.000000 | | | | |
| C | -1.878092 | 0.818821 | 0.000000 | | | | |
| H | -2.195289 | 1.386823 | 0.878137 | | | | |
| H | -2.195289 | 1.386823 | -0.878137 | | | | |
| H | -2.386521 | -0.143481 | 0.000000 | | | | |

**(b)** B3LYP/cc-pVTZ vibrational frequencies and infrared intensities of singlet and triplet $Si_2CH_4$ isomers.

| | $^1$p1 | | $^1$p2 | |
|---|---|---|---|---|
| Normal modes | Frequency($cm^{-1}$) | IR Inten | Frequency($cm^{-1}$) | IR Inten |
| ν1 | 73.65 | 1.8294 | 140.1 | 15.7471 |
| ν2 | 172.32 | 24.0411 | 140.1 | 15.7471 |
| ν3 | 232.56 | 10.8348 | 444.58 | 0 |
| ν4 | 368.36 | 83.6906 | 523.41 | 22.0125 |
| ν5 | 508.34 | 20.1381 | 523.41 | 22.0125 |
| ν6 | 650.83 | 48.3781 | 584.94 | 0 |
| ν7 | 657.42 | 53.6328 | 656.37 | 41.83 |
| ν8 | 925.01 | 331.1129 | 656.37 | 41.83 |
| ν9 | 931.95 | 41.3921 | 963.53 | 0 |
| ν10 | 959.13 | 106.0316 | 967.86 | 247.3809 |
| ν11 | 1283.6 | 14.159 | 1424.12 | 162.6039 |
| ν12 | 2203.33 | 80.2495 | 2240.01 | 173.2868 |
| ν13 | 2209.34 | 109.4522 | 2242.69 | 0 |
| ν14 | 2210.56 | 116.8111 | 2252.07 | 89.9269 |
| ν15 | 2222.69 | 18.7685 | 2252.07 | 89.9269 |
| | $^1$p3 | | $^1$p4 | |
| ν1 | 276.41 | 2.4676 | 81.49 | 3.6098 |
| ν2 | 423.37 | 25.5455 | 235.48 | 1.1566 |
| ν3 | 503.18 | 0.5794 | 535.9 | 6.8137 |
| ν4 | 561.06 | 13.0584 | 536.55 | 21.0076 |
| ν5 | 617.55 | 10.1202 | 684.68 | 97.754 |
| ν6 | 684.88 | 34.4461 | 694.03 | 46.9171 |
| ν7 | 742.93 | 97.9443 | 854.54 | 10.0671 |

| | | | | |
|---|---|---|---|---|
| ν8 | 744.21 | 33.2892 | 930.81 | 25.7654 |
| ν9 | 899.97 | 66.0753 | 942.79 | 207.8957 |
| ν10 | 980.02 | 88.6033 | 967.86 | 157.1935 |
| ν11 | 1041.5 | 93.9686 | 1071.01 | 82.6042 |
| ν12 | 2185.94 | 184.1324 | 2153.35 | 70.9404 |
| ν13 | 2188.96 | 69.3302 | 2200.56 | 123.065 |
| ν14 | 2190.02 | 134.3145 | 2202.98 | 123.2979 |
| ν15 | 3204.36 | 3.2536 | 3174.01 | 1.3631 |
| | $^{1}$p5 | | $^{1}$p6 | |
| ν1 | 98.15 | 1.2905 | 94.75 | 31.9358 |
| ν2 | 128.08 | 4.9445 | 191.2 | 1.3137 |
| ν3 | 396.33 | 3.3854 | 280.64 | 0.5298 |
| ν4 | 474.27 | 22.4828 | 552.77 | 6.8235 |
| ν5 | 482.13 | 0.5534 | 634.08 | 132.3552 |
| ν6 | 493.36 | 0.4757 | 653.68 | 8.6839 |
| ν7 | 660.13 | 1.4837 | 716.2 | 172.1222 |
| ν8 | 712.18 | 66.978 | 743.8 | 3.2571 |
| ν9 | 951.19 | 137.8922 | 892.74 | 36.7363 |
| ν10 | 987.17 | 11.2888 | 1083.01 | 54.4151 |
| ν11 | 1368.16 | 4.4903 | 1347.09 | 7.7855 |
| ν12 | 2154.14 | 99.0141 | 1993.34 | 0.0808 |
| ν13 | 2173.71 | 94.2564 | 2009.85 | 451.8197 |
| ν14 | 3131.59 | 0.5387 | 2964.99 | 0.6583 |
| ν15 | 3220.37 | 0.5899 | 3103.15 | 2.8161 |
| | $^{1}$p7 | | $^{1}$p8 | |
| ν1 | 67.7 | 1.9022 | 81.27 | 5.8144 |
| ν2 | 131.34 | 7.3356 | 345.91 | 0.0849 |

| | | | | |
|---|---|---|---|---|
| ν3 | 165.37 | 0.9255 | 402.55 | 23.0548 |
| ν4 | 485.72 | 20.8879 | 473.93 | 10.0132 |
| ν5 | 741.33 | 4.2431 | 491.49 | 3.1813 |
| ν6 | 762.47 | 0.3182 | 608.81 | 62.6271 |
| ν7 | 776.9 | 3.2492 | 741.22 | 37.9121 |
| ν8 | 1037.74 | 166.5633 | 824 | 36.8951 |
| ν9 | 1268.48 | 0.0881 | 854.91 | 18.5762 |
| ν10 | 1449.15 | 9.6508 | 913.15 | 87.9343 |
| ν11 | 1452.75 | 12.2821 | 1335.33 | 6.5512 |
| ν12 | 1607.73 | 71.1543 | 2215.24 | 73.8412 |
| ν13 | 3034.63 | 2.362 | 2238.19 | 89.6962 |
| ν14 | 3112.13 | 1.636 | 3056.91 | 0.3843 |
| ν15 | 3120.09 | 0.3763 | 3112.39 | 0.5018 |
| | $^{1}$p9 | | $^{1}$p10 | |
| ν1 | 107.45 | 4.2062 | 69.83 | 1.7378 |
| ν2 | 123.59 | 0.376 | 96.36 | 11.1624 |
| ν3 | 309.21 | 0.7344 | 155.87 | 18.0595 |
| ν4 | 476.24 | 23.5844 | 419.75 | 10.5859 |
| ν5 | 603.02 | 11.648 | 483.44 | 4.2763 |
| ν6 | 705.57 | 23.7343 | 715.16 | 31.1314 |
| ν7 | 764.06 | 0.5656 | 753.95 | 8.5853 |
| ν8 | 896.34 | 69.3431 | 787.54 | 0.0506 |
| ν9 | 1280.69 | 1.7867 | 1263.96 | 4.5083 |
| ν10 | 1456.85 | 5.9352 | 1432.76 | 15.4416 |
| ν11 | 1459.79 | 5.6544 | 1454.93 | 10.9252 |
| ν12 | 2169.8 | 85.3546 | 2123.6 | 79.4649 |
| ν13 | 3031.38 | 5.0548 | 3025.15 | 0.1532 |

| | | | | |
|---|---|---|---|---|
| ν14 | 3099.09 | 2.913 | 3098.77 | 5.2547 |
| ν15 | 3116.45 | 3.4199 | 3117.07 | 0.1617 |
| | $^3$p1 | | $^3$p2 | |
| ν1 | 80.94 | 1.3934 | 63.44 | 9.5383 |
| ν2 | 146.97 | 13.2563 | 123.22 | 0.766 |
| ν3 | 353.1 | 9.0596 | 158.64 | 71.1425 |
| ν4 | 400.22 | 7.8358 | 343.15 | 1.6492 |
| ν5 | 507.46 | 30.3601 | 375.23 | 23.576 |
| ν6 | 519.63 | 1.5893 | 453.66 | 54.9842 |
| ν7 | 643.62 | 76.5237 | 519.36 | 39.2432 |
| ν8 | 822.78 | 174.6344 | 784.78 | 7.9021 |
| ν9 | 874.39 | 222.9669 | 858.36 | 281.8871 |
| ν10 | 938.07 | 36.244 | 931.58 | 55.2669 |
| ν11 | 944.74 | 40.493 | 948.77 | 37.3168 |
| ν12 | 2157.38 | 89.9956 | 2180.92 | 74.9459 |
| ν13 | 2208.88 | 58.8674 | 2197.33 | 104.7056 |
| ν14 | 2221.79 | 68.2712 | 2199.99 | 94.5151 |
| ν15 | 2245.75 | 65.93 | 3215.64 | 0.4692 |
| | $^3$p3 | | $^3$p4 | |
| ν1 | 36.63 | 0.0001 | 370.85 | 0.8727 |
| ν2 | 113.35 | 2.7331 | 371.78 | 10.2551 |
| ν3 | 154.14 | 0.1236 | 462.43 | 0 |
| ν4 | 432.98 | 2.9267 | 507.8 | 75.6665 |
| ν5 | 594.39 | 15.3269 | 508.73 | 0 |
| ν6 | 596.06 | 29.4879 | 614.58 | 38.4057 |
| ν7 | 685.53 | 47.1629 | 639.01 | 3.8438 |
| ν8 | 912.45 | 203.9099 | 738.81 | 15.701 |

| | | | | |
|---|---|---|---|---|
| ν9 | 935.46 | 186.2827 | 783.67 | 8.842 |
| ν10 | 945.03 | 39.6527 | 934.36 | 192.1218 |
| ν11 | 1040.14 | 51.4228 | 945.16 | 36.3854 |
| ν12 | 1964.63 | 217.8021 | 2203.03 | 129.2354 |
| ν13 | 2193.34 | 106.7842 | 2206.83 | 13.9027 |
| ν14 | 2204.17 | 71.0246 | 2217.78 | 0 |
| ν15 | 2204.31 | 87.5297 | 2223.78 | 167.4169 |
| | $^3$p5 | | $^3$p6 | |
| ν1 | 122.29 | 2.7311 | 320.35 | 1.9918 |
| ν2 | 165.96 | 9.4373 | 387.47 | 4.5283 |
| ν3 | 302.77 | 14.7806 | 417.77 | 9.7442 |
| ν4 | 388.02 | 1.0029 | 449.4 | 49.6401 |
| ν5 | 493.4 | 54.4771 | 523.25 | 4.7335 |
| ν6 | 519.26 | 32.0781 | 571.08 | 17.5485 |
| ν7 | 570.39 | 4.5515 | 653.1 | 42.7477 |
| ν8 | 635.14 | 72.8765 | 691.93 | 26.4918 |
| ν9 | 910.6 | 164.145 | 774.62 | 9.1511 |
| ν10 | 940.87 | 13.3187 | 894.14 | 35.6155 |
| ν11 | 1153.36 | 6.1834 | 947.59 | 92.6247 |
| ν12 | 2173.09 | 116.5515 | 2044.62 | 126.1127 |
| ν13 | 2198.86 | 102.4811 | 2210.39 | 77.3316 |
| ν14 | 2252.16 | 25.8281 | 2229.39 | 93.743 |
| ν15 | 2270.84 | 66.8773 | 3159.97 | 0.8114 |
| | $^3$p7 | | $^3$p8 | |
| ν1 | 45.23 | 1.0114 | 125.03 | 1.455 |
| ν2 | 179.66 | 0.8578 | 217.83 | 6.0015 |
| ν3 | 466.07 | 0.0947 | 344.84 | 6.1995 |

| | | | | |
|---|---|---|---|---|
| ν4 | 513.12 | 10.0153 | 389.49 | 4.7235 |
| ν5 | 565.01 | 17.6856 | 479.45 | 3.4419 |
| ν6 | 683.27 | 31.7779 | 500.04 | 25.4351 |
| ν7 | 816.02 | 107.5908 | 676.75 | 16.8105 |
| ν8 | 916.85 | 196.3779 | 717.61 | 43.2271 |
| ν9 | 938.72 | 65.5162 | 775.86 | 8.6192 |
| ν10 | 947.6 | 44.6359 | 921.75 | 140.3821 |
| ν11 | 1049.9 | 18.5475 | 1385.23 | 4.6365 |
| ν12 | 2189.06 | 92.9173 | 2159.76 | 96.8715 |
| ν13 | 2189.59 | 84.5235 | 2203.35 | 97.2734 |
| ν14 | 2241.18 | 72.1934 | 3098.86 | 3.604 |
| ν15 | 3055.06 | 6.9827 | 3187.25 | 0.6824 |
| | $^3$p9 | | $^3$p10 | |
| ν1 | 362.08 | 3.3575 | 114.54 | 0.023 |
| ν2 | 389.14 | 0.0764 | 158.45 | 1.1507 |
| ν3 | 404.05 | 7.2681 | 380.96 | 1.5914 |
| ν4 | 487.18 | 23.3081 | 431.51 | 5.5569 |
| ν5 | 558.79 | 2.7413 | 632.65 | 56.687 |
| ν6 | 594.38 | 27.7493 | 686.6 | 3.252 |
| ν7 | 693.65 | 11.9549 | 725.54 | 4.5081 |
| ν8 | 820.12 | 70.8269 | 988.92 | 235.5059 |
| ν9 | 841.03 | 31.9113 | 1255.88 | 13.0873 |
| ν10 | 874.21 | 41.0379 | 1419.2 | 87.6694 |
| ν11 | 1385.37 | 5.2101 | 1440.9 | 3.8933 |
| ν12 | 2099.71 | 144.0428 | 1445.39 | 8.2867 |
| ν13 | 2110.56 | 139.9358 | 3008.83 | 5.495 |
| ν14 | 3059.23 | 2.3187 | 3083.02 | 5.324 |

| | | | | |
|---|---|---|---|---|
| ν15 | 3143.61 | 3.7261 | 3091.22 | 5.8833 |
| | $^3$p11 | | $^3$p12 | |
| ν1 | 46.1 | 0.0321 | 145.73 | 34.2885 |
| ν2 | 146.35 | 1.7127 | 370.23 | 0.0442 |
| ν3 | 158.37 | 1.2794 | 407.7 | 6.7439 |
| ν4 | 379.65 | 3.5537 | 499.49 | 8.7367 |
| ν5 | 532.13 | 38.7137 | 601.58 | 41.5813 |
| ν6 | 660.69 | 32.2663 | 636.54 | 1.7494 |
| ν7 | 683.11 | 1.796 | 703.75 | 40.1631 |
| ν8 | 752.82 | 9.332 | 878.22 | 33.5136 |
| ν9 | 1253.79 | 8.032 | 878.36 | 12.0312 |
| ν10 | 1438.05 | 7.0047 | 946.65 | 126.2253 |
| ν11 | 1442.77 | 12.9347 | 1380 | 6.297 |
| ν12 | 1956.01 | 181.8422 | 2221.53 | 89.63 |
| ν13 | 3010.13 | 3.5111 | 2243.89 | 79.7243 |
| ν14 | 3081.48 | 3.4352 | 3032.66 | 10.8974 |
| ν15 | 3095.38 | 1.8863 | 3094.71 | 1.2942 |
| | $^3$p13 | | | |
| ν1 | 98.68 | 0.0006 | | |
| ν2 | 158.07 | 1.6538 | | |
| ν3 | 303.32 | 4.114 | | |
| ν4 | 429.36 | 9.2134 | | |
| ν5 | 641.57 | 2.543 | | |
| ν6 | 690.16 | 3.1161 | | |
| ν7 | 702.82 | 59.8352 | | |
| ν8 | 916.31 | 117.8766 | | |
| ν9 | 1274.11 | 7.1142 | | |

| | | |
|---|---|---|
| v10 | 1447.11 | 6.5976 |
| v11 | 1451.99 | 5.5667 |
| v12 | 2134.91 | 157.0068 |
| v13 | 3017.16 | 2.0586 |
| v14 | 3076.48 | 3.6013 |
| v15 | 3120.37 | 2.9987 |

**Table S3. (a)** B3LYP/cc-pVTZ optimized cartesian coordinates of doublet $Si_2CH_5$ isomers.

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| **$^2$p1** | | | | **$^2$p2** | | | |
| Si | 0.436645 | 0.566160 | -0.006527 | Si | -0.569962 | -0.795469 | -0.051313 |
| H | 0.678457 | 1.594397 | -1.061982 | C | -1.816375 | 0.664651 | 0.034552 |
| H | 0.406280 | 1.303815 | 1.301472 | H | -1.470303 | 1.558545 | -0.487728 |
| Si | -1.791553 | -0.298954 | -0.010050 | H | -2.773850 | 0.358670 | -0.388947 |
| C | 1.888217 | -0.654679 | -0.000550 | H | -1.992079 | 0.940298 | 1.077905 |
| H | 2.834566 | -0.127519 | 0.129874 | Si | 1.473097 | 0.241202 | 0.066264 |
| H | 1.783932 | -1.379061 | 0.807339 | H | 1.781103 | 1.503693 | -0.674152 |
| H | 1.936171 | -1.204450 | -0.941327 | H | 2.709487 | -0.589386 | 0.056298 |
| **$^2$p3** | | | | **$^2$p4** | | | |
| C | 1.687147 | 1.261284 | 0.000000 | C | 1.960773 | -0.593781 | -0.023311 |
| H | 2.416791 | 0.457597 | 0.000000 | Si | -1.543562 | -0.186985 | -0.085098 |
| H | 2.101711 | 2.260799 | 0.000000 | H | -1.810430 | -1.562871 | 0.401367 |
| Si | 0.000000 | 0.930637 | 0.000000 | H | -2.557152 | 0.779211 | 0.405218 |
| Si | -0.829843 | -1.289822 | 0.000000 | Si | 0.608505 | 0.495122 | 0.048328 |
| H | -1.665751 | -1.505602 | 1.206568 | H | 0.867562 | 1.941841 | -0.137900 |
| H | -1.665751 | -1.505602 | -1.206568 | H | 2.983816 | -0.242536 | -0.059614 |
| H | 0.307927 | -2.246306 | 0.000000 | H | 1.842363 | -1.666871 | 0.045571 |
| **$^2$p5** | | | | **$^2$p6** | | | |
| Si | 1.170098 | -0.379022 | 0.131717 | C | -0.005337 | 1.180163 | 0.000000 |
| C | 0.123116 | 1.204444 | -0.046330 | Si | -0.005337 | -0.249718 | 1.158558 |
| H | -0.004662 | 1.809861 | 0.849102 | H | -1.297247 | -0.668317 | 1.757263 |
| H | 0.219572 | 1.830756 | -0.927614 | H | 1.112189 | -0.430035 | 2.117038 |
| Si | -1.101784 | -0.282507 | -0.017746 | Si | -0.005337 | -0.249718 | -1.158558 |
| H | -1.831608 | -0.616110 | -1.262738 | H | -1.297247 | -0.668317 | -1.757263 |
| H | -1.978238 | -0.340354 | 1.172572 | H | 1.112189 | -0.430035 | -2.117038 |
| H | 1.899846 | -0.649415 | -1.148930 | H | 0.551561 | 2.107828 | 0.000000 |

| $^2$p7 | | | | $^2$p8 | | | |
|---|---|---|---|---|---|---|---|
| Si | 1.787019 | 0.109350 | 0.000000 | Si | 0.627786 | -1.601124 | 0.000000 |
| C | 0.000000 | 0.794347 | 0.000000 | H | 1.455813 | -1.872714 | 1.204319 |
| H | -0.091243 | 1.459419 | 0.869088 | H | -0.518757 | -2.550686 | 0.000000 |
| H | -0.091243 | 1.459419 | -0.869088 | H | 1.455813 | -1.872714 | -1.204319 |
| Si | -1.394221 | -0.478055 | 0.000000 | C | 0.000000 | 0.107363 | 0.000000 |
| H | -2.742243 | 0.155467 | 0.000000 | Si | -0.659624 | 1.661779 | 0.000000 |
| H | -1.287224 | -1.339263 | -1.205576 | H | 0.167884 | 2.885558 | 0.000000 |
| H | -1.287224 | -1.339263 | 1.205576 | H | -2.115020 | 1.917212 | 0.000000 |
| $^2$p9 | | | | $^2$p10 | | | |
| Si | 1.603252 | -0.128271 | 0.081077 | C | 1.612540 | 1.382121 | 0.000000 |
| H | 1.621314 | -1.576823 | -0.245132 | H | -1.455712 | -1.652334 | 1.203873 |
| H | 2.702698 | 0.614362 | -0.586345 | H | -1.455712 | -1.652334 | -1.203873 |
| C | -0.020394 | 0.644245 | -0.015189 | H | 0.582123 | -2.184693 | 0.000000 |
| Si | -1.576105 | -0.132092 | -0.025514 | Si | 0.000000 | 0.906236 | 0.000000 |
| H | -1.709408 | -1.600766 | -0.014601 | H | -1.059165 | 1.943324 | 0.000000 |
| H | -2.838403 | 0.612445 | 0.150496 | H | 2.682832 | 1.441867 | 0.000000 |
| H | -0.033892 | 1.730392 | 0.008832 | Si | -0.640686 | -1.348276 | 0.000000 |
| $^2$p11 | | | | $^2$p12 | | | |
| Si | -0.453915 | -0.684246 | -0.051136 | Si | 1.151927 | -0.327294 | 0.000000 |
| Si | 1.559397 | 0.363842 | -0.063720 | H | 1.933562 | -0.583978 | 1.228806 |
| C | -1.938126 | 0.516304 | 0.012870 | H | 0.037208 | -1.437347 | 0.000000 |
| H | -2.520499 | 0.391848 | -0.903233 | H | 1.933562 | -0.583978 | -1.228806 |
| H | -2.595961 | 0.274237 | 0.849334 | C | 0.000000 | 1.118565 | 0.000000 |
| H | -1.637520 | 1.561083 | 0.091277 | H | 0.050941 | 1.737129 | 0.893688 |
| H | 2.396062 | -0.850229 | 0.282064 | H | 0.050941 | 1.737129 | -0.893688 |
| H | 0.509925 | 0.010891 | 1.211325 | Si | -1.438085 | -0.214159 | 0.000000 |

**(b)** B3LYP/cc-pVTZ vibrational frequencies and infrared intensities of doublet $Si_2CH_5$ isomers.

| | **$^2$p1** | | **$^2$p2** | |
|---|---|---|---|---|
| Normal modes | Frequency($cm^{-1}$) | IR Inten | Frequency($cm^{-1}$) | IR Inten |
| ν1 | 127.49 | 2.3216 | 111.03 | 0.4084 |
| ν2 | 149.77 | 0.4082 | 118.09 | 6.9525 |
| ν3 | 259.23 | 16.8391 | 272.63 | 4.8651 |
| ν4 | 386.02 | 11.1415 | 310.45 | 26.4862 |
| ν5 | 558.76 | 1.8682 | 399.87 | 8.4768 |
| ν6 | 650.88 | 22.6466 | 470.85 | 18.061 |
| ν7 | 682.75 | 52.0366 | 627.86 | 22.0911 |
| ν8 | 875.08 | 155.2215 | 660.99 | 15.7346 |
| ν9 | 887.54 | 87.2962 | 782.33 | 3.9468 |
| ν10 | 913.31 | 50.9365 | 947.61 | 95.5153 |
| ν11 | 1286.19 | 4.7011 | 1264.14 | 9.3064 |
| ν12 | 1463.82 | 3.6346 | 1443.54 | 4.0011 |
| ν13 | 1464.87 | 1.781 | 1456.08 | 8.6607 |
| ν14 | 2118.88 | 92.3017 | 2149.6 | 111.6837 |
| ν15 | 2162.79 | 124.1623 | 2196.36 | 111.027 |
| ν16 | 3028.57 | 10.8209 | 3012.47 | 5.0749 |
| ν17 | 3098.79 | 7.4044 | 3077.75 | 7.9764 |
| ν18 | 3106.51 | 7.9794 | 3094.55 | 6.9543 |
| | **$^2$p3** | | **$^2$p4** | |
| ν1 | 70.18 | 0.0692 | 157.81 | 3.8093 |
| ν2 | 145.64 | 2.0637 | 201.33 | 1.2065 |
| ν3 | 233.31 | 0.7178 | 312.86 | 1.9639 |
| ν4 | 381.57 | 1.432 | 361.4 | 3.7176 |

| | | | | |
|---|---|---|---|---|
| ν5 | 487.42 | 11.0378 | 462.5 | 12.8688 |
| ν6 | 499.53 | 5.5795 | 495.37 | 7.1406 |
| ν7 | 692.77 | 8.3406 | 622.44 | 18.0837 |
| ν8 | 730.91 | 73.424 | 672.21 | 0.6807 |
| ν9 | 867.06 | 341.0349 | 734.91 | 41.3198 |
| ν10 | 931.38 | 34.5285 | 836.3 | 69.7234 |
| ν11 | 945.29 | 29.028 | 880.63 | 22.3006 |
| ν12 | 959.06 | 17.0623 | 922.32 | 66.3193 |
| ν13 | 1374.42 | 5.9294 | 1399.6 | 2.3407 |
| ν14 | 2200.89 | 60.4247 | 2205.42 | 79.6855 |
| ν15 | 2224.84 | 81.3667 | 2230.53 | 12.4961 |
| ν16 | 2227.86 | 78.4516 | 2238.2 | 132.2325 |
| ν17 | 3112.27 | 1.7539 | 3138.51 | 2.4702 |
| ν18 | 3207.26 | 0.3113 | 3226.44 | 0.0783 |
| | **$^2$p5** | | **$^2$p6** | |
| ν1 | 322.17 | 3.9857 | 215.82 | 23.4861 |
| ν2 | 409.89 | 5.9033 | 385.39 | 3.1453 |
| ν3 | 427.83 | 8.3016 | 433.82 | 19.6141 |
| ν4 | 473.99 | 12.8655 | 444.96 | 4.028 |
| ν5 | 517.13 | 5.1732 | 535.57 | 22.25 |
| ν6 | 596.64 | 35.2127 | 545.49 | 29.0828 |
| ν7 | 638.7 | 18.9886 | 635.25 | 28.7301 |
| ν8 | 703.23 | 18.1251 | 668.08 | 51.2214 |
| ν9 | 776.3 | 60.4587 | 688.28 | 25.6067 |
| ν10 | 885.52 | 36.6138 | 790.35 | 10.16 |
| ν11 | 891.46 | 25.915 | 903.24 | 75.4125 |
| ν12 | 931.96 | 104.7429 | 932.52 | 31.5296 |

| | | | | |
|---|---|---|---|---|
| ν13 | 1382.66 | 2.232 | 944.11 | 132.3276 |
| ν14 | 2123.74 | 135.2826 | 2198.63 | 104.1307 |
| ν15 | 2222.5 | 85.2543 | 2203.12 | 33.2828 |
| ν16 | 2247.7 | 86.3541 | 2216.89 | 50.3618 |
| ν17 | 3077.18 | 2.4451 | 2223.18 | 161.6664 |
| ν18 | 3150.6 | 2.0459 | 3176.1 | 3.9665 |
| | **$^2$p7** | | **$^2$p8** | |
| ν1 | 143.75 | 0.4255 | 28 | 0.1133 |
| ν2 | 160.78 | 0.8091 | 116.45 | 2.8814 |
| ν3 | 515.29 | 15.3289 | 154.79 | 7.5449 |
| ν4 | 533.48 | 9.5526 | 483.56 | 11.2334 |
| ν5 | 663.44 | 38.9726 | 486.82 | 13.3656 |
| ν6 | 721.24 | 62.4383 | 580.23 | 6.7573 |
| ν7 | 886.35 | 15.3566 | 647.94 | 83.3041 |
| ν8 | 941.76 | 193.5164 | 666.35 | 37.0978 |
| ν9 | 950.58 | 110.8227 | 928.18 | 386.661 |
| ν10 | 955.12 | 30.4615 | 937.33 | 44.309 |
| ν11 | 987.12 | 37.0963 | 949.69 | 20.0604 |
| ν12 | 1016.22 | 48.7337 | 953.57 | 86.1751 |
| ν13 | 1356.21 | 10.9221 | 1256.27 | 84.0575 |
| ν14 | 2190.13 | 179.4175 | 2190.1 | 98.7962 |
| ν15 | 2214.99 | 68.5248 | 2202.42 | 114.536 |
| ν16 | 2220.72 | 116.9308 | 2206.23 | 122.5862 |
| ν17 | 2982 | 1.6276 | 2244.62 | 29.5905 |
| ν18 | 3039.02 | 4.6519 | 2258.71 | 74.6694 |
| | **$^2$p9** | | **$^2$p10** | |
| ν1 | 167.24 | 0.3039 | 68.92 | 0.2818 |

| | | | | |
|---|---|---|---|---|
| ν2 | 246.87 | 42.3451 | 161.65 | 2.4967 |
| ν3 | 262.69 | 45.6191 | 251.05 | 17.817 |
| ν4 | 328.19 | 7.5349 | 259.42 | 46.4412 |
| ν5 | 503.02 | 52.2849 | 416.32 | 3.2446 |
| ν6 | 560.2 | 2.3342 | 486.41 | 0.464 |
| ν7 | 592.94 | 11.6183 | 522.91 | 10.3767 |
| ν8 | 760.93 | 26.0636 | 636.35 | 51.3095 |
| ν9 | 790.99 | 60.2493 | 767.74 | 118.9811 |
| ν10 | 920.23 | 87.2538 | 882.54 | 248.8087 |
| ν11 | 930.59 | 51.6792 | 937.76 | 36.7724 |
| ν12 | 948.62 | 26.9284 | 949.36 | 44.4684 |
| ν13 | 1121.01 | 8.8027 | 1044.68 | 2.3986 |
| ν14 | 2190.98 | 123.7773 | 2207.2 | 92.5809 |
| ν15 | 2221.95 | 105.5951 | 2217.75 | 81.7424 |
| ν16 | 2255.17 | 42.0801 | 2219.1 | 49.8957 |
| ν17 | 2283.7 | 71.0548 | 2240.6 | 75.0689 |
| ν18 | 3136.07 | 0.1066 | 3319.9 | 8.7207 |
| | **$^{2}$p11** | | **$^{2}$p12** | |
| ν1 | 100.32 | 0.0757 | 248.58 | 0.6517 |
| ν2 | 156.13 | 2.8067 | 259.14 | 17.4207 |
| ν3 | 364.52 | 1.191 | 483.94 | 1.7075 |
| ν4 | 431.35 | 2.1737 | 516.88 | 6.3719 |
| ν5 | 544.03 | 4.7075 | 669.52 | 95.0617 |
| ν6 | 648.68 | 48.3661 | 690.45 | 3.6445 |
| ν7 | 737.41 | 35.3758 | 755.82 | 31.6982 |
| ν8 | 754.65 | 12.2592 | 806.99 | 14.1684 |
| ν9 | 768.48 | 8.395 | 891.88 | 15.2522 |

| | | | | |
|---|---|---|---|---|
| ν10 | 1044.34 | 139.4309 | 895.76 | 15.1415 |
| ν11 | 1267.9 | 8.6394 | 942.54 | 156.8928 |
| ν12 | 1446.41 | 7.8964 | 1051.61 | 140.4952 |
| ν13 | 1453.22 | 16.7597 | 1407.7 | 7.9041 |
| ν14 | 1475.48 | 78.9756 | 1799.14 | 74.8197 |
| ν15 | 2066.39 | 167.7914 | 2239.58 | 82.0679 |
| ν16 | 3019.86 | 5.2168 | 2254.83 | 82.8498 |
| ν17 | 3087.01 | 5.14 | 3067.01 | 5.2973 |
| ν18 | 3105.34 | 5.2223 | 3121.42 | 0.256 |