**SUPPLEMENTARY INFORMATION**

**A Crossed Molecular Beams Investigation of the Reactions of Atomic Silicon (Si(3P)) with C4H6 Isomers (1,3-Butadiene, 1,2-Butadiene, and 1-Butyne)**

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*

Bing-Jian Sun, Tzu-Jung Chou, Agnes H. H. Chang\*

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

 \*E−mail: ralfk@hawaii.edu

**Table S1**. Reaction mechanism and rate equations used to calculate the branching ratios between the SiC4H4 product channels leading to the formation of 1p9 plus H2 and 1p5 plus H2.





**Table S2**. The RRKM rate constants (s−1) computed with B3LYP/cc-pVTZ zero-point energy corrected CCSD(T)/CBS energies, and B3LYP/cc-pVTZ harmonic frequencies at a collision energies of 15 kJ mol−1 for the reaction of atomic silicon (Si) with 1,3-butadiene (CH2CHCHCH2) and its isotopologues.

|  |  |  |  |
| --- | --- | --- | --- |
|  | Si(3P) + CH2CHCHCH2 | Si(3P) + CH2CDCDCH2 | Si(3P) + CD2CHCHCD2 |
| *k1*(i1i2) | 1.13×109 | 8.18×108 | 3.80×108 |
| *k-1*(i2i1) | 1.15×108 | 8.44×107 | 4.20×107 |
| *k2*(i2i3) | 8.43×105 | 4.53×105 | 1.38×105 |
| *k-2*(i3i2) | 1.89×106 | 1.00×106 | 3.06×105 |
| *k3*(i3i4) | 5.64×1012 | 5.33×1012 | 3.64×1012 |
| *k-3*(i4i3) | 7.53×1012 | 7.21×1012 | 4.99×1012 |
| *k4*(i3p9) | 7.46×103 | 3.29×103 | 2.74×102 |
| *k5*(i4p5) | 1.98×106 | 6.76×105 | 6.22×105 |

**Table S3.** Structures and energies of species participating on the SiC4H6 potential energy surface. Energies were determined at the B3LYP/cc-pVTZ//CCSD(T)/CBS level of theory with ZPE correction.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | B3LYP/ cc-pVTZ + Ezpc a | Ezpc b | CCSD(T)/ CBS  | Ec (kJ/mol) |
| **Si(3P)** | -289.396332  | 0.000000  | -288.940006  |  |
| **trans-1,3-butadiene(1Ag)** | -155.970960  | 0.084962  | -155.765380  |  |
| **Si(3P) + 1,3-butadiene(1Ag)** | -445.367292  | 0.084962  | -444.705386  | 0.0  |
| **3i1** | -445.402087  | 0.084957  | -444.740157  | -91  |
| **1i1** | -445.430336  | 0.084629  | -444.777398  | -190  |
| **i1-MSXd** |  | 0.090451  | -444.736523  | -67  |
| **1i2** | -445.438328  | 0.082258  | -444.778804  | -200  |
| **1i3** | -445.434356  | 0.082329  | -444.775531  | -191  |
| **1i4** | -445.432678  | 0.082460  | -444.773880  | -186  |
| **tsi1i2** | -445.389762  | 0.080721  | -444.731847  | -81  |
| **tsi2i3** | -445.377069  | 0.078952  | -444.712114  | -33  |
| **tsi3i4** | -445.427042  | 0.080662  | -444.767174  | -174  |
| **tsi1p23** | -445.295639  | 0.076017  | -444.626339  | 184  |
| **tsi3p9** | -445.366043  | 0.076212  | -444.699987  | -9  |
| **tsi4p5** | -445.375367  | 0.077426  | -444.715994  | -48  |
|  |  |  |  |  |
| **H** | -0.502156  | 0.000000  | -0.500019  |  |
| **H2** | -1.169930  | 0.010069  | -1.174474  |  |
| **D2** | -1.172874  | 0.007125  | -1.174474  |  |
| **HD** | -1.171275  | 0.008724  | -1.174474  |  |
| **p5** | -444.234665  | 0.063062  | -443.564877  |  |
| **p9** | -444.222577  | 0.063417  | -443.546708  |  |
| **p23** | -444.211406  | 0.060727  | -443.530299  |  |
| **p5 + H2** | -445.404595  | 0.073131  | -444.739351  | -120  |
| **p9 + H2** | -445.392507  | 0.073486  | -444.721182  | -72  |
| **p23 + H2** | -445.381336  | 0.070796  | -444.704773  | -36  |

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)/CBS with B3LYP/cc-pVTZ zero-point energy correction.

d The minimum energy crossing point between 3i1 and 1i1 are located with the CPMCSCF/TZVPP.

**Table S4.** Structures and energies of species participating on the SiC4H4D2 potential energy surface. Energies were determined at the B3LYP/cc-pVTZ//CCSD(T)/CBS level of theory with ZPE correction.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | B3LYP/ cc-pVTZ + Ezpc a | Ezpc b | CCSD(T)/ CBS  | Ec (kJ/mol) |
| **Si(3P)** | -289.396332  | 0.000000  | -288.940006  |  |
| **trans-1,3-butadiene(1Ag)-2,3-D2** | -155.977348  | 0.078574  | -155.765380  |  |
| **Si(3P) + 1,3-butadiene(1Ag)-2,3-D2** | -445.373680  | 0.078574  | -444.705386  | 0.0  |
| **3i1-3,4-D2** | -445.408551  | 0.078493  | -444.740157  | -92  |
| **1i1-3,4-D2** | -445.436721  | 0.078244  | -444.777398  | -190  |
| **i1-MSX-3,4-D2d** |  | 0.083615 | -444.736523  | -69 |
| **1i2-3,4-D2** | -445.444772  | 0.075813  | -444.778804  | -200  |
| **1i3-3,4-D2** | -445.440800  | 0.075884  | -444.775531  | -191  |
| **1i4-3,4-D2** | -445.439132  | 0.076006  | -444.773880  | -187  |
| **tsi1i2-3,4-D2** | -445.396199  | 0.074284  | -444.731847  | -81  |
| **tsi2i3-3,4-D2** | -445.383395  | 0.072626  | -444.712114  | -33  |
| **tsi3i4-3,4-D2** | -445.433423  | 0.074281  | -444.767174  | -173  |
| **tsi1p23-3,4-D2** | -445.299982  | 0.071675  | -444.626339  | 189  |
| **tsi3p9-3,4-D2** | -445.372380  | 0.069875  | -444.699987  | -9  |
| **tsi4p5-3,4-D2** | -445.380353  | 0.072439  | -444.715994  | -44  |
|  |  |  |  |  |
| **H** | -0.502156  | 0.000000  | -0.500019  |  |
| **H2** | -1.169930  | 0.010069  | -1.174474  |  |
| **D2** | -1.172874  | 0.007125  | -1.174474  |  |
| **HD** | -1.171275  | 0.008724  | -1.174474  |  |
| **p5-3-D1** | -444.237684  | 0.060043  | -443.564877  |  |
| **p9-3,4-D2** | -444.228852  | 0.057143  | -443.546708  |  |
| **p23** | -444.211406  | 0.060727  | -443.530299  |  |
| **p5-3-D1 + HD** | -445.408959  | 0.068767  | -444.739351  | -115  |
| **p9-3,4-D2 + H2** | -445.398782  | 0.067212  | -444.721182  | -71  |
| **p23 + D2** | -445.384280  | 0.067852  | -444.704773  | -27  |

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)/CBS with B3LYP/cc-pVTZ zero-point energy correction.

d The minimum energy crossing point between 3i1 and 1i1 are located with the CPMCSCF/TZVPP.

**Table S5.** Structures and energies of species participating on the SiC4H2D4 potential energy surface. Energies were determined at the B3LYP/cc-pVTZ//CCSD(T)/CBS level of theory with ZPE correction.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | B3LYP/ cc-pVTZ + Ezpc a | Ezpc b | CCSD(T)/ CBS  | Ec (kJ/mol) |
| **Si(3P)** | -289.396332  | 0.000000  | -288.940006  |  |
| **trans-1,3-butadiene(1Ag)-1,1,4,4-D4** | -155.983441  | 0.072481  | -155.765380  |  |
| **Si(3P) + 1,3-butadiene(1Ag)-1,1,4,4-D4** | -445.379773  | 0.072481  | -444.705386  | 0.0  |
| **3i1-1,2,5,5-D4** | -445.414610  | 0.072434  | -444.740157  | -91  |
| **1i1-1,2,5,5-D4** | -445.442654  | 0.072311  | -444.777398  | -190  |
| **i1-MSX-1,2,5,5-D4d** |  | 0.077026 | -444.736523  | -70 |
| **1i2-1,2,5,5-D4** | -445.449593  | 0.070992  | -444.778804  | -197  |
| **1i3-1,2,5,5-D4** | -445.445678  | 0.071007  | -444.775531  | -188  |
| **1i4-1,2,5,5-D4** | -445.444046  | 0.071092  | -444.773880  | -183  |
| **tsi1i2-1,2,5,5-D4** | -445.400886  | 0.069597  | -444.731847  | -77  |
| **tsi2i3-1,2,5,5-D4** | -445.387734  | 0.068286  | -444.712114  | -29  |
| **tsi3i4-1,2,5,5-D4** | -445.438012  | 0.069692  | -444.767174  | -170  |
| **tsi1p23-1,2,5,5-D4** | -445.307889  | 0.063768  | -444.626339  | 185  |
| **tsi3p9-1,2,5,5-D4** | -445.375826  | 0.066430  | -444.699987  | -2  |
| **tsi4p5-1,2,5,5-D4** | -445.386777  | 0.066016  | -444.715994  | -45  |
|  |  |  |  |  |
| **H** | -0.502156  | 0.000000  | -0.500019  |  |
| **H2** | -1.169930  | 0.010069  | -1.174474  |  |
| **D2** | -1.172874  | 0.007125  | -1.174474  |  |
| **HD** | -1.171275  | 0.008724  | -1.174474  |  |
| **p5-2,5,5-D3** | -444.243951  | 0.053776  | -443.564877  |  |
| **p9-5,5-D2** | -444.228825  | 0.057169  | -443.546708  |  |
| **p23-2,2,5,5-D4** | -444.223398  | 0.048734  | -443.530299  |  |
| **p5-2,5,5-D3 + HD** | -445.415226  | 0.062500  | -444.739351  | -115  |
| **p9-5,5-D2 + D2** | -445.401699  | 0.064294  | -444.721182  | -63  |
| **p23-2,2,5,5-D4 + H2** | -445.393328  | 0.058803  | -444.704773  | -34  |

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)/CBS with B3LYP/cc-pVTZ zero-point energy correction.

d The minimum energy crossing point between 3i1 and 1i1 are located with the CPMCSCF/TZVPP.

**Table S6.** Optimized Cartesian coordinates of intermediates, transition states, and products on the SiC4H6 potential energy surface.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z |  |  |  |  |
| **trans-1,3-butadiene(1Ag)** |  |
| C | 0.599669 | 1.743646 | 0.000000 |  |  |  |  |
| C | 0.599669 | 0.409801 | 0.000000 |  |  |  |  |
| H | 1.518469 | 2.312728 | 0.000000 |  |  |  |  |
| H | -0.325022 | 2.307805 | 0.000000 |  |  |  |  |
| H | 1.546102 | -0.122426 | 0.000000 |  |  |  |  |
| C | -0.599669 | -0.409801 | 0.000000 |  |  |  |  |
| C | -0.599669 | -1.743646 | 0.000000 | 　 |  |  |  |
| H | -1.546102 | 0.122426 | 0.000000 | 　 |  |  |  |
| H | -1.518469 | -2.312728 | 0.000000 | 　 |  |  |  |
| H | 0.325022 | -2.307805 | 0.000000 | 　 | 　 | 　 | 　 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **3i1** | **1i1** |
| C | 1.039158 | 1.136203 | 0.125582 | C | 1.065718 | 1.105038 | 0.05934 |
| C | -0.192417 | 0.63631 | -0.395418 | C | -0.067764 | 0.237943 | -0.438196 |
| H | 1.642013 | 1.750821 | -0.531158 | H | 1.540019 | 1.76806 | -0.65716 |
| H | 1.062254 | 1.432161 | 1.169231 | H | 0.935225 | 1.586936 | 1.024809 |
| H | -0.339903 | 0.651039 | -1.469493 | H | -0.241498 | 0.255875 | -1.510896 |
| C | -1.246942 | 0.107081 | 0.398033 | C | -1.281551 | 0.067598 | 0.370289 |
| C | -2.418465 | -0.364956 | -0.101969 | C | -2.50053 | -0.224333 | -0.084788 |
| H | -1.103191 | 0.118546 | 1.473544 | H | -1.155133 | 0.194781 | 1.443503 |
| H | -3.199134 | -0.732243 | 0.547465 | H | -3.337639 | -0.341017 | 0.588863 |
| H | -2.604316 | -0.394206 | -1.167726 | H | -2.699062 | -0.353399 | -1.141721 |
| Si | 1.532448 | -0.850996 | -0.012802 | Si | 1.547347 | -0.730623 | 0.058052 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **i1-MSX** | **1i2** |
| C | 0.97095334 | 1.17271084 | 0.12469338 | C | 0.363046 | -0.811852 | 0.000000 |
| C | -0.1603975 | 0.5599955 | -0.4010416 | C | 0.000000 | 0.492464 | 0.000000 |
| H | 1.59135125 | 1.77021641 | -0.5140717 | H | -0.016087 | -3.323898 | 0.000000 |
| H | 1.00673874 | 1.41185559 | 1.17078981 | H | 1.429096 | -1.028301 | 0.000000 |
| H | -0.296698 | 0.55431731 | -1.4660431 | H | -1.060248 | 0.741258 | 0.000000 |
| C | -1.2756563 | 0.08191098 | 0.41378823 | C | 0.908342 | 1.620041 | 0.000000 |
| C | -2.4285802 | -0.3213006 | -0.0880765 | C | 0.5019 | 2.893145 | 0.000000 |
| H | -1.1307059 | 0.08972682 | 1.47942302 | H | 1.969445 | 1.393174 | 0.000000 |
| H | -3.2308119 | -0.6410411 | 0.54781676 | H | 1.204594 | 3.714673 | 0.000000 |
| H | -2.6057932 | -0.3464278 | -1.147526 | H | -0.550816 | 3.147587 | 0.000000 |
| Si | 1.7311046 | -0.842204 | -0.0844633 | Si | -0.972551 | -2.129092 | 0.000000 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **1i3** | **1i4** |
| C | -1.167059 | 0.315798 | 0.000000 | C | -1.152314 | 0.271823 | 0.000000 |
| C | 0 | 1.008955 | 0.000000 | C | 0 | 0.991011 | 0.000000 |
| H | -2.810362 | -1.591549 | 0.000000 | H | -0.02917 | -2.044076 | 0.000000 |
| H | -2.067378 | 0.923053 | 0.000000 | H | -2.053781 | 0.882223 | 0.000000 |
| H | -0.033584 | 2.097996 | 0.000000 | H | -0.072901 | 2.078527 | 0.000000 |
| C | 1.338728 | 0.456332 | 0.000000 | C | 1.359523 | 0.497959 | 0.000000 |
| C | 2.434605 | 1.220868 | 0.000000 | C | 2.416351 | 1.317145 | 0.000000 |
| H | 1.435993 | -0.623203 | 0.000000 | H | 1.504893 | -0.574123 | 0.000000 |
| H | 3.426967 | 0.792160 | 0.000000 | H | 3.428702 | 0.937657 | 0.000000 |
| H | 2.367401 | 2.302226 | 0.000000 | H | 2.297025 | 2.393942 | 0.000000 |
| Si | -1.282620 | -1.565172 | 0.000000 | Si | -1.486866 | -1.581555 | 0.000000 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **1tsi1i2** | **1tsi2i3** |
| C | -0.958604 | 0.996158 | 0.299104 | C | 0.705679 | 0.33634 | 0.278602 |
| C | 0.171943 | 0.13725 | 0.442134 | C | -0.617644 | 0.566298 | 0.004518 |
| H | -1.638038 | 0.679244 | -1.088212 | H | 3.113716 | -0.012138 | 1.022022 |
| H | -0.977279 | 2.062697 | 0.109083 | H | 1.152423 | 0.523319 | 1.26919 |
| H | 0.235992 | -0.407032 | 1.378593 | H | -0.929093 | 1.536637 | -0.38886 |
| C | 1.418454 | 0.25558 | -0.310863 | C | -1.670759 | -0.39062 | 0.156452 |
| C | 2.566267 | -0.352816 | -0.005877 | C | -2.953363 | -0.122477 | -0.149414 |
| H | 1.379488 | 0.892171 | -1.190686 | H | -1.392628 | -1.368885 | 0.530686 |
| H | 3.453788 | -0.219715 | -0.608089 | H | -3.732514 | -0.861469 | -0.028119 |
| H | 2.651176 | -1.005081 | 0.854990 | H | -3.248606 | 0.847733 | -0.528950 |
| Si | -1.735249 | -0.587094 | -0.143047 | Si | 2.303801 | -0.214460 | -0.258351 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **1tsi3i4** | **1tsi1p23** |
| C | 0.752641 | 0.900227 | 0.028511 | C | -1.152765 | 1.133344 | 0.162650 |
| C | -0.589503 | 0.85707 | 0.01333 | C | -0.047977 | 0.154980 | -0.043155 |
| H | 2.132193 | -0.768356 | 1.385461 | H | -1.242220 | 1.619778 | 1.133853 |
| H | 1.203831 | 1.897046 | 0.011016 | H | -1.411730 | 1.804661 | -0.658576 |
| H | -1.162442 | 1.780811 | 0.012759 | H | 1.649129 | 1.220565 | -0.866499 |
| C | -1.369794 | -0.367219 | -0.003452 | C | 1.314549 | 0.226159 | -0.091281 |
| C | -2.703049 | -0.422224 | -0.006337 | C | 2.464400 | -0.479034 | 0.117641 |
| H | -0.811921 | -1.302189 | -0.012767 | H | 1.743434 | 1.479205 | -0.024222 |
| H | -3.233849 | -1.363558 | -0.016376 | H | 3.423167 | -0.090178 | -0.183965 |
| H | -3.302514 | 0.479931 | 0.002371 | H | 2.412147 | -1.460616 | 0.561531 |
| Si | 2.045209 | -0.466486 | -0.112484 | Si | -1.574512 | -0.770436 | -0.059803 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **1tsi3p9** | **1tsi4p5** |
| C | -0.672197 | 0.203156 | -0.012644 | C | -1.184217 | 1.006364 | 0.038747 |
| C | 0.610450 | 0.525698 | 0.092419 | C | 0.136254 | 1.269997 | 0.010306 |
| H | -2.453654 | 0.347655 | -1.415791 | H | -0.768889 | -1.256318 | 1.430132 |
| H | -1.684711 | 0.834238 | -0.962882 | H | -1.975667 | 1.74362 | 0.054784 |
| H | 0.890562 | 1.554316 | 0.318997 | H | 0.632922 | 2.239188 | 0.027383 |
| C | 1.711741 | -0.406967 | -0.087186 | C | 0.829495 | -0.017572 | 0.026411 |
| C | 2.998792 | -0.066973 | 0.019747 | C | 2.126617 | -0.316171 | -0.062099 |
| H | 1.439520 | -1.430519 | -0.318341 | H | 0.085291 | -0.828366 | 1.083171 |
| H | 3.788015 | -0.792718 | -0.116437 | H | 2.485837 | -1.333939 | 0.021961 |
| H | 3.298647 | 0.948423 | 0.247837 | H | 2.877440 | 0.451597 | -0.223132 |
| Si | -2.369364 | -0.213634 | 0.155186 | Si | -1.056130 | -0.905107 | -0.176749 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **1p5** | **1p9** |
| Si | -0.884921 | -0.996101 | -0.073803 | C | 2.142206 | 1.929304 | 0.000000 |
| C | -1.31497 | 0.799266 | 0.253963 | C | 1.449885 | 0.785296 | 0.000000 |
| C | -0.066634 | 1.167891 | -0.158745 | H | 3.223139 | 1.938818 | 0.000000 |
| C | 0.782155 | -0.01099 | -0.003774 | H | 1.642072 | 2.889956 | 0.000000 |
| H | -2.1845 | 1.439712 | 0.304758 | H | 1.962425 | -0.169219 | 0.000000 |
| H | 0.230661 | 2.1069 | -0.632888 | C | 0.000000 | 0.741187 | 0.000000 |
| C | 2.10082 | -0.151876 | 0.088463 | C | -0.736213 | -0.370203 | 0.000000 |
| H | 2.774674 | 0.699826 | 0.086480 | H | -0.491728 | 1.717024 | 0.000000 |
| H | 2.559831 | -1.126777 | 0.195452 | Si | -1.676513 | -1.777863 | 0.000000 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z |  |  |  |  |
| **1p23** |  |  |  |  |
| C | 2.645696 | -0.174571 | -0.000072 |  |  |  |  |
| C | 1.351968 | -0.008012 | 0.000034 |  |  |  |  |
| H | 3.202759 | -0.243279 | -0.926168 |  |  |  |  |
| H | 3.202953 | -0.24333 | 0.925904 |  |  |  |  |
| H | -1.125995 | 1.74843 | -0.902266 |  |  |  |  |
| C | 0.065829 | 0.113713 | 0.000337 |  |  |  |  |
| C | -1.009393 | 1.151524 | -0.000065 |  |  |  |  |
| H | -1.126758 | 1.748522 | 0.901963 |  |  |  |  |
| Si | -1.605540 | -0.679020 | -0.000060 |  |  |  |  |

**Table S7.** Vibrational frequencies and infrared intensities for intermediates, transition states, and products on the SiC4H6 potential energy surface.

|  |  |
| --- | --- |
| trans-1,3-butadiene(1Ag) |  |
| Normal modes | Frequency(cm-1) | IR Inten |  |  |  |
| ν1 | 174.3783 | 0.4162 |  |  |  |
| ν2 | 299.7798 | 2.8113 |  |  |  |
| ν3 | 519.8144 | 0 |  |  |  |
| ν4 | 538.4075 | 11.3063 |  |  |  |
| ν5 | 783.7131 | 0 |  |  |  |
| ν6 | 901.5539 | 0 |  |  |  |
| ν7 | 943.3092 | 81.6143 |  |  |  |
| ν8 | 943.4798 | 0 |  |  |  |
| ν9 | 1004.4204 | 0 |  |  |  |
| ν10 | 1007.6772 | 1.9007 |  |  |  |
| ν11 | 1058.5437 | 32.305 |  |  |  |
| ν12 | 1230.2891 | 0 |  |  |  |
| ν13 | 1319.0154 | 0 |  |  |  |
| ν14 | 1325.2723 | 2.1749 |  |  |  |
| ν15 | 1420.3454 | 4.0514 |  |  |  |
| ν16 | 1479.8527 | 0 |  |  |  |
| ν17 | 1655.0238 | 19.6064 |  |  |  |
| ν18 | 1705.8009 | 0 |  |  |  |
| ν19 | 3125.7972 | 0 |  |  |  |
| ν20 | 3135.7145 | 22.5669 |  |  |  |
| ν21 | 3138.3394 | 0 |  |  |  |
| ν22 | 3138.6341 | 9.5277 |  |  |  |
| ν23 | 3222.2217 | 0 |  |  |  |
| ν24 | 3222.6365 | 24.6804 | 　 | 　 | 　 |

|  |  |
| --- | --- |
| 3i1 | 1i1 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 95.6949 | 1.352 | ν1 | 106.8038 | 0.075 |
| ν2 | 214.6459 | 0.197 | ν2 | 143.2156 | 0.7731 |
| ν3 | 291.5502 | 0.6988 | ν3 | 271.194 | 1.0715 |
| ν4 | 309.0402 | 6.6735 | ν4 | 415.5012 | 17.3019 |
| ν5 | 403.9863 | 14.4187 | ν5 | 490.5012 | 2.6147 |
| ν6 | 515.5228 | 1.6835 | ν6 | 548.0123 | 7.5632 |
| ν7 | 602.1432 | 3.1509 | ν7 | 623.5465 | 30.5674 |
| ν8 | 744.8946 | 3.0689 | ν8 | 685.7617 | 12.4409 |
| ν9 | 850.8776 | 0.5701 | ν9 | 835.0889 | 7.2763 |
| ν10 | 877.2898 | 37.3031 | ν10 | 870.1868 | 17.6983 |
| ν11 | 881.3975 | 52.1213 | ν11 | 903.6795 | 41.6758 |
| ν12 | 912.9909 | 5.7165 | ν12 | 955.6597 | 0.8484 |
| ν13 | 994.7352 | 12.5495 | ν13 | 991.2588 | 2.6732 |
| ν14 | 1015.4186 | 6.0988 | ν14 | 1029.9782 | 8.2495 |
| ν15 | 1204.3062 | 9.784 | ν15 | 1102.8661 | 33.0178 |
| ν16 | 1237.4343 | 7.2946 | ν16 | 1204.8797 | 35.1084 |
| ν17 | 1295.2246 | 4.3963 | ν17 | 1299.8412 | 0.3805 |
| ν18 | 1365.3811 | 0.7637 | ν18 | 1337.1984 | 2.1805 |
| ν19 | 1464.0471 | 0.8082 | ν19 | 1414.3948 | 4.9932 |
| ν20 | 1497.7942 | 13.4086 | ν20 | 1462.5367 | 4.4904 |
| ν21 | 1559.0755 | 12.369 | ν21 | 1673.9329 | 62.4945 |
| ν22 | 3099.0837 | 2.6557 | ν22 | 3081.1466 | 5.6063 |
| ν23 | 3138.7633 | 2.6391 | ν23 | 3093.9855 | 1.2803 |
| ν24 | 3144.6035 | 2.2003 | ν24 | 3104.2229 | 18.5156 |
| ν25 | 3153.1207 | 3.3873 | ν25 | 3134.1609 | 6.5044 |
| ν26 | 3185.4406 | 1.0542 | ν26 | 3150.3713 | 5.6182 |
| ν27 | 3237.2298 | 6.3985 | ν27 | 3218.0301 | 15.2954 |

|  |  |
| --- | --- |
| i1-MSX | 1i2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 63.08 | 51.21 | ν1 | 108.944 | 0.0563 |
| ν2 | 116.13 | 2.06 | ν2 | 153.7133 | 0.3952 |
| ν3 | 196.61 | 1.14 | ν3 | 196.7439 | 0.3804 |
| ν4 | 295.68 | 10.64 | ν4 | 259.2841 | 0.8216 |
| ν5 | 325.73 | 3.61 | ν5 | 346.8408 | 2.2633 |
| ν6 | 537.64 | 14.59 | ν6 | 451.3673 | 15.7517 |
| ν7 | 691.17 | 14.53 | ν7 | 636.8275 | 1.8255 |
| ν8 | 809.07 | 22.22 | ν8 | 742.8703 | 43.2039 |
| ν9 | 931.56 | 3.66 | ν9 | 844.6262 | 151.9051 |
| ν10 | 950.5 | 20.04 | ν10 | 882.1404 | 10.0733 |
| ν11 | 967.59 | 5.66 | ν11 | 958.6401 | 7.7884 |
| ν12 | 1069.08 | 90.08 | ν12 | 972.0853 | 28.2275 |
| ν13 | 1086.96 | 2.62 | ν13 | 1011.3573 | 5.4227 |
| ν14 | 1126.02 | 8.52 | ν14 | 1060.6322 | 49.7401 |
| ν15 | 1301.83 | 100 | ν15 | 1150.809 | 10.333 |
| ν16 | 1324.51 | 36.65 | ν16 | 1255.6224 | 12.0306 |
| ν17 | 1425.52 | 4.28 | ν17 | 1320.3012 | 16.8945 |
| ν18 | 1483.68 | 8.73 | ν18 | 1336.2685 | 10.0231 |
| ν19 | 1584.78 | 4.82 | ν19 | 1445.6763 | 1.6916 |
| ν20 | 1646.32 | 29.72 | ν20 | 1585.6095 | 167.036 |
| ν21 | 1815.12 | 89.25 | ν21 | 1672.3415 | 35.7427 |
| ν22 | 3283.59 | 4.43 | ν22 | 2001.7487 | 339.46 |
| ν23 | 3288.07 | 9.92 | ν23 | 3097.2956 | 2.9378 |
| ν24 | 3307.24 | 9.26 | ν24 | 3106.0592 | 17.5248 |
| ν25 | 3324.98 | 4.47 | ν25 | 3137.4495 | 8.2152 |
| ν26 | 3374.58 | 2.54 | ν26 | 3145.6619 | 7.7562 |
| ν27 | 3376.22 | 22.39 | ν27 | 3226.2061 | 7.4013 |

|  |  |
| --- | --- |
| 1i3 | 1i4 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 123.0669 | 0.1554 | ν1 | 96.5266 | 0.0785 |
| ν2 | 162.4145 | 1.2543 | ν2 | 191.5087 | 0.8308 |
| ν3 | 193.1152 | 0.0048 | ν3 | 205.2946 | 0.073 |
| ν4 | 264.4364 | 0.6482 | ν4 | 244.285 | 0.7546 |
| ν5 | 332.1286 | 7.8779 | ν5 | 338.8392 | 10.2967 |
| ν6 | 572.3119 | 6.1186 | ν6 | 570.2416 | 1.2547 |
| ν7 | 619.652 | 16.1642 | ν7 | 628.3019 | 13.9832 |
| ν8 | 666.945 | 67.3962 | ν8 | 647.2241 | 99.335 |
| ν9 | 831.7748 | 9.0234 | ν9 | 844.3298 | 3.141 |
| ν10 | 855.6655 | 68.9059 | ν10 | 862.2714 | 50.4866 |
| ν11 | 940.4016 | 6.5157 | ν11 | 946.174 | 4.8038 |
| ν12 | 968.8928 | 45.8319 | ν12 | 971.6043 | 43.3496 |
| ν13 | 1022.1503 | 3.8563 | ν13 | 1028.5831 | 3.8604 |
| ν14 | 1066.4683 | 4.2128 | ν14 | 1070.3116 | 4.5357 |
| ν15 | 1123.9619 | 7.3835 | ν15 | 1141.5171 | 0.8679 |
| ν16 | 1265.5159 | 12.2584 | ν16 | 1280.3882 | 11.99 |
| ν17 | 1323.6085 | 3.6561 | ν17 | 1319.4688 | 5.571 |
| ν18 | 1376.8201 | 16.9457 | ν18 | 1392.6026 | 23.4344 |
| ν19 | 1448.2201 | 3.3237 | ν19 | 1452.7016 | 15.9909 |
| ν20 | 1571.3136 | 164.9845 | ν20 | 1573.9369 | 255.8563 |
| ν21 | 1674.7392 | 27.5555 | ν21 | 1671.56 | 42.0875 |
| ν22 | 2011.1901 | 333.7001 | ν22 | 2005.5802 | 239.0845 |
| ν23 | 3084.466 | 11.2763 | ν23 | 3074.5973 | 7.3815 |
| ν24 | 3124.4332 | 21.3145 | ν24 | 3101.2105 | 33.6342 |
| ν25 | 3135.1313 | 10.6976 | ν25 | 3135.1848 | 9.1855 |
| ν26 | 3155.0783 | 1.3871 | ν26 | 3177.2603 | 2.2101 |
| ν27 | 3224.2929 | 7.6883 | ν27 | 3224.1624 | 8.1666 |

|  |  |
| --- | --- |
| 1tsi1i2 | 1tsi2i3 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -942.5115 | 266.8344 | ν1 | -1150.029 | 3.904 |
| ν2 | 111.9808 | 0.1702 | ν2 | 107.0546 | 0.7163 |
| ν3 | 214.211 | 7.6706 | ν3 | 142.5642 | 2.5563 |
| ν4 | 264.4032 | 1.155 | ν4 | 296.6049 | 20.8157 |
| ν5 | 392.7294 | 13.4057 | ν5 | 363.8097 | 11.5092 |
| ν6 | 502.642 | 0.3517 | ν6 | 432.9656 | 2.2964 |
| ν7 | 689.284 | 15.9834 | ν7 | 504.4521 | 16.6092 |
| ν8 | 725.5708 | 34.1382 | ν8 | 655.8573 | 23.0687 |
| ν9 | 810.813 | 16.0772 | ν9 | 711.4446 | 131.106 |
| ν10 | 908.1363 | 16.3468 | ν10 | 757.1711 | 35.619 |
| ν11 | 920.1711 | 9.3897 | ν11 | 818.0555 | 334.9284 |
| ν12 | 925.981 | 51.3143 | ν12 | 942.9332 | 34.5623 |
| ν13 | 980.2214 | 22.9582 | ν13 | 966.9309 | 29.4015 |
| ν14 | 1031.678 | 17.2274 | ν14 | 981.3691 | 24.0603 |
| ν15 | 1114.91 | 14.3464 | ν15 | 1036.9935 | 18.0469 |
| ν16 | 1165.1425 | 3.915 | ν16 | 1203.2499 | 4.7628 |
| ν17 | 1244.7915 | 17.7061 | ν17 | 1291.7818 | 3.0429 |
| ν18 | 1321.0898 | 3.2521 | ν18 | 1312.6086 | 8.5452 |
| ν19 | 1360.1659 | 1.4812 | ν19 | 1437.4955 | 0.7259 |
| ν20 | 1468.8911 | 0.3905 | ν20 | 1516.7238 | 62.5917 |
| ν21 | 1671.8018 | 21.4312 | ν21 | 1627.2745 | 2.284 |
| ν22 | 1857.1502 | 48.0594 | ν22 | 1988.7441 | 345.1211 |
| ν23 | 3117.8785 | 6.6962 | ν23 | 2977.2106 | 105.9337 |
| ν24 | 3130.3511 | 5.6152 | ν24 | 3047.4789 | 15.8639 |
| ν25 | 3134.6599 | 5.7354 | ν25 | 3140.9964 | 3.146 |
| ν26 | 3147.6882 | 10.8292 | ν26 | 3161.7907 | 5.6141 |
| ν27 | 3220.0817 | 12.525 | ν27 | 3232.2518 | 5.4592 |

|  |  |
| --- | --- |
| 1tsi3i4 | 1tsi1p23 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -305.9308 | 15.9825 | ν1 | -1076.5247 | 365.3606 |
| ν2 | 96.7507 | 0.5006 | ν2 | 132.7224 | 6.5265 |
| ν3 | 129.0874 | 0.5498 | ν3 | 145.0821 | 2.5797 |
| ν4 | 315.8099 | 0.1431 | ν4 | 189.024 | 14.685 |
| ν5 | 325.6982 | 4.81 | ν5 | 466.694 | 18.6345 |
| ν6 | 565.9941 | 7.1605 | ν6 | 528.8584 | 33.3089 |
| ν7 | 573.129 | 18.8216 | ν7 | 561.6698 | 13.5073 |
| ν8 | 608.8081 | 15.639 | ν8 | 585.7145 | 27.8362 |
| ν9 | 746.8899 | 16.5767 | ν9 | 648.9847 | 10.8461 |
| ν10 | 820.2501 | 105.8013 | ν10 | 712.4173 | 16.2069 |
| ν11 | 924.8117 | 0.0697 | ν11 | 749.3176 | 66.3628 |
| ν12 | 937.2248 | 43.3408 | ν12 | 844.2297 | 9.1912 |
| ν13 | 978.1396 | 0.2907 | ν13 | 864.2918 | 10.2286 |
| ν14 | 1028.3338 | 14.0538 | ν14 | 892.5487 | 72.3336 |
| ν15 | 1090.1841 | 3.9215 | ν15 | 997.8445 | 117.0246 |
| ν16 | 1243.9982 | 1.1201 | ν16 | 1050.1831 | 2.1559 |
| ν17 | 1328.6707 | 7.0291 | ν17 | 1126.765 | 9.8125 |
| ν18 | 1360.3074 | 0.6572 | ν18 | 1300.0592 | 17.3543 |
| ν19 | 1452.4947 | 0.7937 | ν19 | 1458.5073 | 13.819 |
| ν20 | 1600.2243 | 6.5096 | ν20 | 1482.6784 | 17.425 |
| ν21 | 1682.7796 | 11.5004 | ν21 | 1606.4371 | 40.1841 |
| ν22 | 1995.1968 | 267.9702 | ν22 | 1697.438 | 704.1337 |
| ν23 | 3035.9622 | 8.515 | ν23 | 2806.5952 | 36.9655 |
| ν24 | 3089.3722 | 11.0514 | ν24 | 3007.7695 | 70.5938 |
| ν25 | 3116.0124 | 24.4898 | ν25 | 3062.7255 | 34.6363 |
| ν26 | 3136.9459 | 4.7881 | ν26 | 3175.2767 | 7.5551 |
| ν27 | 3223.6224 | 9.6319 | ν27 | 3273.8903 | 1.4935 |

|  |  |
| --- | --- |
| 1tsi3p9 | 1tsi4p5 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -1333.357 | 253.7629 | ν1 | -1230.7031 | 284.7611 |
| ν2 | 112.4177 | 0.8399 | ν2 | 211.812 | 0.9396 |
| ν3 | 135.4935 | 1.3912 | ν3 | 264.1671 | 2.5761 |
| ν4 | 289.211 | 3.7635 | ν4 | 395.515 | 6.6392 |
| ν5 | 362.0388 | 4.8637 | ν5 | 489.8884 | 31.8949 |
| ν6 | 382.9712 | 8.8383 | ν6 | 532.6875 | 21.0613 |
| ν7 | 489.4189 | 12.5843 | ν7 | 603.3135 | 2.2176 |
| ν8 | 660.3881 | 8.6617 | ν8 | 689.2733 | 9.4388 |
| ν9 | 715.9103 | 8.6603 | ν9 | 726.1245 | 14.8622 |
| ν10 | 771.1862 | 6.8535 | ν10 | 808.0211 | 19.2479 |
| ν11 | 898.0767 | 8.9975 | ν11 | 895.8519 | 62.6853 |
| ν12 | 932.4787 | 86.733 | ν12 | 941.9002 | 1.1888 |
| ν13 | 945.1156 | 26.1276 | ν13 | 946.8065 | 43.1244 |
| ν14 | 966.7696 | 12.2875 | ν14 | 997.4467 | 5.444 |
| ν15 | 1036.0773 | 17.9856 | ν15 | 1057.2166 | 3.5606 |
| ν16 | 1175.8922 | 4.5255 | ν16 | 1168.7011 | 1.0124 |
| ν17 | 1280.4474 | 9.0749 | ν17 | 1218.7334 | 19.3289 |
| ν18 | 1320.5246 | 3.1527 | ν18 | 1301.3534 | 18.0999 |
| ν19 | 1453.1882 | 2.0804 | ν19 | 1449.1366 | 1.7313 |
| ν20 | 1656.1604 | 66.6814 | ν20 | 1559.174 | 5.8781 |
| ν21 | 1668.9165 | 13.0967 | ν21 | 1661.2222 | 6.8952 |
| ν22 | 1796.6059 | 181.5815 | ν22 | 1714.909 | 38.9633 |
| ν23 | 1811.7558 | 3.4856 | ν23 | 1778.7082 | 173.517 |
| ν24 | 3077.5267 | 8.2146 | ν24 | 3087.9681 | 39.909 |
| ν25 | 3136.6792 | 7.5036 | ν25 | 3108.1274 | 14.7494 |
| ν26 | 3153.7099 | 6.3916 | ν26 | 3183.8234 | 15.1002 |
| ν27 | 3224.3359 | 10.5804 | ν27 | 3194.2885 | 5.8019 |

|  |  |
| --- | --- |
| 1p5 | 1p9 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 183.1405 | 0.4239 | ν1 | 96.9224 | 0.9211 |
| ν2 | 275.5198 | 0.3599 | ν2 | 128.2337 | 2.504 |
| ν3 | 322.6247 | 8.212 | ν3 | 250.8504 | 2.1958 |
| ν4 | 523.9323 | 2.8227 | ν4 | 366.5114 | 15.664 |
| ν5 | 604.8113 | 43.0539 | ν5 | 480.0111 | 14.9839 |
| ν6 | 683.3588 | 20.5327 | ν6 | 626.464 | 11.071 |
| ν7 | 753.2015 | 24.4568 | ν7 | 807.1429 | 33.5025 |
| ν8 | 831.5068 | 39.2118 | ν8 | 916.126 | 0.0685 |
| ν9 | 927.453 | 21.4567 | ν9 | 973.0915 | 1.8662 |
| ν10 | 933.0473 | 16.7068 | ν10 | 974.1588 | 42.3581 |
| ν11 | 997.9336 | 2.9786 | ν11 | 1037.4072 | 13.2906 |
| ν12 | 1052.0626 | 4.1793 | ν12 | 1183.0359 | 4.8035 |
| ν13 | 1154.5467 | 8.5232 | ν13 | 1293.6396 | 0.7557 |
| ν14 | 1287.0887 | 28.5574 | ν14 | 1316.1519 | 9.063 |
| ν15 | 1452.1204 | 4.7189 | ν15 | 1453.5399 | 6.5333 |
| ν16 | 1482.1026 | 10.3139 | ν16 | 1656.837 | 1.4026 |
| ν17 | 1694.5121 | 1.7907 | ν17 | 1702.3698 | 335.9909 |
| ν18 | 3042.5248 | 60.589 | ν18 | 3045.2583 | 22.2737 |
| ν19 | 3102.6638 | 27.9981 | ν19 | 3137.9669 | 7.4982 |
| ν20 | 3184.3077 | 11.8049 | ν20 | 3164.2247 | 4.2696 |
| ν21 | 3192.7744 | 6.717 | ν21 | 3227.1135 | 7.3422 |

|  |  |  |  |
| --- | --- | --- | --- |
| 1p23 |  |  |  |
| Normal modes | Frequency(cm-1) | IR Inten |  |  |  |
| ν1 | 94.5084 | 1.5774 |  |  |  |
| ν2 | 156.0295 | 1.301 |  |  |  |
| ν3 | 367.2852 | 1.8468 |  |  |  |
| ν4 | 464.3254 | 51.8425 |  |  |  |
| ν5 | 467.8352 | 2.1881 |  |  |  |
| ν6 | 559.6736 | 21.1217 |  |  |  |
| ν7 | 579.1157 | 0.612 |  |  |  |
| ν8 | 645.2693 | 18.1242 |  |  |  |
| ν9 | 797.1383 | 59.9652 |  |  |  |
| ν10 | 852.6324 | 54.676 |  |  |  |
| ν11 | 961.0238 | 10.1589 |  |  |  |
| ν12 | 993.6599 | 0.0342 |  |  |  |
| ν13 | 1012.5863 | 0.0252 |  |  |  |
| ν14 | 1305.9329 | 16.5766 |  |  |  |
| ν15 | 1412.8525 | 5.5217 |  |  |  |
| ν16 | 1469.8667 | 6.4374 |  |  |  |
| ν17 | 2019.9461 | 625.5822 |  |  |  |
| ν18 | 3055.0551 | 10.0765 |  |  |  |
| ν19 | 3117.843 | 5.8988 |  |  |  |
| ν20 | 3125.8148 | 1.4278 |  |  |  |
| ν21 | 3197.6834 | 0.2115 |  |  |  |

**Table S8.** Vibrational frequencies and infrared intensities for intermediates, transition states, and products on the SiC4H4D2 potential energy surface.

|  |  |
| --- | --- |
| trans-1,3-butadiene(1Ag)-2,3-D2 |  |
| Normal modes | Frequency(cm-1) | IR Inten |  |  |  |
| ν1 | 164.2271 | 0.2688 |  |  |  |
| ν2 | 288.7587 | 2.6384 |  |  |  |
| ν3 | 493.7177 | 13.0992 |  |  |  |
| ν4 | 504.9364 | 0 |  |  |  |
| ν5 | 777.2148 | 0 |  |  |  |
| ν6 | 836.0776 | 0 |  |  |  |
| ν7 | 859.2303 | 0.6719 |  |  |  |
| ν8 | 883.0367 | 13.4174 |  |  |  |
| ν9 | 895.4102 | 0 |  |  |  |
| ν10 | 943.311 | 82.1585 |  |  |  |
| ν11 | 947.5578 | 0 |  |  |  |
| ν12 | 957.2984 | 0 |  |  |  |
| ν13 | 1148.3703 | 1.8766 |  |  |  |
| ν14 | 1242.6193 | 0 |  |  |  |
| ν15 | 1413.5327 | 4.3864 |  |  |  |
| ν16 | 1462.9728 | 0 |  |  |  |
| ν17 | 1643.3317 | 20.2551 |  |  |  |
| ν18 | 1682.2093 | 0 |  |  |  |
| ν19 | 2314.196 | 0 |  |  |  |
| ν20 | 2316.8641 | 12.7655 |  |  |  |
| ν21 | 3136.3231 | 12.6255 |  |  |  |
| ν22 | 3136.4437 | 0 |  |  |  |
| ν23 | 3221.2048 | 19.344 |  |  |  |
| ν24 | 3221.2816 | 0 | 　 | 　 | 　 |

|  |  |
| --- | --- |
| 3i1-3,4-D2 | 1i1-3,4-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 94.9329 | 1.3502 | ν1 | 103.1852 | 0.045 |
| ν2 | 192.6246 | 0.2007 | ν2 | 130.8346 | 0.6696 |
| ν3 | 281.4132 | 0.5069 | ν3 | 261.1794 | 0.922 |
| ν4 | 293.5169 | 5.5278 | ν4 | 406.3013 | 15.9682 |
| ν5 | 402.0857 | 12.3724 | ν5 | 466.2845 | 4.1791 |
| ν6 | 498.6629 | 2.5916 | ν6 | 540.7193 | 7.7578 |
| ν7 | 559.3145 | 8.2541 | ν7 | 603.8384 | 21.3872 |
| ν8 | 701.5165 | 7.8089 | ν8 | 630.1201 | 14.9138 |
| ν9 | 755.8748 | 0.7552 | ν9 | 749.8605 | 6.7942 |
| ν10 | 801.6592 | 7.4786 | ν10 | 812.3956 | 16.5458 |
| ν11 | 858.2237 | 13.3148 | ν11 | 856.942 | 6.3994 |
| ν12 | 873.776 | 33.7925 | ν12 | 862.2776 | 4.7973 |
| ν13 | 876.0589 | 34.0814 | ν13 | 903.3425 | 42.7025 |
| ν14 | 901.1847 | 1.2051 | ν14 | 937.4178 | 11.7121 |
| ν15 | 963.9781 | 8.4338 | ν15 | 954.7167 | 4.1101 |
| ν16 | 1131.4209 | 2.1567 | ν16 | 1073.5958 | 3.8391 |
| ν17 | 1209.9982 | 3.2128 | ν17 | 1158.6826 | 0.9578 |
| ν18 | 1316.7867 | 4.596 | ν18 | 1230.5441 | 35.8211 |
| ν19 | 1414.9994 | 11.8156 | ν19 | 1413.8859 | 5.1325 |
| ν20 | 1478.1401 | 7.8961 | ν20 | 1444.0914 | 9.6859 |
| ν21 | 1541.2621 | 13.6972 | ν21 | 1655.016 | 67.3105 |
| ν22 | 2320.2518 | 1.9824 | ν22 | 2278.7662 | 3.0714 |
| ν23 | 2323.5874 | 1.0715 | ν23 | 2289.8368 | 9.7389 |
| ν24 | 3099.1041 | 2.743 | ν24 | 3081.4341 | 5.6011 |
| ν25 | 3143.8571 | 3.8774 | ν25 | 3133.8738 | 7.1473 |
| ν26 | 3183.8487 | 0.613 | ν26 | 3148.8725 | 3.6251 |
| ν27 | 3236.2856 | 5.5969 | ν27 | 3217.0758 | 12.7766 |

|  |  |
| --- | --- |
| i1-MSX-3,4-D2 | 1i2-3,4-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 63.06 | 52.15 | ν1 | 104.8062 | 0.032 |
| ν2 | 113.85 | 2.11 | ν2 | 151.4245 | 0.3754 |
| ν3 | 179.72 | 0.99 | ν3 | 185.2457 | 0.3132 |
| ν4 | 281.8 | 11.15 | ν4 | 249.98 | 0.6431 |
| ν5 | 310.25 | 2.22 | ν5 | 332.1766 | 1.6131 |
| ν6 | 520.13 | 14.21 | ν6 | 439.3815 | 15.479 |
| ν7 | 605.98 | 4.87 | ν7 | 580.7284 | 4.3548 |
| ν8 | 759.39 | 25 | ν8 | 736.0832 | 45.032 |
| ν9 | 863.43 | 13.67 | ν9 | 825.3131 | 0.5752 |
| ν10 | 921.77 | 3.03 | ν10 | 833.1104 | 131.8099 |
| ν11 | 928.25 | 14.16 | ν11 | 857.9499 | 1.948 |
| ν12 | 942.79 | 7.89 | ν12 | 881.285 | 13.3148 |
| ν13 | 950.59 | 22.52 | ν13 | 927.2123 | 38.6555 |
| ν14 | 1025.11 | 19.16 | ν14 | 959.6014 | 8.4633 |
| ν15 | 1071.87 | 75.13 | ν15 | 975.7206 | 35.4949 |
| ν16 | 1226.14 | 17.21 | ν16 | 1047.0646 | 12.6395 |
| ν17 | 1305.14 | 5.77 | ν17 | 1205.0802 | 8.7584 |
| ν18 | 1426.6 | 75.23 | ν18 | 1257.2283 | 2.3543 |
| ν19 | 1558.41 | 17.92 | ν19 | 1432.7354 | 0.9005 |
| ν20 | 1633.54 | 29.52 | ν20 | 1563.7565 | 206.1695 |
| ν21 | 1790.46 | 100 | ν21 | 1651.2588 | 24.4348 |
| ν22 | 2447.21 | 9.53 | ν22 | 2001.7214 | 339.0033 |
| ν23 | 2454.57 | 1.51 | ν23 | 2286.8869 | 6.3695 |
| ν24 | 3284.3 | 6.2 | ν24 | 2324.1979 | 5.5418 |
| ν25 | 3289.94 | 7.2 | ν25 | 3104.8051 | 17.008 |
| ν26 | 3373.66 | 6.99 | ν26 | 3138.398 | 5.6224 |
| ν27 | 3374.92 | 14.14 | ν27 | 3225.015 | 5.5881 |

|  |  |
| --- | --- |
| 1i3-3,4-D2 | 1i4-3,4-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 115.3412 | 0.0819 | ν1 | 90.2933 | 0.0983 |
| ν2 | 159.5327 | 1.271 | ν2 | 187.4686 | 0.8718 |
| ν3 | 185.8288 | 0.0167 | ν3 | 198.4277 | 0.0219 |
| ν4 | 247.3252 | 0.5814 | ν4 | 229.3624 | 0.6591 |
| ν5 | 322.6027 | 6.9614 | ν5 | 330.3513 | 9.2091 |
| ν6 | 549.4095 | 15.5709 | ν6 | 554.1303 | 0.2141 |
| ν7 | 554.2581 | 6.8818 | ν7 | 556.9385 | 13.3156 |
| ν8 | 651.5561 | 60.6901 | ν8 | 628.9606 | 92.454 |
| ν9 | 804.6886 | 1.0207 | ν9 | 809.1294 | 0.0032 |
| ν10 | 838.1045 | 55.1448 | ν10 | 851.6424 | 49.9555 |
| ν11 | 859.7812 | 12.7716 | ν11 | 863.0964 | 9.1857 |
| ν12 | 890.1584 | 10.4185 | ν12 | 885.6347 | 3.1361 |
| ν13 | 936.6744 | 7.3656 | ν13 | 950.6849 | 5.276 |
| ν14 | 971.628 | 4.6263 | ν14 | 970.6805 | 11.9717 |
| ν15 | 972.144 | 32.8211 | ν15 | 974.4783 | 31.6546 |
| ν16 | 998.3715 | 21.0118 | ν16 | 1013.9026 | 2.5408 |
| ν17 | 1191.7724 | 4.7089 | ν17 | 1197.3322 | 3.7429 |
| ν18 | 1324.0586 | 1.9042 | ν18 | 1352.4035 | 6.464 |
| ν19 | 1434.5856 | 0.2359 | ν19 | 1437.0942 | 1.5771 |
| ν20 | 1548.0518 | 196.2699 | ν20 | 1552.3908 | 306.7148 |
| ν21 | 1652.4532 | 15.8535 | ν21 | 1649.5749 | 23.0655 |
| ν22 | 2011.1537 | 334.3017 | ν22 | 2005.5087 | 239.3458 |
| ν23 | 2278.8937 | 16.5098 | ν23 | 2273.7381 | 19.1253 |
| ν24 | 2332.6017 | 0.9581 | ν24 | 2349.3522 | 2.2175 |
| ν25 | 3120.4798 | 12.9408 | ν25 | 3092.8447 | 15.7877 |
| ν26 | 3135.1306 | 8.8324 | ν26 | 3135.1624 | 8.3809 |
| ν27 | 3222.8417 | 6.6026 | ν27 | 3221.9917 | 6.6682 |

|  |  |
| --- | --- |
| 1tsi1i2-3,4-D2 | 1tsi2i3-3,4-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -922.5498 | 266.1017 | ν1 | -1117.4327 | 2.1341 |
| ν2 | 107.0252 | 0.1448 | ν2 | 105.0733 | 0.652 |
| ν3 | 199.6999 | 6.0559 | ν3 | 134.8205 | 2.1948 |
| ν4 | 254.9211 | 1.2746 | ν4 | 283.0006 | 17.7945 |
| ν5 | 382.4491 | 13.7315 | ν5 | 348.073 | 11.2516 |
| ν6 | 488.9066 | 0.2681 | ν6 | 422.6863 | 3.379 |
| ν7 | 616.5108 | 24.3502 | ν7 | 493.4369 | 15.9719 |
| ν8 | 707.8424 | 1.414 | ν8 | 611.3135 | 12.2911 |
| ν9 | 723.4643 | 53.3916 | ν9 | 685.8036 | 118.8963 |
| ν10 | 847.7507 | 1.0616 | ν10 | 728.1326 | 41.756 |
| ν11 | 861.3617 | 6.8815 | ν11 | 794.2764 | 219.6992 |
| ν12 | 876.5973 | 8.9657 | ν12 | 845.8947 | 12.9239 |
| ν13 | 925.408 | 42.4122 | ν13 | 869.6015 | 36.8243 |
| ν14 | 932.0994 | 22.3816 | ν14 | 897.8673 | 137.8809 |
| ν15 | 959.4954 | 11.1998 | ν15 | 964.7238 | 30.814 |
| ν16 | 1040.4428 | 4.8651 | ν16 | 969.9291 | 2.2766 |
| ν17 | 1114.6765 | 6.9086 | ν17 | 1057.2254 | 0.6775 |
| ν18 | 1192.9509 | 6.7614 | ν18 | 1223.1793 | 9.9121 |
| ν19 | 1311.3039 | 7.2585 | ν19 | 1422.0798 | 0.4281 |
| ν20 | 1446.2073 | 1.2616 | ν20 | 1493.4065 | 64.4205 |
| ν21 | 1652.83 | 25.0365 | ν21 | 1608.9954 | 2.1125 |
| ν22 | 1855.8768 | 49.1864 | ν22 | 1988.7421 | 345.09 |
| ν23 | 2301.5009 | 0.575 | ν23 | 2243.7607 | 11.2797 |
| ν24 | 2307.1512 | 6.9449 | ν24 | 2337.5458 | 4.6586 |
| ν25 | 3134.0087 | 6.9518 | ν25 | 2977.2894 | 107.0835 |
| ν26 | 3147.4766 | 10.7776 | ν26 | 3141.2716 | 2.9337 |
| ν27 | 3218.988 | 10.2198 | ν27 | 3230.9655 | 4.381 |

|  |  |
| --- | --- |
| 1tsi3i4-3,4-D2 | 1tsi1p23-3,4-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -304.5351 | 15.9962 | ν1 | -850.3663 | 240.9569 |
| ν2 | 95.2821 | 0.4905 | ν2 | 118.4002 | 5.5865 |
| ν3 | 118.1819 | 0.3858 | ν3 | 142.7615 | 2.714 |
| ν4 | 296.0658 | 0.2086 | ν4 | 179.1942 | 8.3383 |
| ν5 | 314.3741 | 4.187 | ν5 | 443.2694 | 4.7311 |
| ν6 | 506.8814 | 18.7131 | ν6 | 475.6234 | 29.9759 |
| ν7 | 557.847 | 2.5955 | ν7 | 524.7511 | 10.091 |
| ν8 | 586.9027 | 20.8714 | ν8 | 548.0644 | 12.6727 |
| ν9 | 744.6718 | 15.9543 | ν9 | 603.3931 | 18.5223 |
| ν10 | 783.6752 | 63.0512 | ν10 | 653.5092 | 16.6412 |
| ν11 | 840.6534 | 33.466 | ν11 | 705.7624 | 31.7562 |
| ν12 | 874.6328 | 0.8824 | ν12 | 732.2785 | 5.9176 |
| ν13 | 889.195 | 13.268 | ν13 | 759.9373 | 66.1816 |
| ν14 | 940.4601 | 36.0924 | ν14 | 891.2467 | 80.8126 |
| ν15 | 955.1345 | 1.9428 | ν15 | 968.7576 | 84.2775 |
| ν16 | 972.6686 | 0.1613 | ν16 | 1040.3171 | 6.4103 |
| ν17 | 1180.5582 | 4.5192 | ν17 | 1089.0631 | 5.0004 |
| ν18 | 1290.7766 | 2.1931 | ν18 | 1172.6735 | 19.942 |
| ν19 | 1436.333 | 0.7592 | ν19 | 1271.3744 | 28.9886 |
| ν20 | 1585.0747 | 4.4 | ν20 | 1458.4287 | 13.9825 |
| ν21 | 1662.129 | 12.4485 | ν21 | 1476.481 | 19.6052 |
| ν22 | 1995.1857 | 267.6805 | ν22 | 1677.7886 | 697.9441 |
| ν23 | 2283.2586 | 7.2324 | ν23 | 2009.1983 | 24.5306 |
| ν24 | 2297.9591 | 10.5056 | ν24 | 3007.751 | 71.0027 |
| ν25 | 3038.1167 | 9.818 | ν25 | 3062.6994 | 34.865 |
| ν26 | 3136.6746 | 4.7514 | ν26 | 3175.2288 | 7.3756 |
| ν27 | 3222.8167 | 7.8951 | ν27 | 3273.6305 | 1.5326 |

|  |  |
| --- | --- |
| 1tsi3p9-3,4-D2 | 1tsi4p5-3,4-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -1330.6909 | 254.6323 | ν1 | -945.2478 | 149.6384 |
| ν2 | 108.1678 | 0.6906 | ν2 | 203.4925 | 0.7022 |
| ν3 | 131.8305 | 1.24 | ν3 | 259.8057 | 2.2472 |
| ν4 | 276.2328 | 4.3417 | ν4 | 364.6973 | 8.4948 |
| ν5 | 348.5254 | 4.5018 | ν5 | 464.4153 | 25.8983 |
| ν6 | 373.7474 | 8.767 | ν6 | 515.8516 | 18.5754 |
| ν7 | 476.8047 | 10.8705 | ν7 | 559.7921 | 1.1763 |
| ν8 | 600.0781 | 11.0303 | ν8 | 648.0738 | 8.3135 |
| ν9 | 701.6677 | 9.9956 | ν9 | 718.9213 | 13.2312 |
| ν10 | 744.8095 | 4.9183 | ν10 | 776.3627 | 10.406 |
| ν11 | 777.8163 | 0.0607 | ν11 | 838.0523 | 22.3791 |
| ν12 | 860.9052 | 7.4511 | ν12 | 865.9464 | 39.5594 |
| ν13 | 864.9422 | 0.4671 | ν13 | 908.6104 | 13.433 |
| ν14 | 932.0677 | 93.6014 | ν14 | 941.2001 | 1.3375 |
| ν15 | 942.8993 | 28.4277 | ν15 | 945.9969 | 26.2006 |
| ν16 | 961.6844 | 0.4813 | ν16 | 972.1975 | 21.5334 |
| ν17 | 1062.7823 | 11.1218 | ν17 | 1123.0731 | 3.5192 |
| ν18 | 1208.586 | 6.6559 | ν18 | 1226.1314 | 27.5471 |
| ν19 | 1436.3484 | 1.519 | ν19 | 1292.784 | 4.9679 |
| ν20 | 1645.5662 | 33.891 | ν20 | 1445.311 | 1.7541 |
| ν21 | 1651.4094 | 37.8273 | ν21 | 1531.8274 | 6.4405 |
| ν22 | 1792.9465 | 189.5263 | ν22 | 1662.5614 | 3.6746 |
| ν23 | 1811.569 | 3.6118 | ν23 | 1759.5215 | 148.2457 |
| ν24 | 2269.1991 | 4.9525 | ν24 | 2287.8097 | 23.159 |
| ν25 | 2331.1165 | 4.6536 | ν25 | 3108.043 | 13.7494 |
| ν26 | 3137.1019 | 6.9437 | ν26 | 3182.4441 | 11.761 |
| ν27 | 3222.8847 | 8.3118 | ν27 | 3194.2814 | 6.0929 |

|  |  |
| --- | --- |
| 1p5-3-D1 | 1p9-3,4-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 170.6096 | 0.3364 | ν1 | 94.012 | 0.8151 |
| ν2 | 271.5999 | 0.3325 | ν2 | 125.3064 | 2.3292 |
| ν3 | 305.3863 | 7.5594 | ν3 | 238.0316 | 2.3312 |
| ν4 | 515.1996 | 3.0469 | ν4 | 354.8493 | 15.1124 |
| ν5 | 600.5608 | 42.7349 | ν5 | 469.0902 | 13.6297 |
| ν6 | 650.302 | 21.0713 | ν6 | 555.6632 | 9.7829 |
| ν7 | 749.1686 | 27.3181 | ν7 | 766.9613 | 28.3017 |
| ν8 | 787.7448 | 9.1444 | ν8 | 809.659 | 1.675 |
| ν9 | 853.4416 | 2.3367 | ν9 | 858.7043 | 7.9221 |
| ν10 | 906.545 | 22.9136 | ν10 | 869.4475 | 0.1894 |
| ν11 | 931.4786 | 31.778 | ν11 | 964.7013 | 6.7576 |
| ν12 | 944.2411 | 1.9148 | ν12 | 973.5219 | 34.0158 |
| ν13 | 1119.3495 | 5.2974 | ν13 | 1075.2698 | 1.1948 |
| ν14 | 1225.6728 | 29.4954 | ν14 | 1214.7498 | 5.7398 |
| ν15 | 1437.484 | 10.5103 | ν15 | 1434.864 | 11.9194 |
| ν16 | 1464.0177 | 5.1923 | ν16 | 1638.9532 | 4.4164 |
| ν17 | 1693.0036 | 1.7462 | ν17 | 1690.6614 | 325.0352 |
| ν18 | 2251.0914 | 40.324 | ν18 | 2244.5198 | 22.0666 |
| ν19 | 3102.6378 | 27.4014 | ν19 | 2340.0549 | 3.3188 |
| ν20 | 3184.304 | 11.9225 | ν20 | 3138.2511 | 7.205 |
| ν21 | 3192.1062 | 5.4463 | ν21 | 3225.597 | 5.6922 |

|  |  |  |  |
| --- | --- | --- | --- |
| 1p23 |  |  |  |
| Normal modes | Frequency(cm-1) | IR Inten |  |  |  |
| ν1 | 94.5084 | 1.5774 |  |  |  |
| ν2 | 156.0295 | 1.301 |  |  |  |
| ν3 | 367.2852 | 1.8468 |  |  |  |
| ν4 | 464.3254 | 51.8425 |  |  |  |
| ν5 | 467.8352 | 2.1881 |  |  |  |
| ν6 | 559.6736 | 21.1217 |  |  |  |
| ν7 | 579.1157 | 0.612 |  |  |  |
| ν8 | 645.2693 | 18.1242 |  |  |  |
| ν9 | 797.1383 | 59.9652 |  |  |  |
| ν10 | 852.6324 | 54.676 |  |  |  |
| ν11 | 961.0238 | 10.1589 |  |  |  |
| ν12 | 993.6599 | 0.0342 |  |  |  |
| ν13 | 1012.5863 | 0.0252 |  |  |  |
| ν14 | 1305.9329 | 16.5766 |  |  |  |
| ν15 | 1412.8525 | 5.5217 |  |  |  |
| ν16 | 1469.8667 | 6.4374 |  |  |  |
| ν17 | 2019.9461 | 625.5822 |  |  |  |
| ν18 | 3055.0551 | 10.0765 |  |  |  |
| ν19 | 3117.843 | 5.8988 |  |  |  |
| ν20 | 3125.8148 | 1.4278 |  |  |  |
| ν21 | 3197.6834 | 0.2115 |  |  |  |

**Table S9.** Vibrational frequencies and infrared intensities for intermediates, transition states, and products on the SiC4H2D4 potential energy surface.

|  |  |
| --- | --- |
| trans-1,3-butadiene(1Ag)-1,1,4,4-D4 |  |
| Normal modes | Frequency(cm-1) | IR Inten |  |  |  |
| ν1 | 159.6802 | 0.4512 |  |  |  |
| ν2 | 259.0083 | 1.9859 |  |  |  |
| ν3 | 404.6504 | 5.5115 |  |  |  |
| ν4 | 459.9526 | 0 |  |  |  |
| ν5 | 630.2497 | 0 |  |  |  |
| ν6 | 749.1149 | 0 |  |  |  |
| ν7 | 754.7358 | 0 |  |  |  |
| ν8 | 755.1031 | 52.9548 |  |  |  |
| ν9 | 828.0886 | 2.4781 |  |  |  |
| ν10 | 970.2473 | 0 |  |  |  |
| ν11 | 996.6228 | 28.816 |  |  |  |
| ν12 | 1047.0686 | 5.2391 |  |  |  |
| ν13 | 1062.2228 | 0 |  |  |  |
| ν14 | 1194.1883 | 0 |  |  |  |
| ν15 | 1303.0204 | 1.213 |  |  |  |
| ν16 | 1330.0038 | 0 |  |  |  |
| ν17 | 1587.9077 | 13.814 |  |  |  |
| ν18 | 1670.8075 | 0 |  |  |  |
| ν19 | 2291.4365 | 0 |  |  |  |
| ν20 | 2294.5159 | 3.6448 |  |  |  |
| ν21 | 2398.7802 | 9.966 |  |  |  |
| ν22 | 2399.4815 | 0 |  |  |  |
| ν23 | 3128.9369 | 0 |  |  |  |
| ν24 | 3139.7538 | 25.4761 | 　 | 　 | 　 |

|  |  |
| --- | --- |
| 3i1-1,2,5,5-D4 | 1i1-1,2,5,5-D4 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 91.9947 | 1.3325 | ν1 | 99.7762 | 0.042 |
| ν2 | 195.2037 | 0.1868 | ν2 | 130.2137 | 0.6184 |
| ν3 | 253.2181 | 0.4427 | ν3 | 236.3694 | 0.5681 |
| ν4 | 294.9078 | 6.856 | ν4 | 369.9284 | 12.1515 |
| ν5 | 393.0693 | 11.6345 | ν5 | 385.5333 | 3.1305 |
| ν6 | 458.423 | 1.6782 | ν6 | 496.0985 | 10.3809 |
| ν7 | 477.2987 | 1.2853 | ν7 | 564.4746 | 28.4413 |
| ν8 | 561.8684 | 1.1235 | ν8 | 588.4779 | 0.9992 |
| ν9 | 659.5392 | 24.1413 | ν9 | 686.4708 | 4.3622 |
| ν10 | 695.9358 | 17.2433 | ν10 | 726.5138 | 27.4933 |
| ν11 | 749.2731 | 3.1157 | ν11 | 749.9028 | 3.4538 |
| ν12 | 814.2247 | 1.1802 | ν12 | 799.9645 | 2.2517 |
| ν13 | 861.2197 | 17.7564 | ν13 | 900.0073 | 9.4552 |
| ν14 | 967.6087 | 15.2664 | ν14 | 967.8284 | 9.0261 |
| ν15 | 1016.1744 | 1.9968 | ν15 | 987.0532 | 14.9896 |
| ν16 | 1047.1796 | 2.1312 | ν16 | 1050.9066 | 1.835 |
| ν17 | 1204.2265 | 5.7255 | ν17 | 1109.9725 | 12.0867 |
| ν18 | 1223.0329 | 12.648 | ν18 | 1171.1958 | 52.369 |
| ν19 | 1296.6406 | 3.9064 | ν19 | 1278.6607 | 1.8713 |
| ν20 | 1401.4929 | 11.7638 | ν20 | 1349.9576 | 0.6004 |
| ν21 | 1517.2787 | 10.3707 | ν21 | 1629.6705 | 63.1385 |
| ν22 | 2250.354 | 0.7892 | ν22 | 2237.395 | 1.5032 |
| ν23 | 2287.9798 | 1.5513 | ν23 | 2290.2017 | 1.5498 |
| ν24 | 2370.0921 | 0.4256 | ν24 | 2337.503 | 1.9763 |
| ν25 | 2411.1921 | 3.5309 | ν25 | 2395.7797 | 6.1351 |
| ν26 | 3140.6686 | 1.7737 | ν26 | 3095.0031 | 1.8552 |
| ν27 | 3154.7745 | 3.8598 | ν27 | 3106.1136 | 22.4024 |

|  |  |
| --- | --- |
| i1-MSX-1,2,5,5-D4 | 1i2-1,2,5,5-D4 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 62.58 | 58.23 | ν1 | 92.5068 | 0.0184 |
| ν2 | 109.17 | 2.79 | ν2 | 142.1499 | 0.4056 |
| ν3 | 184.83 | 1.11 | ν3 | 181.2932 | 0.4091 |
| ν4 | 266.53 | 4.86 | ν4 | 210.5811 | 0.4949 |
| ν5 | 296 | 9.46 | ν5 | 329.9586 | 0.892 |
| ν6 | 480.53 | 10.75 | ν6 | 408.7635 | 11.2564 |
| ν7 | 543.38 | 6.69 | ν7 | 505.4791 | 0.3921 |
| ν8 | 637.06 | 26.83 | ν8 | 574.4723 | 8.8878 |
| ν9 | 712.9 | 7.26 | ν9 | 722.408 | 134.9447 |
| ν10 | 780.19 | 5.72 | ν10 | 732.9618 | 12.934 |
| ν11 | 847.64 | 54.62 | ν11 | 776.7525 | 17.8598 |
| ν12 | 872.59 | 5.62 | ν12 | 798.91 | 1.7679 |
| ν13 | 932.43 | 3.94 | ν13 | 961.5284 | 30.6195 |
| ν14 | 1068.63 | 18.69 | ν14 | 981.2404 | 0.3063 |
| ν15 | 1103.21 | 30.34 | ν15 | 999.0634 | 34.0157 |
| ν16 | 1137.87 | 3.49 | ν16 | 1060.4489 | 1.8352 |
| ν17 | 1252.58 | 59.18 | ν17 | 1190.0325 | 5.8422 |
| ν18 | 1342.42 | 78 | ν18 | 1309.395 | 3.7375 |
| ν19 | 1411.91 | 3.64 | ν19 | 1321.114 | 28.0238 |
| ν20 | 1542.55 | 34.65 | ν20 | 1440.2387 | 168.2692 |
| ν21 | 1762.6 | 100 | ν21 | 1555.863 | 123.0259 |
| ν22 | 2390 | 3.14 | ν22 | 1636.7819 | 90.5638 |
| ν23 | 2409.96 | 2.53 | ν23 | 2289.3565 | 6.2357 |
| ν24 | 2514.19 | 8.75 | ν24 | 2293.4229 | 3.7029 |
| ν25 | 2515.36 | 4.99 | ν25 | 2402.6071 | 2.8519 |
| ν26 | 3307.03 | 15.63 | ν26 | 3098.7628 | 5.5675 |
| ν27 | 3326.52 | 6.98 | ν27 | 3145.9526 | 10.3618 |

|  |  |
| --- | --- |
| 1i3-1,2,5,5-D4 | 1i4-1,2,5,5-D4 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 100.4584 | 0.0869 | ν1 | 84.0052 | 0.1595 |
| ν2 | 154.0161 | 1.304 | ν2 | 160.2338 | 0.0345 |
| ν3 | 158.115 | 0.0106 | ν3 | 179.7076 | 0.9871 |
| ν4 | 245.7627 | 0.95 | ν4 | 228.8397 | 0.9534 |
| ν5 | 303.7716 | 4.9059 | ν5 | 307.7156 | 5.4963 |
| ν6 | 499.5286 | 8.3177 | ν6 | 497.2452 | 8.5459 |
| ν7 | 502.3794 | 3.5306 | ν7 | 505.8132 | 6.9657 |
| ν8 | 597.8449 | 41.9774 | ν8 | 614.6916 | 99.409 |
| ν9 | 658.4154 | 4.4953 | ν9 | 668.2465 | 1.4754 |
| ν10 | 716.6195 | 76.5409 | ν10 | 698.3812 | 16.9582 |
| ν11 | 764.7023 | 2.0463 | ν11 | 770.9969 | 1.6321 |
| ν12 | 774.1201 | 27.3347 | ν12 | 776.4111 | 25.8473 |
| ν13 | 905.6651 | 0.9309 | ν13 | 927.2114 | 6.0128 |
| ν14 | 990.707 | 2.7933 | ν14 | 994.6563 | 1.6808 |
| ν15 | 1011.4992 | 8.6803 | ν15 | 1012.7234 | 10.2669 |
| ν16 | 1054.4815 | 5.1274 | ν16 | 1054.2424 | 3.73 |
| ν17 | 1208.098 | 3.6317 | ν17 | 1212.1345 | 1.939 |
| ν18 | 1309.9993 | 3.5381 | ν18 | 1302.705 | 6.286 |
| ν19 | 1347.7069 | 22.0154 | ν19 | 1356.5927 | 38.8544 |
| ν20 | 1447.485 | 178.6162 | ν20 | 1442.5168 | 114.4427 |
| ν21 | 1540.8523 | 123.1049 | ν21 | 1543.7416 | 191.4573 |
| ν22 | 1638.4066 | 66.4963 | ν22 | 1635.9747 | 108.4205 |
| ν23 | 2291.1496 | 5.9914 | ν23 | 2276.5767 | 9.6304 |
| ν24 | 2300.367 | 3.1072 | ν24 | 2291.1537 | 4.6289 |
| ν25 | 2400.6411 | 4.4536 | ν25 | 2400.0855 | 4.4703 |
| ν26 | 3088.8824 | 21.883 | ν26 | 3083.4204 | 27.2306 |
| ν27 | 3156.6814 | 2.9398 | ν27 | 3179.567 | 3.4364 |

|  |  |
| --- | --- |
| 1tsi1i2-1,2,5,5-D4 | 1tsi2i3-1,2,5,5-D4 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -727.1958 | 151.7152 | ν1 | -875.4365 | 2.843 |
| ν2 | 103.8075 | 0.1658 | ν2 | 100.2199 | 0.5049 |
| ν3 | 200.8566 | 5.8257 | ν3 | 131.6679 | 1.9633 |
| ν4 | 232.6955 | 0.7966 | ν4 | 270.5566 | 16.2766 |
| ν5 | 354.8142 | 13.0843 | ν5 | 325.1317 | 8.3278 |
| ν6 | 439.8784 | 0.3695 | ν6 | 348.0739 | 5.8668 |
| ν7 | 564.3092 | 34.0176 | ν7 | 457.029 | 11.0924 |
| ν8 | 593.297 | 3.6802 | ν8 | 513.4855 | 31.8211 |
| ν9 | 727.3538 | 7.3404 | ν9 | 563.7755 | 77.8769 |
| ν10 | 743.2021 | 13.805 | ν10 | 600.682 | 187.6555 |
| ν11 | 759.5413 | 7.4616 | ν11 | 709.2809 | 12.1872 |
| ν12 | 785.379 | 5.9766 | ν12 | 767.2399 | 24.1937 |
| ν13 | 845.6265 | 29.8574 | ν13 | 830.1841 | 1.7972 |
| ν14 | 908.6307 | 6.8887 | ν14 | 928.2603 | 10.3223 |
| ν15 | 982.748 | 17.1891 | ν15 | 997.9048 | 15.1308 |
| ν16 | 1049.8952 | 4.6586 | ν16 | 1047.6338 | 6.959 |
| ν17 | 1117.3177 | 4.2422 | ν17 | 1189.7934 | 3.0435 |
| ν18 | 1228.5233 | 25.5206 | ν18 | 1287.2293 | 3.975 |
| ν19 | 1297.5947 | 7.8167 | ν19 | 1309.0977 | 2.4749 |
| ν20 | 1332.2206 | 17.5575 | ν20 | 1430.3788 | 183.9144 |
| ν21 | 1390.604 | 3.628 | ν21 | 1486.4751 | 54.8951 |
| ν22 | 1626.6345 | 18.5002 | ν22 | 1579.3205 | 10.544 |
| ν23 | 2290.2777 | 1.6625 | ν23 | 2190.6315 | 90.3846 |
| ν24 | 2326.6241 | 6.1519 | ν24 | 2292.3633 | 0.8859 |
| ν25 | 2397.2354 | 5.0564 | ν25 | 2407.264 | 3.5463 |
| ν26 | 3119.4705 | 6.3447 | ν26 | 3047.4385 | 14.971 |
| ν27 | 3130.9343 | 7.421 | ν27 | 3163.0033 | 6.8816 |

|  |  |
| --- | --- |
| 1tsi3i4-1,2,5,5-D4 | 1tsi1p23-1,2,5,5-D4 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -222.8512 | 8.5598 | ν1 | -1071.7579 | 362.5938 |
| ν2 | 92.8197 | 0.4862 | ν2 | 120.4958 | 5.2809 |
| ν3 | 117.0128 | 0.4094 | ν3 | 132.2251 | 2.1434 |
| ν4 | 283.8284 | 0.9594 | ν4 | 172.6087 | 10.115 |
| ν5 | 293.1642 | 2.8029 | ν5 | 428.3949 | 10.956 |
| ν6 | 440.4305 | 8.8718 | ν6 | 458.4969 | 36.5412 |
| ν7 | 532.7049 | 4.7683 | ν7 | 477.6024 | 11.5368 |
| ν8 | 576.3303 | 7.295 | ν8 | 525.4369 | 11.216 |
| ν9 | 597.924 | 16.789 | ν9 | 543.8018 | 39.1574 |
| ν10 | 659.6143 | 70.9591 | ν10 | 616.7654 | 15.0055 |
| ν11 | 749.7188 | 27.8562 | ν11 | 629.993 | 18.6551 |
| ν12 | 755.193 | 0.7988 | ν12 | 712.252 | 14.2466 |
| ν13 | 880.8933 | 4.9646 | ν13 | 764.831 | 4.5846 |
| ν14 | 948.0914 | 0.3789 | ν14 | 808.6958 | 28.4806 |
| ν15 | 968.4457 | 19.4543 | ν15 | 838.4195 | 3.6415 |
| ν16 | 1051.965 | 3.4238 | ν16 | 960.8283 | 115.1235 |
| ν17 | 1192.2132 | 0.6327 | ν17 | 1010.9247 | 5.6122 |
| ν18 | 1313.4109 | 5.3446 | ν18 | 1038.8285 | 39.9542 |
| ν19 | 1346.5069 | 0.6122 | ν19 | 1100.7034 | 1.9256 |
| ν20 | 1435.5863 | 141.2576 | ν20 | 1353.5701 | 19.4679 |
| ν21 | 1573.3298 | 9.1569 | ν21 | 1599.2812 | 64.0484 |
| ν22 | 1650.1901 | 5.1445 | ν22 | 1684.3519 | 672.7839 |
| ν23 | 2233.7744 | 4.6388 | ν23 | 2176.5946 | 33.7989 |
| ν24 | 2292.6335 | 0.8595 | ν24 | 2276.0573 | 19.1956 |
| ν25 | 2400.2895 | 4.681 | ν25 | 2311.8093 | 27.6306 |
| ν26 | 3090.38 | 10.0938 | ν26 | 2440.7814 | 0.7312 |
| ν27 | 3114.6613 | 26.3634 | ν27 | 2807.2709 | 35.9177 |

|  |  |
| --- | --- |
| 1tsi3p9-1,2,5,5-D4 | 1tsi4p5-1,2,5,5-D4 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | -963.7775 | 129.3607 | ν1 | -1175.658 | 280.0619 |
| ν2 | 103.4779 | 0.6941 | ν2 | 192.208 | 0.9903 |
| ν3 | 129.8428 | 1.1666 | ν3 | 240.2209 | 1.5448 |
| ν4 | 249.6055 | 1.8116 | ν4 | 359.2148 | 4.2187 |
| ν5 | 310.427 | 0.6859 | ν5 | 444.4571 | 7.0897 |
| ν6 | 339.8432 | 9.2803 | ν6 | 464.7273 | 17.5415 |
| ν7 | 470.5989 | 10.4616 | ν7 | 506.7642 | 20.7921 |
| ν8 | 500.0615 | 4.3026 | ν8 | 540.6835 | 10.5851 |
| ν9 | 564.4468 | 5.4066 | ν9 | 644.9675 | 7.1054 |
| ν10 | 700.3228 | 18.0933 | ν10 | 661.7166 | 15.9664 |
| ν11 | 734.0392 | 42.4638 | ν11 | 708.4665 | 54.8323 |
| ν12 | 750.9506 | 41.214 | ν12 | 765.8662 | 4.2067 |
| ν13 | 839.0937 | 0.9052 | ν13 | 786.6726 | 7.3034 |
| ν14 | 895.0396 | 7.3943 | ν14 | 865.8215 | 9.0046 |
| ν15 | 985.8204 | 13.7101 | ν15 | 949.2785 | 8.4951 |
| ν16 | 1047.5867 | 4.654 | ν16 | 1055.7249 | 3.7731 |
| ν17 | 1154.9113 | 5.4318 | ν17 | 1123.8554 | 1.5032 |
| ν18 | 1242.4047 | 61.6584 | ν18 | 1163.3298 | 19.4276 |
| ν19 | 1278.1299 | 55.5237 | ν19 | 1266.3387 | 31.549 |
| ν20 | 1294.1944 | 4.8402 | ν20 | 1295.4158 | 87.1684 |
| ν21 | 1330.3239 | 15.0247 | ν21 | 1541.0032 | 9.1736 |
| ν22 | 1614.6397 | 4.6188 | ν22 | 1620.6308 | 1.6121 |
| ν23 | 1697.9048 | 0.5209 | ν23 | 1687.6738 | 40.5108 |
| ν24 | 2292.4535 | 1.8653 | ν24 | 2269.723 | 5.0652 |
| ν25 | 2400.5877 | 4.8348 | ν25 | 2355.3132 | 3.9161 |
| ν26 | 3077.5368 | 8.8106 | ν26 | 2377.6234 | 3.6068 |
| ν27 | 3154.9818 | 9.1273 | ν27 | 3089.8799 | 45.1102 |

|  |  |
| --- | --- |
| 1p5-2,5,5-D3 | 1p9-5,5-D2 |
| Normal modes | Frequency(cm-1) | IR Inten | Normal modes | Frequency(cm-1) | IR Inten |
| ν1 | 172.9109 | 0.4204 | ν1 | 91.5442 | 0.7057 |
| ν2 | 247.7653 | 0.1504 | ν2 | 123.9589 | 2.1195 |
| ν3 | 306.6338 | 8.0232 | ν3 | 247.0728 | 2.0989 |
| ν4 | 446.169 | 0.3378 | ν4 | 332.6026 | 12.1513 |
| ν5 | 530.998 | 15.0858 | ν5 | 473.5985 | 15.3985 |
| ν6 | 600.3228 | 31.9079 | ν6 | 498.3799 | 6.3777 |
| ν7 | 656.8958 | 28.7545 | ν7 | 735.9004 | 27.1257 |
| ν8 | 677.7325 | 13.9815 | ν8 | 772.1917 | 21.5396 |
| ν9 | 747.3948 | 20.131 | ν9 | 876.4893 | 10.8811 |
| ν10 | 799.9163 | 14.8574 | ν10 | 912.1536 | 8.9126 |
| ν11 | 876.5146 | 5.2892 | ν11 | 991.5677 | 12.4253 |
| ν12 | 962.9998 | 8.9558 | ν12 | 1048.6887 | 5.8448 |
| ν13 | 1064.3251 | 6.4665 | ν13 | 1165.8731 | 7.5014 |
| ν14 | 1103.3401 | 6.593 | ν14 | 1281.629 | 1.2132 |
| ν15 | 1254.6653 | 15.5551 | ν15 | 1326.8896 | 0.9825 |
| ν16 | 1458.4873 | 13.9208 | ν16 | 1606.6449 | 2.5162 |
| ν17 | 1655.8295 | 2.0468 | ν17 | 1702.3586 | 336.0996 |
| ν18 | 2266.5015 | 11.3499 | ν18 | 2292.9671 | 4.6572 |
| ν19 | 2362.3166 | 0.9994 | ν19 | 2402.9979 | 3.6525 |
| ν20 | 2369.7369 | 8.2293 | ν20 | 3045.2912 | 22.9295 |
| ν21 | 3043.6356 | 62.5976 | ν21 | 3165.6791 | 5.9189 |

|  |  |  |  |
| --- | --- | --- | --- |
| 1p23-2,2,5,5-D4 |  |  |  |
| Normal modes | Frequency(cm-1) | IR Inten |  |  |  |
| ν1 | 85.2554 | 1.2335 |  |  |  |
| ν2 | 146.0057 | 1.2668 |  |  |  |
| ν3 | 289.0263 | 2.0251 |  |  |  |
| ν4 | 369.9203 | 0.3157 |  |  |  |
| ν5 | 439.4666 | 0.3976 |  |  |  |
| ν6 | 441.7085 | 48.1541 |  |  |  |
| ν7 | 515.5338 | 20.425 |  |  |  |
| ν8 | 621.2 | 6.9238 |  |  |  |
| ν9 | 649.3528 | 35.9591 |  |  |  |
| ν10 | 746.9314 | 2.9158 |  |  |  |
| ν11 | 783.5303 | 0.0448 |  |  |  |
| ν12 | 831.381 | 0.0003 |  |  |  |
| ν13 | 839.0002 | 64.8154 |  |  |  |
| ν14 | 1001.0878 | 4.2231 |  |  |  |
| ν15 | 1062.8499 | 3.5655 |  |  |  |
| ν16 | 1375.1477 | 18.4493 |  |  |  |
| ν17 | 1997.6641 | 578.3201 |  |  |  |
| ν18 | 2214.2469 | 3.7448 |  |  |  |
| ν19 | 2288.706 | 51.1338 |  |  |  |
| ν20 | 2315.0309 | 3.5499 |  |  |  |
| ν21 | 2378.8893 | 0.1917 |  |  |  |