

**Scheme 1.** Molecular structures, electronic ground state wave functions, point groups, and the relative energies of C3H2 (**1**-**3**) and SiC2H2 (**4**-**9**) isomers. Energies are shown in kJ mol-1.



**Scheme 2.** Molecular structures of singlet ethyl­silane­diyl carbene (HCCSiH; X1A1) and triplet propargylene (HCCCH; X3B). Bond angles are presented in degrees, bond lengths are provided in Angstroms.

图表, 直方图

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**Figure 1.** (a) Time-of-flight (TOF) spectra recorded at *m/z* = 54 (C2SiH2+) for reaction of dicarbon (C2;X1Σg+ / a3Πu) with silane (SiH4; X1A1). The open circles are experimental data; the fits in blue and red result from the QCT-based and ‘best fit’ center-of-mass translational energy distributions. (b) Laboratory angular distribution obtained at *m/z* = 54 (C2SiH2+) from the reaction of dicarbon (C2;X1Σg+/a3Πu) with silane (SiH4; X1A1). The circles are experimental data; the fits in blue and red result from the QCT-based and ‘best fit’ center-of-mass translational energy distributions.

图表, 折线图

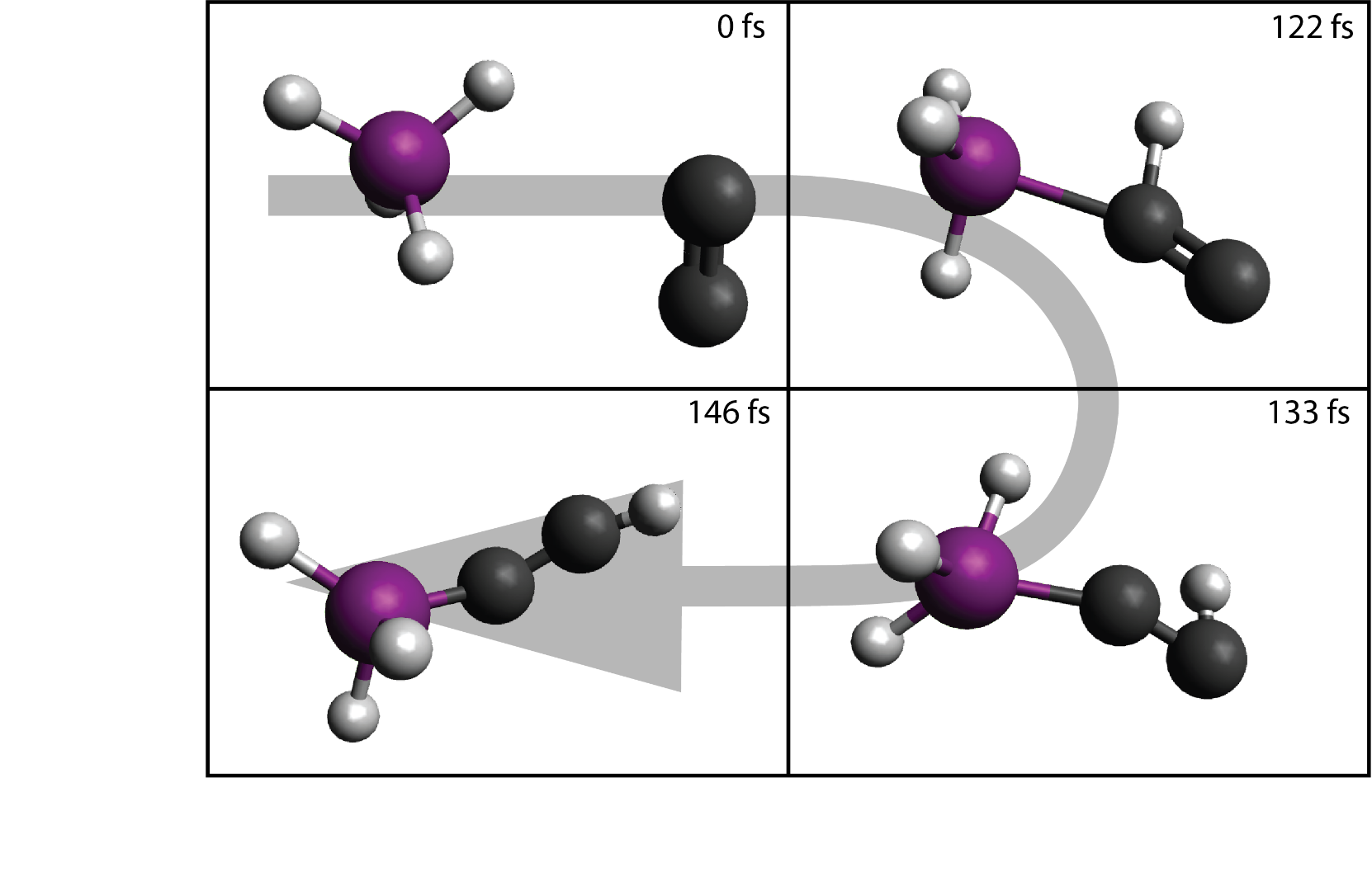
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**Figure 2:** Center-of-mass translational energy (a) and angular (b) flux distributions for the formation of C2SiH2 isomersplus molecular hydrogen via the reaction of dicarbon (C2;X1Σg+/a3Πu) with silane (SiH4; X1A1). The hatched areas define regions of acceptable fits. QCT calculations provide the center-of-mass translational energy distribution color coded in blue.



**Fig. 3.** Potential energy surfaces (PESs) in kJ mol-1 for the reactions of singlet dicarbon with silane alogn with electronic ground state wave functions and point groups of intermediates and products. Atoms are color coded in white (hydrogen), purple (silicon), and black (carbon). Structures along with the vibrational frequencies of the reactants, intermediates, products, and transition states are compiled in the Supplementary Material (Table S2).

a)



b)

A picture containing accessory, necklet

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**Fig. 4.** Snapshots along the reaction coordinate for a) an initial barrierless 1,1-insertion of singlet dicarbon into a silicon – hydrogen bond of silane followed by hydrogen migration leading to the 3-sila-methyl­acetylene (HCCSiH3) intermediate [i1] and b) a hydrogen abstraction leading to the ethynyl and silyl radical pair followed by radical-radical recombination to 3-sila-methyl­acetylene (HCCSiH3) intermediate [i1].