

FTIR OBSERVATION VIBRATIONAL FUNDAMENTALS OF SiCH AND H₂SiC₂H IN SOLID Ar

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Fourier transform infrared studies have resulted in the first observation of vibrational spectra of the linear SiCH and non-planar H₂SiCCH radicals produced by trapping the products of the vacuum ultraviolet photolysis of a mixture of SiH₄ silane, and C₂H₂ acetylene, in an Ar matrix at about 10 K. The silicon-carbon stretching mode $\nu_1(\sigma)$ of SiCH has been observed at 1010.4 cm⁻¹. Two vibrational fundamentals of H₂SiC₂H have been identified, the $\nu_3(a')$, silicon-carbon stretching mode at 2055.6 cm⁻¹ and the $\nu_4(a')$, hydrogen-silicon bending mode at 926.8 cm⁻¹. The results of extensive measurements of D and ¹³C isotopic shifts are in good agreement with the predictions of coupled cluster ab initio calculations performed at the CCSD(T)/6-31G** level and confirm the proposed identifications.

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