FTIR OBSERVATION VIBRATIONAL FUNDAMENTALS OF SiCH AND H_2SiC_2H 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 H_2SiCCH radicals produced by trapping the products of the vacuum ultraviolet photolysis of a mixture of SiH_4 silane, and C_2H_2 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 H_2SiC_2H have been identified, the ν_3(a'), silicon-carbon stretching mode at 2055.6 cm^{-1} and the ν_4(a'), hydrogen-silicon bending mode at 926.8 cm^{-1}. The results of extensive measurements of D and ^{13}C 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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