FIRST OBSERVATION OF A VIBRATIONAL FUNDAMENTAL OF SiC_6Si TRAPPED IN SOLID Ar

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We report here the first results from a Fourier transform infrared (FTIR) and density functional theory (DFT) study on SiC_6Si, which follows earlier investigations of the SiC_nSi (n = 3, 4) chains. The new molecule has been produced by ablating a rod made of silicon and graphite powder with a Nd:YAG laser and trapping the products in solid Ar at $\sim$15 K. Isotopic shift measurements on FTIR spectra produced using ^{13}C-enriched rods combined with DFT calculations have resulted in the assignment of the most intense infrared active mode, $\nu_1(\sigma)$ = 1848.2 cm^{-1} of linear SiC_6Si. A new isotopic perturbation model (IPM) has been developed to investigate the isotopic vibrational spectrum that is complicated by mode mixing. This is part of an effort directed toward understanding the structures and bonding of silicon-carbon molecules and may help in identifying SiC_6Si in circumstellar and interstellar environments.