VIBRATIONAL SPECTRA OF A HEXA-ATOMIC SILICON-CARBON CLUSTER: LINEAR SiC_4Si [a]

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Ongoing Fourier transform infrared investigations of the spectra and structures of silicon-carbon clusters trapped in Ar at 10 K, have resulted in the observation of the first six-member cluster, Si_2C_4 cluster. Two vibrational fundamentals of the linear SiC_4Si structure have been assigned, the C=C stretching mode $\nu_4(\sigma_u) = 1807.4$ cm^{-1}, and the Si-C stretching mode $\nu_5(\sigma_u) = 719.1$ cm^{-1}. The measured frequencies, relative intensities, and ^{13}C and ^{29,30}Si isotopic shifts are in very good agreement with the predictions of DFT calculations and confirm the previously predicted, linear symmetric geometry for the ground state of SiC_4Si.

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