

Abstract Submitted
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FTIR Argon Matrix and DFT Study of the Vibrational Spectrum of SiC₅¹ T.H. LE, W.R.M. GRAHAM, Texas Christian University, TCU MOLECULAR PHYSICS LAB TEAM — This is the first Fourier transform infrared (FTIR) study on SiC₅, which is a part of ongoing FTIR and density functional theory (DFT) research, investigating the structures and vibrations of silicon-carbon molecules. Vibrational spectra of SiC₅ were obtained by Nd:YAG laser ablation of a sintered rod, made of ¹³C-enriched graphite and silicon, and trapping the resulting vapor in solid Ar at ~15 K. The $\nu_4(\sigma_u)$ asymmetric stretching fundamental of SiC₅ has been observed at $936.9 \pm 0.2 \text{ cm}^{-1}$. The measured isotopic shifts are in good agreement with the predictions of DFT calculations. This information will help in identifying SiC₅ in circumstellar and interstellar environments. Also, it has potential applications for optoelectronic and semi-conductor devices.

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