FTIR ISOTOPIC AND DFT STUDIES OF SiC_5 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_5. This species 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. In the only previous observation of SiC_5, McCarthy *et al*. reported the microwave rotational spectrum[a]. In the present work, extensive FTIR measurements of vibrational frequencies and isotopic shifts from ^{13}C enrichment and the naturally occurring ^{29,30}Si isotopes have been compared with the predictions of density functional theory calculations at the B3LYP/cc-pVDZ level. The excellent agreement between experiment and theory has enabled the assignment of the $\nu_4(\sigma)$ fundamental of linear SiC_5 at 936.9 $\pm$ 0.2 cm^{-1}. This information may help in identifying SiC_5 in circumstellar and interstellar environments.

[a] M.C. McCarthy, A.J. Apponi, C.A. Gottlieb, and P. Thaddeus, *Astrophys. J.* **538**, 766 (2000)