FTIR AND DFT STUDY OF THE VIBRATIONAL SPECTRUM OF SiC_5 TRAPPED IN SOLID Ar

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This paper follows preliminary results on the SiC_5 molecule presented earlier. An absorption at 936.9 ± 0.2 cm^{-1} has been identified as the $\nu_4(\sigma)$ Si-C stretching fundamental of linear SiC_5. Its assignment has been confirmed by the close agreement between DFT predicted and observed ^{13}C isotopic shifts. DFT-B3LYP calculations predict that two other C-C fundamentals, $\nu_1(\sigma)$ and $\nu_2(\sigma)$ of SiC_5 should have intensities 10 to 15 times stronger than $\nu_4(\sigma)$, but would appear in the C-C stretching frequency regions.
Refinements of the Si-C laser ablation techniques have helped to reveal the isotopic ^{13}C shifts for two additional absorptions at 2045.0 and 1992.9 cm^{-1}. Comparison of their observed isotopic shifts with the predictions of DFT calculations at the MPW1PW91/6-311+G(3fd) level have led to their assignment to the $\nu_1(\sigma)$ and $\nu_2(\sigma)$ fundamentals of SiC_5.