

## FTIR AND DFT STUDY OF THE VIBRATIONAL SPECTRUM OF SiC<sub>5</sub> TRAPPED IN SOLID Ar

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This paper follows preliminary results on the SiC<sub>5</sub> molecule presented earlier. An absorption at  $936.9 \pm 0.2 \text{ cm}^{-1}$  has been identified as the  $\nu_4(\sigma)$  Si-C stretching fundamental of linear SiC<sub>5</sub>. Its assignment has been confirmed by the close agreement between DFT predicted and observed <sup>13</sup>C isotopic shifts. DFT-B3LYP calculations predict that two other C-C fundamentals,  $\nu_1(\sigma)$  and  $\nu_2(\sigma)$  of SiC<sub>5</sub> 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 <sup>13</sup>C shifts for two additional absorptions at 2045.0 and 1992.9  $\text{cm}^{-1}$ . 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<sub>5</sub>.