FTIR MATRIX AND DFT STUDY OF THE VIBRATIONAL SPECTRUM OF NiC_3Ni

R. E. KINZER, JR., C. M. L. RITTBY, and W. R. M. GRAHAM, *Department of Physics and Astronomy, Texas Christian University, Fort Worth, TX 76129*.

This study of NiC_3Ni is part of continuing Fourier transform infrared (FTIR) and density functional theory (DFT) research investigating the structures and vibrations of small transition-metal carbide clusters. These studies are motivated by the potential for identifying metal carbide species in astrophysical environments and interest in understanding their role in the formation and bonding mechanisms of larger transition-metal carbide structures such as metallocarbohedrenes. FTIR spectra of NiC_3Ni were obtained by trapping the vapors produced during dual ablation of ^{13}C-enriched graphite and Ni rods with Nd:YAG lasers in solid Ar at $\sim$10 K. An asymmetric carbon stretching mode of NiC_3Ni has been observed at $1950.8 \pm 0.2\ \mathrm{cm}^{-1}$. The measured isotopic shifts are in good agreement with shifts calculated using DFT simulations. Although other small nickel-carbon clusters have been the subject of considerable theoretical research[a], this is the first report on NiC_3Ni.

[a] R. C. Longo, M. M. G. Alemany, B. Fernández, and L. J. Gallego, *Phys. Rev. B* **68**, 167401 (2003).