FTIR MATRIX AND DFT STUDY OF THE VIBRATIONAL SPECTRUM OF CYCLIC ScC_3

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This report on the vibrational spectrum of ScC_3 is part of a continuing research project investigating the structures and infrared spectra of small, novel transition-metal carbide clusters. This study is motivated by the potential for observation of such clusters in astrophysical environments and the possible insight they may provide in understanding the structures and bonding mechanisms of larger transition-metal carbide clusters such as metallocarbohedrenes. FTIR spectra of ScC_3 were obtained by trapping the vapors produced by the simultaneous ablation of Sc and ^{13}C-enriched graphite rods with Nd:YAG lasers in solid Ar at $\sim$10 K and annealing at temperatures $\sim$25 - 30 K. Three vibrational fundamentals including the $\nu_5(b_2)$ = 1478.0 cm^{-1} asymmetric carbon stretch, the $\nu_3(a_1)$ = 557.0 cm^{-1} symmetric metal-carbon stretch, and the $\nu_1(a_1)$ = 1190.7 cm^{-1} symmetric carbon stretch have been observed. The measured isotopic spectra are in good agreement with DFT-B3LYP simulated spectra.