FTIR OBSERVATION AND DFT STUDY OF CoC_3 TRAPPED IN SOLID Ar

SARAH A. BATES, J. A. RHODES, C. M. L. RITTBY, and W. R. M. GRAHAM, *Department of Physics and Astronomy, Texas Christian University, Fort Worth, TX 76129*.

Fourier transform infrared (FTIR) and density functional theory (DFT) isotopic studies have been initiated on cobalt-carbon species and have resulted in the detection of linear CoC_3. The CoC_3 chain was produced by the dual laser ablation of carbon and cobalt rods, followed by trapping the products in solid Ar at $\sim$10 K. FTIR measurements of ^{13}C isotopic shifts are in good agreement with DFT predictions using both the BPW91 and B3LYP functionals with a 6-311+G(3*df*) basis set, confirming the assignment of the $\nu_1(\sigma)$ fundamental of linear CoC_3 at 1918.2 cm^{-1}.