FTIR ISOTOPIC AND DFT STUDIES OF TRANSITION METAL-CARBON CLUSTERS CONDENSED IN SOLID ARGON: CrC_3

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We report here the first results from Fourier transform infrared (FTIR) and density functional theory (DFT) studies that have been initiated on the structures and vibrational fundamentals of transition metal-carbon clusters, including chromium-carbon (Cr_nC_m) species. CrC_3 has been produced by ablating carbon and chromium rods with a Nd:YAG laser and trapping the products in solid Ar at $\sim$10 K. Earlier gas phase work using photoelectron spectroscopy and DFT calculations had given evidence of both C_{2v} (fan-shaped) and linear isomers for CrC_3.[a] In the present work, extensive FTIR measurements of vibrational frequencies and ^{13}C isotopic shifts measurements compared with the predictions of DFT calculations at the B3LYP/6-311G+(3*df*) level confirm the assignment of the $\nu_1(\sigma)$ fundamental of the linear isomer of CrC_3 at 1789.5 cm^{-1}.

[a]H. -J. Zhai, L. -S. Wang, P. Jena, G. L. Gustev, and C. W. Bauschlicher, Jr., *J. Chem. Phys.* **120**, 8996 (2004).