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FTIR Isotopic Study of the $\nu_1(\sigma)$ Stretching Mode of Linear CrC_3 Condensed in Solid Ar S.A. BATES, C.M.L. RITTBY, W.R.M. GRAHAM, Texas Christian University — Earlier gas phase investigations of chromium-carbon species using photoelectron spectroscopy (PES) and density functional theory (DFT) calculations have shown the existence of both the C_{2v} (fan-shaped) and linear isomers of CrC_3 .¹ We report the first results from Fourier transform infrared (FTIR) spectroscopic studies on CrC_3 , produced by Nd:YAG laser ablation of carbon and chromium rods and trapping the products in solid Ar at ~ 10 K.² Extensive ^{13}C isotopic shift measurements and predictions from DFT calculations at the B3LYP/6-311G+(3df) level show that linear CrC_3 is the ground state isomer and enables the assignment of its $\nu_1(\sigma)$ fundamental at 1789.5 cm^{-1} .

¹H. -J. Zhai, L. -S. Wang, P. Jena, G. L. Gustev, and C. W. Bauschlicher, Jr., *J. Chem. Phys.* **120**, 8996 (2004).

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Sarah Bates
Texas Christian University

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