MATRIX ISOLATION FTIR SPECTROSCOPIC AND DFT STUDIES OF MnC_3

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This study on MnC_3 is part of an ongoing project investigation of the structures and vibrations of small metal-carbon clusters using Fourier transform infrared (FTIR) spectroscopy and density functional theory (DFT). These species are of interest as potential species in astronomical environments and for understanding the structure and bonding of larger metal-carbide molecules such as metallocarbohedrenes. MnC_3 was produced by trapping the products from the dual laser Nd-YAG lased ablation of carbon and manganese rods in solid Ar at $\sim$12 K. Fourier transform infrared measurements of frequencies and ^{13}C isotopic shifts were compared with the predictions of density functional theory calculations performed for three possible structures: two cyclic isomers with transannular C-C or C-Mn bonds and an asymmetric linear form. Based on this analysis the asymmetric stretching fundamental $\nu_1(\sigma)$ has been identified at 1846.9 cm^{-1}. This is the first optical detection of any isomer of MnC_3. A previous study by photoelectron spectroscopy reported evidence for the cyclic isomer with transannular Mn-C stretch based on preliminary DFT calculations[a]. The results of calculations performed in conjunction with the present work will also be reported.

[a] L. S. Wang and X. Li *J. Chem. Phys.* **112**(8), 22 February 2000.