Abstract Submitted
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Structures and Vibrational Spectra of Potential Astrophysical Molecules: MnC_3 MICHELINE BEJJANI, MAGNUS RITTBY, WILLIAM GRAHAM, Texas Christian University — 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 circumstellar shells or other 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 ∼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 [1] reported evidence for the cyclic isomer with transannular Mn-C stretch based on preliminary DFT calculations. The results of calculations performed in conjunction with the present work will also be reported.

[1] L. S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

Micheline Bejjani
Texas Christian University

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