

Abstract Submitted  
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**FTIR Matrix Study of Transition-Metal Carbon Clusters and Potential Circumstellar Molecules:  $\text{TiC}_3$**  R.E. KINZER, JR., C.M.L. RITTBY, W.R.M. GRAHAM, Texas Christian University — Results will be presented of recently initiated studies on the structures and infrared spectra of transition metal-carbon clusters that may be of interest in circumstellar shells or other astrophysical environments. Such clusters are also of interest as fundamental building blocks for larger metal-carbon structures, such as metallocarbohedrenes. The FTIR (Fourier transform infrared) spectrum of  $\text{TiC}_3$  was observed by trapping the vapors produced during dual Nd:YAG laser ablation of Ti and C rods in solid Ar at  $\sim 10$  K. Measurements of frequencies and  $^{13}\text{C}$  isotopic shifts have enabled the identification of the fan-like ( $C_{2v}$ ) isomer of  $\text{TiC}_3$  with vibrational fundamentals  $\nu_3(a_1) = 624.3$  and  $\nu_5(b_2) = 1484.2 \text{ cm}^{-1}$ . The results are in good agreement with the predictions of DFT calculations at the B3LYP/6-311G(3*df*, 3*pd*) level. The observed  $C_{2v}$  structure is also consistent with the results from an earlier photoelectron spectroscopy study.

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