FTIR MATRIX STUDY OF POTENTIAL CIRCUMSTELLAR MOLECULES: TiC_3

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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. The FTIR (Fourier transform infrared) spectrum of TiC_3 was observed by trapping the vapor produced during dual Nd:YAG laser ablation of Ti and C rods in solid Ar at $\sim$10 K. Measurements of frequencies and ^{13}C isotopic shifts have enabled the identification of the fan-like (C_{2v}) isomer of TiC_3 with vibrational fundamentals $\nu_3(a_1)$ = 624.3 and $\nu_5(b_2)$ = 1484.2 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.[a]

[a]X. B. Wang, C. F. Ding, L. S. Wang, *J. Phys. Chem. A* **101**, 7699 (1997).