FTIR AND DFT STUDIES OF THE MgC_3^- ANION IN SOLID Ar

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This study on MgC_3^- anion is part of an ongoing investigation of the structures and vibrational fundamentals of small metal-carbon clusters using Fourier transform infrared (FTIR) spectroscopy and density functional theory (DFT). In part, these studies are motivated by the potential presence of small metal carbide molecules in astronomical environments. Binary carbon compounds containing silicon and sulfur, including SiC_2, SiC_3, and SC_3, as well as metal-containg molecules such as MgCN and MgCN have already been detected in interstellar space and circumstellars shells. In the present work, the linear MgC_3^- was produced by trapping the products from the dual laser Nd-YAG laser ablation of carbon and magnesium rods in solid Ar at $\sim$12 K. Measurements of ^{13}C isotopic shifts confirm the identification of the $\nu_1(\sigma)$ vibrational fundamental at 1797.5 cm^{-1}. A second fundamental $\nu_2(\sigma)$, has been tentatively identified at 1190.1 cm^{-1}. The results are in very good agreement with the predictions of density functional theory calculations using the B3LYP functional with both the 6-311+G(d) and the cc-pVDZ basis sets. This is the first optical detection of the linear isomer of MgC_3^-.