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Vibrational Spectroscopy and Structures of Novel Metal-Carbon Species of Astrophysical Interest MICHELINE BEJJANI, WILLIAM GRAHAM, MAGNUS RITTBY, Texas Christian University — This study on metal-carbon molecules is part of an ongoing investigation of the structures and vibrational frequencies of small metal carbide clusters using Fourier transform infrared spectroscopy (FTIR) and density functional theory (DFT). These studies are motivated by the potential presence of small metal carbide molecules in astrophysical environments. Binary carbon compounds containing silicon and sulfur, including SiC_2 , SiC_3 , and SC_3 , have been observed in interstellar space and circumstellar shells. In addition several metal-containing molecules, such as MgCN and MgNC have also been detected. Hence, metal carbides have been suggested as possible interstellar molecules although a lack of information on their spectral properties may so far have prevented their detection. Recent studies by this laboratory on the infrared spectroscopy of matrix-isolated metal tricarbide clusters, such as fanlike TiC_3 and ScC_3 , linear CrC_3 and CoC_3 and floppy NiC_3Ni have begun to provide some of this information. Here, we report the structures and vibrational spectra of MnC_3 , ZnC_3 and MgC_3^- .

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