NEW METAL DICARBIDES IN THE LABORATORY AND IN SPACE

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We present a joint laboratory, theoretical, and astronomical study of several new metal-carbon clusters including the alkaline earth metal-bearing molecules MgC_2, CaC_2, and SrC_2, as well as the closely related rare earth molecule YbC_2. We have synthesized these species in the laboratory with a laser-ablation supersonic expansion source and detected their rotational spectra at high resolution with cavity Fourier transform microwave spectroscopy. Combining extensive isotopic measurements with highly accurate *ab initio* rovibrational calculations, we have derived their precise semi-experimental equilibrium geometries, which are all T-shaped with highly ionic metal-carbon bonds. Our measured laboratory rest frequencies have enabled the identification of MgC_2 and CaC_2 as the carriers of several strong, previously unassigned radio emission lines in the circumstellar envelope of the well known evolved carbon-rich star IRC+10216. These laboratory and astronomical discoveries yield fundamental insights into the chemical structure and bonding of s- and f-block metal compounds, and place critical new constraints on the postulated astrochemical pathways that incorporate metal atoms into complex polyatomic molecules. Our work suggests that larger metal-carbon clusters may now be detectable in the laboratory and in circumstellar environments, providing a new probe of the formation of refractory metal-carbon particles.