

UNRAVELING THE COMPLEX NEAR-UV SPECTRUM OF Si₂C

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Though it has yet to be detected in space, there is good reason to believe that the disilicon carbide molecule, Si₂C, is an abundant constituent of circumstellar shells such as IRC+10216, in which the isovalent ionic ring SiC₂ is highly conspicuous. Si₂C exhibits a surprisingly complicated R2C2PI spectrum, which EOM-CCSD calculations indicate arises from a bent-to-linear transition involving several interacting electronic states in the region of vertical excitation. Some of the observed spectral features show well-resolved emission spectra when probed by LIF/DF, yielding vibrational frequencies in excellent agreement with *ab initio* and matrix IR studies of the ground electronic state. Partially resolved rotational structure for these bands, which appear to be dominated by a vibronically allowed transition to a dark *A*₂ state, suggests a ground state bond angle significantly larger than predicted by theory. Owing to the presence of overlapping, unresolved bands, in addition to spectral contamination from Si₂ and SiC, further experimental characterization would appear ideally suited to a two-dimensional fluorescence approach.