HIGH RESOLUTION INFRARED SPECTROSCOPY AND SEMI-EXPERIMENTAL STRUCTURES OF Si_2C_3 AND Ge_2C_3

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Molecular species of group 14 elements e.g. carbon, silicon, and germanium are well suited to study cumulenic bond properties and to compare experimental results with high level quantum chemical calculations. In our recent investigation of SiC_3Si and GeC_3Ge, a high resolution laser spectrometer has been used to record rotationally resolved spectra of selected isotopologues at 5 μm.

We derived semi-empirical values for Si-C and Ge-C bond distances based on spectroscopic data and corresponding zero-point vibrational corrections calculated at the CCSD(T)/cc-pVXZ level of theory (with X = T and Q). Comparison of semi-empirical structural parameters with those from quantum chemical calculations reveals very good agreement for both molecules. Relativistic effects are found negligible for SiC_3Si and small for GeC_3Ge.