A THEORETICAL INVESTIGATION OF THE SILICON-CARBON CHAIN MOLECULE SiC_8

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Large-scale coupled cluster calculations have been carried out for linear SiC_8, a molecule of interest to astrochemistry. An accurate equilibrium structure has been established and a large equilibrium dipole moment of μ_e = -9.96 D is predicted, where the positive end of the dipole is located at the silicon site. Most promising for future detection by infrared spectroscopy are the stretching vibrations at 1973 and 2103 cm^{-1} with absolute intensities of 6662 and 3699 km mol^{-1}, respectively. The lowest bending vibration has a harmonic wavenumber of 38 cm^{-1}. The collinear fragmentation process $SiC_8 \rightarrow SiC_6 + C_2$ has been investigated in detail and the corresponding dissociation energy is predicted to be D_0 = 568 kJ mol^{-1}.