SPECTROSCOPIC OBSERVATION OF CS_2 DIMER

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Infrared spectra of the CS_2 dimer are observed in the region of the CS_2 ν_3 fundamental band ($\sim$ 1535 cm^{-1}) using a tuneable diode laser spectrometer. The weakly-bound complex is formed in a pulsed supersonic slit-jet expansion of a dilute gas mixture of carbon disulfide in helium. Contrary to the planar slipped-parallel geometry previously observed for $(CO_2)_2$, $(N_2O)_2$ and $(OCS)_2$, the CS_2 dimer exhibits a cross-shaped structure with D_{2d} symmetry. Two bands were observed and analyzed: the fundamental (C–S asymmetric stretch) and a combination involving this mode plus an intermolecular vibration. In both cases, the rotational structure corresponds to a perpendicular ($\Delta K = \pm 1$) band of a symmetric rotor molecule. The intermolecular center of mass separation (C–C distance) is determined to be 3.539(7) Å. Thanks to symmetry, this is the only parameter required to characterize the structure, if the monomer geometry is assumed to remain unchanged in the dimer. From the band centers of the fundamental and combination band an intermolecular frequency of 10.96 cm^{-1} is obtained, which we assign as the torsional bending mode. This constitutes the first high resolution spectroscopic investigation of CS_2 dimer.