INFRARED SPECTRA OF CS₂ TRIMER: OBSERVATION OF AN ISOMER WITH D₃ SYMMETRY

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Infrared spectra of carbon disulfide trimer formed in a pulsed supersonic slit-jet expansion are obtained via direct absorption of a tuneable diode laser in the region of the CS₂ ν₃ fundamental band (~1535 cm⁻¹). Two bands sharing the same lower state were assigned to (C₃²S₂)₃. These correspond to the two infrared active vibrations (a parallel and a perpendicular band) of the constituent CS₂ asymmetric stretches. The weaker perpendicular band is centered at 1524.613 cm⁻¹. It is shifted by −10.74 cm⁻¹ with respect to the free CS₂ monomer. The parallel band which is significantly stronger is centered at 1545.669 cm⁻¹. It has a vibrational shift of +10.31 cm⁻¹. The transitions with K ≠ 3n and those with J = odd and K = 0 in the ground state are absent in both bands. This rigorously establishes that this isomer of carbon disulfide trimer has D₃ symmetry. Thanks to the symmetry, only two parameters, the C-C distance and the angle between a monomer axis and the plane containing the C atoms, are required to fully define the structure of the trimer. These were determined to be 3.811 Å and 61.8°, respectively. In addition, a parallel band corresponding to a single ³⁴S substitution was observed around 1544.46 cm⁻¹. Results from this band are in complete agreement with those of the two bands for (C₃²S₂)₃.