INFRARED SPECTRA OF CS_2 TRIMER: OBSERVATION OF AN ISOMER WITH D_3 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 CS_2 ν_3 fundamental band ($\sim$ 1535 cm^{-1}). Two bands sharing the same lower state were assigned to $(C^{32}S_2)_3$. These correspond to the two infrared active vibrations (a parallel and a perpendicular band) of the constituent CS_2 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 CS_2 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 $K \neq 3n$ 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 D_3 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 ^{34}S substitution was observed around 1544.46 cm^{-1}. Results from this band are in complete agreement with those of the two bands for $(C^{32}S_2)_3$.