

## INFRARED SPECTRA OF CS<sub>2</sub> TRIMER: OBSERVATION OF AN ISOMER WITH D<sub>3</sub> SYMMETRY

M. REZAEI, J. NOROOZ OLIAEE, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada*; A.R.W. MCKELLAR, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON K1A 0R6, Canada*.

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<sub>2</sub>  $\nu_3$  fundamental band ( $\sim 1535$  cm<sup>-1</sup>). Two bands sharing the same lower state were assigned to (C<sup>32</sup>S<sub>2</sub>)<sub>3</sub>. These correspond to the two infrared active vibrations (a parallel and a perpendicular band) of the constituent CS<sub>2</sub> asymmetric stretches. The weaker perpendicular band is centered at 1524.613 cm<sup>-1</sup>. It is shifted by  $-10.74$  cm<sup>-1</sup> with respect to the free CS<sub>2</sub> monomer. The parallel band which is significantly stronger is centered at 1545.669 cm<sup>-1</sup>. It has a vibrational shift of  $+10.31$  cm<sup>-1</sup>. The transitions with  $K \neq 3n$  and those with  $J = \text{odd}$  and  $K = 0$  in the ground state are absent in both bands. This rigorously establishes that this isomer of carbon disulfide trimer has D<sub>3</sub> 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 <sup>34</sup>S substitution was observed around 1544.46 cm<sup>-1</sup>. Results from this band are in complete agreement with those of the two bands for (C<sup>32</sup>S<sub>2</sub>)<sub>3</sub>.