COMBINATION BANDS OF THE NONPOLAR OCS DIMER INVOLVING INTERMOLECULAR MODES

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Spectra of the nonpolar carbonyl sulfide in the region of the OCS ν_1 fundamental band were observed in a supersonic slit-jet apparatus. The expansion gas was probed using radiation from a tunable diode laser employed in a rapid-scan signal averaging mode. Three bands centered at 2085.906, 2103.504, and 2114.979 cm^{-1} were observed and anlysed. The rotational assignment and fitting of the bands were made by fixing the lower state parameters to those for the ground state of nonpolar $(OCS)_2$, thus confirming that they were indeed combination bands of the of the most stable isomer of OCS dimer. The band centered at 2085.906 cm^{-1} is a combination of the forbidden A_g intramolecular mode plus the geared bend intermolecular mode and that centered at 2114.979 cm^{-1} is a combination of the allowed B_u intramolecular mode plus the intermolecular van der Waals stretch. The combination at 2103.504 cm^{-1} can be assigned as a band whose upper state involves four quanta of the intramolecular bend or the B_u intramolecular mode plus two quanta of the intermolecular torsional mode. Isotopic work is needed to conclusively identify the vibrational assignment of this band. Our experimental frequencies for the geared bend and van der Waals modes are in good agreement with a recent high level ab initio calculation by Brown et al. [a]

[a] J. Brown, Xiao-Gang Wang, T. Carrington Jr. and Richard Dawes, Journal of Chemical Physics, submitted.