HIGH RESOLUTION FTIR SPECTRA OF METHYL NITRITE AND ASSIGNMENT OF THE ν_8 FUNDAMENTAL OF THE CIS CONFORMER

LISA M. GOSS, *Department of Chemistry, Idaho State University, Campus Box 8023, Pocatello ID, 83209*; THOMAS A. BLAKE, *Pacific Northwest National Laboratory, P. O. Box 999, Mail Stop K8-88, Richland, WA 99352*.

The infrared spectrum of gas phase methyl nitrite (CH_3ONO) has been recorded at high resolution between 600 and 4000 cm^{-1}. The conformational doublets due to the cis and trans conformers are clearly separated in a number of the fundamentals. Previous work in the microwave has established that the barrier to rotation of the methyl group in the trans form is very low[a] and the infrared bands observed in this study are very congested. The barrier in the cis conformer is much higher[b]. The ν_8 at 841 cm^{-1} was assigned by previous workers to the N-O stretch of the cis conformer[c] and is partially overlapped by the ν_8 of the trans conformer. In this study, spectra taken at 0.0015 cm^{-1} resolution on the PNNL IFS120/HR in a 20 cm cell were used to assign more than 800 A-type rovibrational lines of the cis ν_8 between 815 and 865 cm^{-1}.

[a]Turner, P. H., et al., J. Phys. Chem. 83 (11), 1473 1979.
[b]Ghosh, P. N., et al., Chem. Phys. 53 (1-2), 39 1980.
[c]Stidham, H. D., et al. J. Raman Spec. 21 (1-2), 615 1990; da Silva, J. B. P., et al. J. Molec. Struct. 375 (1/2), 153 1996; and references therein.