

ROVIBRATIONAL INTERACTIONS IN THE GROUND AND TWO LOWEST EXCITED VIBRATIONAL STATES OF METHOXY ISOCYANATE

*Anastasiiia PIENKINA¹, Roman MOTIYENKO¹, Laurent MARGULES¹,
J.-C. GUILLEMIN²*

¹ *Laboratoire PhLAM, UMR 8523 CNRS – Université de Lille 1, Villeneuve d'Asq, France.*

² *Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS - ENSCR, Rennes, France.*

Recent detection of methyl isocyanate (CH_3NCO) in the Orion [1], towards Sgr B2(N) [2] and on the surface of the comet 67P/Churyumov-Gerasimenko [3] motivated us to study another isocyanate, methoxy isocyanate (CH_3ONCO) as a possible candidate molecule for searches in the interstellar clouds. Neither identification or laboratory rotational spectra of CH_3ONCO has been reported up to now. Methoxy isocyanate was synthesized by the flash vacuum pyrolysis of N-Methoxycarbonyl-O-methyl-hydroxylamine (MeOC(O)NHOMe) at a temperature of 800 K. Experimental spectrum of CH_3ONCO was recorded in situ in the millimeter-wave range (75-105 GHz and 150-330 GHz) using Lille's fast-scan fully solid-state DDS spectrometer. The recorded spectrum is strongly perturbed due to the interaction between the overall rotation and the skeletal torsion. Perturbations affect even rotational transitions with low K_a levels of the ground vibrational state, appearing in shifting frequency predictions and intensities distortions of the lines. The interactions are significant due to the relatively small vibrational energy difference (50 cm^{-1}) between the states and different representations of the C_s symmetry point group for the ground (A'), $\nu_{18} = 1$ (A'') and $\nu_{18} = 2$ (A') vibrational states, thus leading to a "ladder" of multiple resonances by means of a-, and b-type Coriolis coupling. The global fit analysis of the rotational spectrum of methoxy isocyanate using Coriolis coupling terms in the ground and two lowest vibrational states ($\nu_{18} = 1$ and $\nu_{18} = 2$) will be presented.

This work was funded by the French ANR under the Contract No. ANR-13-BS05-0008-02 IMOLABS.

[1] J. Cernicharo, N. Marcelino, E. Roueff et al. 2012, ApJ, 759, L43

[2] D. T. Halfen, V. V. Ilyushin, & L. M. Ziurys, 2015, ApJ, 812, L5

[3] F. Goesmann, H. Rosenbauer, J. H. Bredehöft et al. 2015, Science, 349.6247, aab0689