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

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Recent detection of methyl isocyanate ($\mathrm{CH_3NCO}$) in the Orion[a], towards Sgr B2(N)[b] and on the surface of the comet 67P/Churyumov-Gerasimenko[c] motivated us to study another isocyanate, methoxy isocyanate ($\mathrm{CH_3ONCO}$) as a possible candidate molecule for searches in the interstellar clouds. Neither identification or laboratory rotational spectra of $\mathrm{CH_3ONCO}$ 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 $\mathrm{CH_3ONCO}$ 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 $\mathrm{cm^{-1}}$) 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.

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