IR spectroscopy and energetic processing of methyl isocyanate ice

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Methyl isocyanate was recently detected in the interstellar medium [1-2] (the reported detection on comet 67P/CG [3] could not be confirmed[4]). Although it was usually neglected in astrochemical networks, this new evidence fosters new studies on this species. We present here our work on the IR spectra and on the energetic processing of ices of this molecule.

We have recorded in our lab the IR spectra of amorphous CH_3NCO and CD_3NCO obtained by vapor deposition at 20 K. The most intense band corresponds to the NCO asymmetric stretching (ν_a-NCO). It has a characteristic quadruplet structure, usually attributed to the interaction with the CH_3 torsion. CD_3NCO was used to help the spectral assignment. We have also measured the band strengths for the absorptions of CH_3NCO in ice at 20 K.

Since no X-ray structure for crystalline CH_3NCO had been reported, we put forward a tentative theoretical structure, derived taking as a starting point the crystal of isocyanic acid. We have predicted a spectrum for the proposed structure, and compared it with our experimental observation [5] (see Fig. 1).

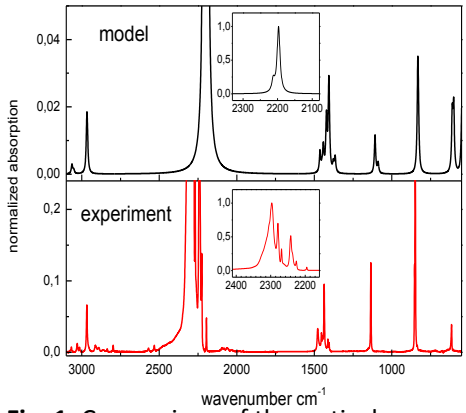

Fig. 1. Comparison of theoretical spectrum of the crystal with experiment.

We have studied the stability of CH_3NCO under heating, UV irradiation with a D_2 lamp (UV photons ≈ 10.3-6.9 eV), and cosmic ray bombardment, simulated with high energy electrons (5 keV) [6]. The samples were either pure CH_3NCO or CH_3NCO diluted in H_2O. Heating of the ices leads to variations in the ν_a-NCO band profile but not to an appreciable depletion of CH_3NCO until H_2O sublimation (beyond T=150 K) and thus rules out hydrolysis in the ice. UV irradiation and electron bombardment at 20 K lead to the destruction of CH_3NCO and to the formation of CO, CO_2 and OCN^- ions in the processed ices.

These results indicate that the lifetime of hypothetical CH_3NCO present in the ice mantels of dust grains in a typical dense cloud might be longer than the cloud's lifetime.

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References

[1] Halfen, D. T., Ilyushin, V.V., & Ziurys, L. M. 2015, ApJ, 812, L5
[2] Cernicharo, J., Kisiel, Z., Tercero, B. et al. 2016, A&A, 587, L4
[3] Goesmann, F., Rosenbauer, H., Brederhöft, J. H. et al. 2015, Sci, 349, aab0689
[4] Altwegg, K., Balsiger, H., Berthelier, J. J., et al. 2017, MNRAS, 469, S130
[5] B. Maté et al. MNRAS 2017, 470, 4222.
[6] B. Maté et al. 2018, A&A, 861:61