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Spectroscopy of 4(5)-Methylimidazole and its Hydrates in He Droplets

F. Grollau¹, J.-M. Mestdagh¹, B. Soep, E. Gloaguen¹, V. Brenner¹, L. Poisson¹, M. Mons¹ and M. Briant^{2*}

* presenter

¹Univ. Paris-Saclay, CEA, CNRS, LIDYL, 91191 Gif-sur-Yvette, France

²marc.briant@cea.fr, Univ. Paris-Saclay, CEA, CNRS, NIMBE, 91191 Gif-sur-Yvette, France

Histidine, one of two amino acids with a tautomeric equilibrium, is both a proton acceptor and a proton donor. It plays therefore an essential role in biological processes where proton transfer is involved (*e.g.* regulation of blood pH). Studies have shown that the tautomeric equilibrium of this molecule is modified by the environment^[1], making its intrinsic properties difficult to obtain experimentally. However, knowledge of these properties is important for a full understanding of the behaviour of this molecule when surrounded. The above-mentioned characteristics are carried by the imidazole ring that constitutes the side chain of histidine. Hence, the 4(5)-methylimidazole (MeIm) (Figure 1) may appear as an adequate model to study these properties specifically.

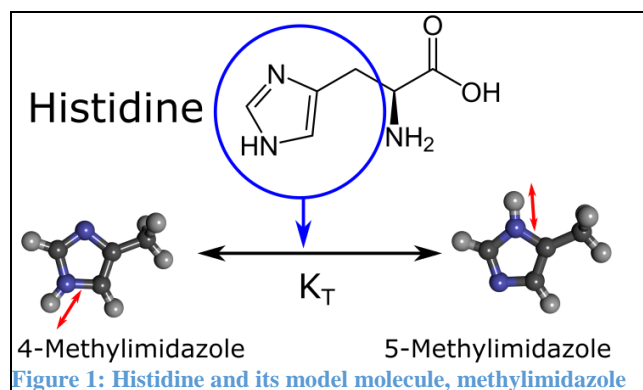


Figure 1: Histidine and its model molecule, methylimidazole

Experimentally, we characterized the tautomers of MeIm and its hydrates by infrared spectroscopy (IR). The Gouttelium setup^[2] was used to record the IR spectra of these species using the "Helium NanoDroplet Isolation" technique^[3]. Helium droplets are cold (0.37 K^[4]), superfluid^[5] and very fragile quantum systems. They thermalize the hosted species and loosely interact with them. This allows obtaining sort of IR

absorption spectra that are close to those expected for the totally isolated molecule. This concerns essentially the vibrational structure of the spectra since the rotational structure is often affected by the presence of the droplet.

We have unambiguously characterized the two MeIm tautomers via the NH stretching whose frequency is very sensitive to the position of the methyl group. The assignment of the observed IR bands to a specific tautomer was done by comparison with DFT-D calculations. The relative intensities between bands allowed us to estimate the tautomerization constant, $K_{5\leftrightarrow 4}(T=43^\circ\text{C}) = 5.3 \pm 0.8$, which yet, was not known precisely. The rotational constants of 4-MeIm in the droplets were determined by the simulation of the spectrum and show a strong rotational interaction with the helium droplet as expected with this type of molecule.

Finally, 4(5)-MeIm-water complexes were formed by the deposition of both species in the helium droplets. Spectra involving the NH stretching of MeIm and the symmetric and asymmetric OH stretching of water will be presented and discussed.

¹ Vila, J. A.; *et al.*, PNAS **2011**, 108 (14), 5602-5607

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