FREE JET ABSORPTION MILLIMETER-WAVE SPECTROSCOPY OF MOLECULES OF BIOLOGICAL INTEREST AND OF THEIR COMPLEXES WITH WATER

W. CAMINATI, P. G. FAVERO, A. MARIS, S. MELANDRI, P. OTTAVIANI, *Dipartimento di Chimica "G.Ciamician", Universita' di Bologna, Via Selmi I-40126, Italy*.

By applying free jet millimeter wave spectroscopy we could study several molecules of biological interest, such as purine.[a] In addition, the rotational spectra of molecular adducts of biological basis with a water molecule have been investigated (those of the three diazines with water:[b] pyrazine-water, pyrimidine-water and pyridazine-water) obtaining detailed information on the shape, energetics and dynamics of the interaction water-biochemical basis, which takes place through a planar O-H—N H-bond. Precise information have been obtained also for another interaction of great relevance in biochemistry, the O-H—O H-bond,[c] from the the rotational spectra of the molecular complexes of water with cyclic ethers and phenols. The interaction energy of this H-bond is ca. 20 kJ/mol. The studies of small oligomers of ethers, stabilized by C-H—O "improper blue shifted" H-bond (interaction energies of ca. 2 kJ/mol), supply also interesting information for the numerous interactions of this kind which take place in the biological systems.

Here some details will be given on the results obtained by our more recent investigations, concerning the pure rotational spectra of: 1) *Lactamide.* Two conformers have been observed, with the relative energies governed by the proton donor/acceptor double role of the peptidic group. 2) *Tyramine.* Four conformational species have been observed. Their relative energies are determined by secondary non bonding interactions. 3) *2-Hydroxy-pyridine/2-pyridone—water.* Only the adduct of pyridone with water has been observed so far, in agreement with the results from rotationally resolved fluorescence excitation spectra.[d] 4) *Dimethyl ether dimer:* stabilized by "improper blue shifted" H-bonds

Advantages and disadvantages with respect to the complimentary technique, molecular beam Fourier transform microwave spectroscopy, will be discussed.

---

[a] W. Caminati, G. Maccaferri, P. G. Favero, and L. B. Favero, *Chem. Phys. Lett.* **251**, 189 (1996).

[b] see, for example, S. Melandri, M. E. Sanz, W. Caminati, P. G. Favero, and Z. Kisiel, *J. Am. Chem. Soc.* **120**, 11504 (1998).

[c] see, for example, W. Caminati, P. Moreschini, I. Rossi, and P. G. Favero, *J. Am. Chem. Soc.* **120**, 11144 (1998).

[d] A. Held and D. W. Pratt, *J. Am. Chem. Soc.* **115**, 9708 (1993).