THE INTERACTIONS OF THE PEPTIDE FUNCTIONAL GROUP WITH WATER: A JET COOLED ROTATIONAL STUDY OF THE FORMAMIDE-$(H_2O)_n$ AND 2-AZETIDINONE-$(H_2O)_n$ (n=1,2) CLUSTERS

JUAN C. LÓPEZ, SUSANA BLANCO, RAQUEL SÁNCHEZ, ALBERTO LESARRI, and JOSÉ L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47005 Valladolid, Spain*.

Microsolvated clusters constitute models that allow the investigation of molecular properties in the transition from isolation to solvation and the understanding of solute-solvent interactions and solvent-enhanced chemical reactivity. In this work we have analyzed the jet-cooled rotational spectra of the formamide-$(H_2O)_n$ and 2-azetidinone-$(H_2O)_n$ (n=1, 2) clusters in order to investigate the diverse hydrogen bond interactions of water with the peptide functional group. Formamide (NH_2–CHO) and 2-azetidinone (C_3H_5NO), a lactam four-membered ring that forms part of penicillin- and cephallosporin-type antibiotics, are two of the most simple molecules carrying a peptide group. A molecular beam Fourier Transform microwave spectrometer[a] equipped with a heating nozzle[b] has been used for this research. We have observed thre 1:1 forms of the formamide-H_2O complex, two 1:1 forms of the 2-azetidinone-H_2O complex and the trimers formamide-$(H_2O)_2$ and 2-azetidinone-$(H_2O)_2$. The most stable conformer of the formamide-H_2O complex, previously observed by Lovas *et al.*,[c] and the most stable form of the 2-azetidinone-H_2O complex are stabilized by two hydrogen bonds O-H$\cdots$O=C and N-H$\cdots$O with water closing a cycle with the peptide functional group. In the second most stable 1:1 conformers water is placed on the other side of the carbonyl group stabilized by O-H$\cdots$O=C hydrogen bonds and by C-H$\cdots$O weak hydrogen bonds. In the third formamide-H_2O form, water is bonded to the amino group by a N-H$\cdots$O hydrogen bond. For the trimers, the two molecules of water close a cycle with the peptide group with three different hydrogen bonds (O-H$\cdots$O=C, O-H$\cdots$O and N-H$\cdots$O). The spectra of the parent and several D/H, $^{15}N/^{14}N$, $^{13}C/^{12}C$ and $^{18}O/^{16}O$ isotopomers have been measured in order to investigate the structures of these clusters.

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[c] F. J. Lovas, R. D. Suenram, G. T. Fraser, C. W. Gillies and J. Zozom, *J. Chem. Phys.*, **88** 722 (1988)