MICROSOLVATION OF BUILDING BLOCKS

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Laser ablation molecular beam Fourier transform microwave spectroscopy LA-MB-FTMW has provided the first observation of the rotational spectra of the glycine-H_2O complex.[a] As a continuation of this work we present the study of monohydrated complexes of alanine, uracil and thymine and the first observations of the dihydrated clusters glycine-$(H_2O)_2$ and alanine-$(H_2O)_2$. For the microsolvated amino acids only the conformer with *cis*-COOH configuration and bifurcated $NH_2\cdots$O=C H-bond has been observed. Both alanine-H_2O and glycine-H_2O have similar shapes: the water molecule being bonded through two O-H$\cdots$O hydrogen bonds to the carboxylic group of the amino acid. The dihydrated clusters have also comparable structures where the two water molecules form a cycle with the COOH group through sequential H-bonds. The rotational spectra of uracyl-H_2O and thymine-H_2O show the same complexity than those of the bare molecules[b,c] due to the hyperfine structure of two quadrupolar ^{14}N atoms. The detected conformers show comparable structures with the water molecule bonded through two N-H$\cdots$O and O-H$\cdots$O=C hydrogen bonds to the N bases. The structure of hydrogen bond has been investigated by isotopic substitution.

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[c] J.C. López, M.I. Peña, M.E. Sanz and J.L. Alonso, *J. Chem. Phys.* 126, 191103 (2007)