THE FORMAMIDE-$(H_2O)_n$ (n=1,2) CLUSTERS BY ROTATIONAL SPECTROSCOPY

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Formamide (NH_2-COH) is the most simple molecule carrying the peptide linkage and its microsolvated clusters can be used to investigate the diverse hydrogen bond interactions of water with this functional group. A molecular beam Fourier Transform microwave spectrometer[a] equipped with a heating nozzle[b] has been used for this research. The most stable conformer of the formamide-H_2O complex, previously observed by Lovas *et al.*,[c] is stabilized by two hydrogen bonds O-H···O=C and N-H···O with water closing a cycle with the peptide functional group. In the present work we have observed two new formamide-H_2O conformers and the trimer formamide-$(H_2O)_2$. In the second most stable 1:1 conformer water is placed on the other side of the carbonyl group stabilized by a O-H···O=C hydrogen bond and by a C-H···O weak hydrogen bond. In the third 1:1 complex, water is bonded to the amino group by a N-H···O hydrogen bond. For the formamide-$(H_2O)_2$ complex the two molecules of water close a cycle with the peptide group with three different hydrogen bonds (O-H···O=C, O-H···O and N-H···O). The rotational spectra of the parent and several D/H, $^{15}N/^{14}N$, $^{13}C/^{12}C$ and $^{18}O/^{16}O$ isotopically substituted species have been measured for the formamide monomer, the most stable conformer of the formamide-H_2O adduct and the formamide-$(H_2O)_2$ complex in order to investigate their structures. High level *ab initio* computations have been performed in order to complement the experimental results.

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[b] S. Blanco, J. C. López, J. L. Alonso, P. Ottaviani and W. Caminati; *J. Chem. Phys.*, **119**, 880 (2003)
[c] F. J. Lovas, R. D. Suenram, G. T. Fraser, C. W. Gillies and J. Zozom, *J. Chem. Phys.*, **88** 722 (1988)