IR-SPECTROSCOPY OF GLYCINE AND ITS COMPLEXES WITH WATER IN HELIUM NANODROPLETS

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Glycine is the smallest amino acid, and therefore it is of special interest as a model and starting point for theoretical and experimental studies. Whereas the crystalline form of glycine consists of zwitterions $NH_3^+ - CH_2 - COO^-$ [a], gas phase glycine is known to exist in the nonionized form $NH_2 - CH_2 - COOH$ [b]. The interaction between glycine and water has been widely studied using a large variety of theoretical methods. Depending on the theoretical level used, a stabilisation of the zwitterionic form is predicted for complexes containing from 2 to 7 water molecules. In low-temperature Ar matrices a set of characteristic IR absorption bands for the zwitterionic form has been observed. The higher stoichiometry complexes (glycine)$\cdots(H_2O)_n$ with n larger than 3 are demonstrated to be zwitterionic H-bonded complexes [c]. The multitude of conformations expected for these glycine-water complexes makes a combination of low temperature and high resolution spectroscopy essential. We want to use the advantages of our experiment to investigate glycine and its complexes with water in helium-nanodroplets at ultracold temperatures in the range from 3000-3800 cm^{-1}. Our measurements were carried out using a high power IR-OPO (cw: 2.7 W) as radiation source and a helium nanodroplet spectrometer. Helium-nanodroplets are formed by expansion of helium at 55 bar through a 5 μm nozzle which is kept at a temperature of 16 K. The status of the project is presented.

[a] P.-G. Jönsson et al., Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem. 28, 1827 (1972)
[b] G. Junk et al., J. Am. Chem. Soc. 85, 839 (1963)
[c] R. Ramaekers et al., J. Chem. Phys., 120 (2004)