AN EXPERIMENTAL SETUP TO STUDY THE INFLUENCE OF HYDRATION ON SMALL CHARGED MOLECULAR SYSTEMS BY ROTATIONALLY RESOLVED VIBRATIONAL SPECTROSCOPY

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Many biomolecules exhibit several structural isomers, which govern their functionality. The structure and thus the function of biomolecules are strongly influenced due to hydration with single water molecules and further by hydration shells.[a] This influence can be observed in different molecular systems e.g. in the change of the selective binding in host-guest complexes involving crown ethers [b], in the influence on the delocalized proton in charged water complexes [c] or in intramolecular vibrational energy redistribution after excitation by photons or collisions. Spectroscopy plays an increasingly important role in the study of structural details and thereby the function in molecular systems. [d] In this contribution an experimental setup to study the structure of small biomolecular ions and the influence of hydration by means of rotationally resolved pre-dissociation spectroscopy will be presented.

The setup consists of a nano-ESI, followed by two skimmers, enabling a gentle transfer into vacuum and avoiding breaking apart of the loosely bound water molecules. Further, the ions are confined in a cryogenic 16-pole wire ion trap, reaching temperatures below 3 K [e], leading to the binding of up to four helium atoms on protonated glycine ions.[f]

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[a] Laage, Chem. Rev. 2017
[b] Glendening, JACS 1999
[c] Tuckerman, Science 1997
[d] Wolk, Acc. Chem. Res. 2014
[e] Geistlinger, Rev. Sci. Instrum. 2021
[f] Geistlinger, J. Mol. Spectrosc. 2021