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Influence of nanohydration on the structure and radiation induced fragmentation of gas-phase biomolecules

Water plays an important role in the structure and properties of biomolecules. For example, hydrophobic interactions provide the dominant force driving protein folding. One native structure of the protein is encoded in the amino acid sequence because of these interactions [1]. Isolation of biomolecules in the gas phase removes all interactions with the solvent, but also enables stepwise control of these interactions by progressively increasing the number of the bound water molecules, ultimately bridging the gap between the gas phase and aqueous conditions. Already a single water molecule can induce significant structural changes in the molecule, such as the location of the protonation site of a small peptide [2]. And it has been shown that the addition of about a dozen water molecules to deprotonated molecules can induce folding, as the hydrogen bond network leads to a decrease in Coulomb repulsion [3] or can be sufficient to protect the molecules from fragmentation under collision-induced dissociation with neutral atoms [4].

Over the last thirty years, there have been massive efforts to develop experimental techniques to study hydrated species in the gas phase using electrospray ionization sources. Already in the late 1990s, John Fenn, the recipient of the Nobel prize for developing the electrospray technique, studied solvated biomolecules with a dedicated source that produced hydrated biomolecules with up to 30 water molecules [5], which has then been further optimized by Nonose et al. to reach hydration with up to 40 water molecules [6]. Based on these earlier developments, we are building a hydration electrospray source and integrate it into our tandem mass spectrometer setup designed for experiments at large photon facilities. I will introduce what we can learn from hydrated species in the gas phase and present the new source we are developing for the controlled production of hydrated (de)protonated species.

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