Theoretical study of solvated peptides

Context:

In the last 20 years, there has been a growing interest for ion-mobility spectrometry (IMS) as a powerful tool to unravel the structure of isolated molecular systems, especially when coupled to mass spectrometry. Experimentally, molecular ions are discriminated by their cross-section of collision with a gas such as helium or nitrogen, and these collision cross-sections (CCS) can be compared to those calculated for given structures. This way, one may further perform experiment on conformer-selected molecular systems by storing and irradiating them in an ion trap by means of synchrotron radiation in the VUV and soft X-ray ranges. VUV and soft X-ray action spectroscopy techniques are powerful methods to investigate the electronic and some aspects of the geometric structure of biomolecules. Combining IMS with mass spectrometry technique will make possible the irradiation of conformer-selected molecules.

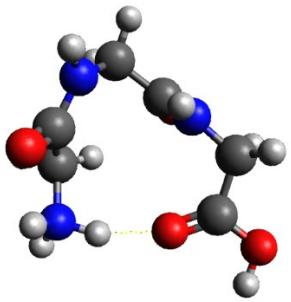
In the thesis of Juliette LEROUX, they will combine both action spectroscopy and structural approaches to investigate radiation-induced processes in conformer-selected biomolecular systems (peptides and proteins), by adding an IMS stage to the already existing tandem mass spectrometer installed in Hamburg, going one step further by making possible the irradiation of conformer-selected biomolecules by synchrotron beams in an ion trap. They will also study the influence of a controlled number of water molecules on the radiation-induced processes in peptides and proteins.

Project:

The protonated triglycine has been studied theoretically and experimentally by many groups mostly to understand its structure (linear or folded) and protonation sites (N-terminus or an amine O) that remains controversial. Adding water molecules can change the structure of the peptide and its protonation site. In this context, the master student will study theoretically two small model protonated peptides : the triglycine (see figure below) and the pentaglycine.

First, the student will have to generate different isomers for the isolated and hydrated peptides (1 to 5 water molecules). This exploration of potential energy surface (PES) will be done using Molecular Dynamics simulations.

In a second step, the student will have to reoptimize these geometries with Density Functional Theory (DFT) calculations. These calculations will be done with ORCA program. For the lowest-isomers the student will calculate infrared spectra to analyse the role of the water environment.



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