PROTON TRANSFER IN NEUTRAL PEPTIDES EXAMINED BY CONFORMATIONAL SPECIFIC IR AND UV SPECTROSCOPY

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The combination of UV and IR spectroscopy offers a powerful probe to study molecular structure and intramolecular interactions. With resonance enhanced multi photon ionization (REMPI), the electronically excited state of biomolecules can be probed. As different conformations have different excited state energies, peaks in the REMPI spectrum can be attributed to different conformations. This allows us to perform conformation specific IR absorption spectroscopy using IR-UV ion-dip spectroscopy (IR-IDS) in the 1800-1000 cm^{-1} region by employing the free electron laser FELIX. IR-IDS in combination with DFT calculations allows us to determine the gas phase conformations of biomolecules. Here, we used these techniques on Z-Glu-OH and Z-Arg-OH to reveal their conformational structure and the possible presence of proton transfer. There is an ongoing debate on the gas phase structure of arginine. Proton transfer has been suggested to occur from the C-terminal COOH group to the guanidium side chain of arginine to form a zwitterion. Moreover, there can be two tautomers of canonical arginine. Here, we will elucidate the gas phase structure of arginine. In order to promote intramolecular proton transfer, we designed a peptide which contains both the most acid (Glu) as well as the most basic residue (Arg): Z-Glu-Arg-NHMe and Z-Glu-Ala$_n$-Arg-NHMe. Here, the occurrence of proton transfer will be probed via the carboxylic acid C=O stretch vibration.