Formation of Phenylalanine-Water-Clusters: gas phase spectra in comparison to theoretical calculations

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We investigated the formation of amino-acid water clusters experimentally by R2PI and IR/UV-double resonance spectroscopy as well as theoretically by means of semiempirical and DFT-D calculations. The latter includes empirical correction terms to adequately describe the effect of dispersion, which influences the relative cluster energies to a non-negligible extent. Amino-acid water clusters with a varying number of water molecules are of general interest to the scientific community, because they open the path to investigate the transition from the neutral to the zwitter-ionic form of the amino acid. Our setup will eventually allow the simultaneous observation of the O-H- and C=O-stretching vibrations of the carboxyl group in a size- and conformer-selective experiment, which will enable us to unambiguously determine the structure and the number of water molecules at the transition point.

The calculations are based on a common scheme, where we randomly generated amino acid conformers with randomly positioned water molecules using a home build program. These randomly generated structures (typically several thousands) are pre-optimized using semiempricial methods. For the most stable structures the geometries, energies and vibrational frequencies are then calculated at the DFT-D level for comparison with experiment.