EFFECTS OF MICROSOLVATION ON A MODEL PEPTIDE CHAIN INVESTIGATED BY IR/UV DOUBLE RESONANCE SPECTROSCOPY

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IR/UV double resonance spectroscopy of gas phase 1:1 complexes of the capped phenylalanine amino acid with water or methanol has been carried out. The IR spectra in the amide NH and water OH stretches spectral region of UV-selected conformations have resolved absorption bands which have been assigned by comparison with scaled harmonic frequency calculations of the most stable conformations optimized at the B97-D/TZVPP level. The effects of solvation on the structural properties have been investigated by comparison with the conformations observed on the isolated capped phenylalanine. The solvation by one molecule turns out to strongly impact the energy landscape by favoring specific folded structures.