

SECONDARY STRUCTURES IN GAS -PHASE MODEL PEPTIDES AS REVEALED BY IR/UV DOUBLE RESONANCE SPECTROSCOPY

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Thanks to progress in computer science, quantum calculations become now feasible on small biomolecules and are often the main source of structural data used to parameterise the interaction potentials in molecular biomodelling. Unfortunately, so far, the experimental gas-phase counterparts of these theoretical studies remain sparse. Our group has started a series of experimental and theoretical studies on protected peptides, which aims at characterising the intrinsic properties of the peptide backbone in terms of hydrogen bonding, under solvent-free conditions to allow an easier comparison to calculations.

The use of simple **protected peptides** (N-acetyl-Phe-NH₂) enables us to focus onto the **local conformational preferences** of the peptide backbone on a phenylalanine (Phe) residue. The study of model tripeptides (N-acetyl-Phe-Xxx-NH₂ or N-acetyl-Xxx-Phe-NH₂, Xxx = Gly, Ala, Val and Pro) enables us to address the issue of the **competition between these local conformational preferences** (on the Phe and Xxx residues) **and secondary structures, which results from H bond bonding between two remote amide bonds.**

The combination of UV data and IR/UV double resonance spectroscopy reveal that, under supersonic beam conditions, only a reduced number of conformations are formed, indicating efficient conformational relaxation processes in these species. The IR spectroscopy in the NH stretch range (3 μ m spectral region) combined with DFT calculations proves to be a very efficient tool to assign the structure of the species populated in terms of intramolecular H-bonding.

Both UV and IR spectroscopic results will be presented on model di-, tri- and tetra- peptides, showing the capability of gas phase experiments to provide precise spectroscopic data upon secondary structures of biology, such as γ -turns, double γ -turns, β -turns and the 3₁₀ helix.