IR-UV spectroscopic studies of a cold peptide ion in the gas phase

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The biological function of proteins is largely determined by the three-dimensional structure they adopt in *vivo*. It is a great challenge for theory to predict this structure which is determined by a delicate interplay between various non-covalent forces. To verify that theoretical models describe the underlying physics correctly, comparison with benchmark experiments is essential, and the most rigorous test is perhaps to compare theoretical and experimental data on small peptides in the gas phase.

Infrared spectroscopy of gas phase biomolecular ions can be used to obtain information on the ion structure (conformation) as the vibrational frequencies are sensitive to the local environment. Here we measure infrared spectra by studying photofragmentation of ions trapped in a linear radiofrequency multipole ion trap [1,2]. Under the experimental conditions multiple structures are present, and furthermore many quantum states are thermally populated if the ions are studied at room temperature, two factors that severely complicate spectral analysis. To eliminate thermal congestion, the ions are cooled to low temperatures (here approximately 10 K) which offers the possibility to obtain conformation-specific infrared spectra by employing IR-UV double resonance techniques [3]. This talk will demonstrate how such conformation-specific spectra can be measured in the gas phase and the results obtained with a peptide consisting of nine amino acids (150 atoms) are presented.

References:
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Invited talk