CONFORMATION-SPECIFIC DOUBLE RESONANCE SPECTROSCOPY OF SYNTHETIC FOLDAMERS, CROWN ETHERS, AND 'BIOLOGICAL WATER' IN THE GAS PHASE: ANOTHER WAY TO LOOK UNDERNEATH THE 1D-IR AND 1D-UV SPECTRA

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While Raman and infrared are powerful vibrational spectroscopy methods, their utility as structural tools in the face of the conformational complexity of a large, flexible biomolecule is limited by the fact that the spectrum contains contributions from an unspecified number of molecular conformations with unknown spectral signatures. This talk will describe a series of double and triple resonance methods which, when applied to jet-cooled isolated molecules or molecular clusters, can provide the infrared and ultraviolet spectral signatures of individual conformations free from interference from one another. Applications will be drawn from several of our recent studies. In particular, the talk will describe recent single-conformation spectra in the near-IR and mid-IR of a series of beta-peptides and alpha-beta peptides, including the innate C=O stretch spectral signatures. The single-conformation IR and UV spectra of benzo-15-crown-5 and its water-containing complexes provide signatures of crown buckling and how the crown adjusts its conformation in order to accept hydrogen bonds from water. The spectroscopic signatures of this bound water will also be described and compared to those of the free water molecule.