CONFORMATION-SPECIFIC INFRARED SPECTROSCOPY OF GAS-PHASE PROTONATED HELICAL PEPTIDES

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Infrared spectroscopy is a powerful probe of molecular structure, especially under conditions of high resolution and when multiple conformations can be separated using double resonance techniques. We use electrospray ionization to generate protonated peptides in the gas phase, and collisionally cool them in a 6 K 22-pole ion trap in order to perform infrared-ultraviolet double resonance spectroscopy. At 10-15 K, even peptides of twelve or more amino acids have vibrationally resolved ultraviolet and infrared spectra, allowing for assignment of N-H and C=O vibrations and identification of the conformations present, particularly when high-level harmonic frequency calculations are feasible. We have recently used these techniques to study a series of helical protonated peptides based on lysine-capped polyalanines, which contain at least one of the three aromatic amino acids as an ultraviolet chromophore. We have observed differences in the number and types of conformations present depending on the chromophore and its location, as well as spectral and conformational differences due to multiple protonation sites.