INFRARED-ULTRAVIOLET DOUBLE RESONANCE SPECTROSCOPY OF COLD BIOMOLECULAR IONS IN THE GAS PHASE

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The use of a nanospray source and a liquid-helium cooled 22-pole ion trap allows us to produce biomolecular ions in the gas phase in sufficient quantities to study them spectroscopically, and at temperatures conducive to obtaining vibrationally resolved spectra. We describe here an infrared-ultraviolet double resonance spectroscopy which relies on changes produced by the absorption of an infrared photon on the subsequent ultraviolet-induced photofragmentation. By recording the infrared-induced changes in the fragment ion signal as a function of infrared frequency, we can obtain conformer-specific hydride stretch infrared spectra of cold, protonated biomolecules. We have applied this method to protonated tryphophan, tyrosine, and their water clusters. In each case conformational assignments were made with the assistance of density functional theory calculations. There are fewer low energy conformers than were observed previously in the neutral molecules, because of the stabilization requirements of the charged amino group. Additionally, the protonated amino acids bind water preferentially at the charged site.