ULTRAVIOLET AND INFRARED SPECTROSCOPY OF HELICAL PEPTIDES AND THEIR WATER COMPLEXES

JAIME A. STEARNS, MONIA GUIDI, CAROLINE SEAIBY, ANNETTE SVENDSEN, OLEG V. BOYARKIN, and THOMAS R. RIZZO, *Laboratoire de Chimie Physique Moléculaire, Ecole Polytechnique Fédérale de Lausanne, CH-1015, Lausanne, Switzerland*.

We have developed methods to study large, gas-phase molecules at low temperatures by combining electrospray ionization with collisional cooling in a 6 K, 22-pole ion trap, and using ultraviolet photofragmentation and infrared-ultraviolet double resonance spectroscopy to probe molecular structure. An important goal of our studies has been to understand the conformational preferences of increasingly large peptides, and to identify spectroscopic signatures of important secondary structure elements such as helices. In addition to transferring large molecules into the gas phase, electrospray affords the opportunity to create complexes between the ion of interest and a selected number of solvent molecules. We have systematically studied the effects of microsolvation on the small helical peptide Ac-Phe-$(Ala)_5$-Lys-H^+, determining how the structure of the helix changes as up to ten water molecules begin to compete with intramolecular hydrogen bonds.