CONFORMATION-SPECIFIC INFRARED SPECTROSCOPY OF COLD, PROTONATED Ac-PHE-$(ALA)_5$-LYS AND PHE-$(ALA)_{10}$-LYS: SPECTROSCOPIC SIGNATURES OF HELIX FORMATION

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*.

The α-helix is an important structural motif in biological molecules, although the factors governing helix formation are still being determined. One approach to studying helix formation is to remove the peptide to the gas phase to determine the characteristics intrinsic to the peptide which stabilize helical structures. Previous studies using ion mobility have suggested that helical structures persist in the gas phase for polyalanines capped at the C-terminus with a lysine residue.[a] We have studied similar peptides, Ac-Phe-$(Ala)_5$-$LysH^+$ and Phe-$(Ala)_{10}$-$LysH^+$, using conformation-specific infrared spectroscopy in a cold ion trap. We observed at least four conformers of the smaller peptide, but a single major conformer of the larger. The amide N-H stretch frequencies provide signatures of the different types of hydrogen bonding present in each conformer. The bonding environments range from the free N-H groups at the N-terminus of the peptides to amide groups in the center and C-terminus which are in strong helical N-H$\cdots$O=C hydrogen bonds.

[a] M. Kohtani and M. F. Jarrold *J. Am. Chem. Soc.* **126**, 8454, 2004.