CONFORMATION-SPECIFIC SPECTROSCOPY OF A PROTOTYPICAL γ-PEPTIDE-WATER COMPLEX: Ac-γ^2-hPhe-NHMe-$(H_2O)_1$

EVAN G. BUCHANAN, WILLIAM H. JAMES III, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*; LI GUO, and SAMUEL H. GELLMAN, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*.

The prototypical γ-peptide, Ac-γ^2-hPhe-NHMe, has been previously studied in a supersonic jet expansion, with three different conformers observed. Two of the monomers form nine atom, intramolecular hydrogen bonded rings, which differ by the position of the aromatic chromophore relative to the backbone. The third monomer conformer has no intramolecular H-bonds, but forms instead an intramolecular, amide-amide stacked structure unique to the γ-peptide backbone. This talk focuses attention on the conformation-specific IR spectra of the Ac-γ^2-hPhe-NHMe-$(H_2O)_1$ complex, which is observed to form six unique conformational isomers, all of which preserve the two distinct monomer structural motifs. Three conformers are assigned to the nine atom intramolecular hydrogen bond family with the water hydrogen bonded to it as donor in different locations. The other three belong to the amide-amide stacking family with the water forming a bridge between the two amide planes. Infrared photodissocation of the water molecule from the complex to form γ-peptide monomer conformations will also be discussed.