WATER CLUSTERS OF A MODEL DIPEPTIDE: N-ACETYLTRYPTOPHAN METHYLAMIDE

ASIER LONGARTE, BRIAN C. DIAN and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-1393*.

Most molecules of biological relevance have considerable conformational flexibility. Our recent work on the model dipeptide N-acetyltryptophan methylamide, has found that there exist only a few low lying energy structures populated in the pre-nozzle gas mixture. However, this model dipeptide offers numerous hydrogen bonding sites to which water molecules can bind. These water molecules can also influence the conformation of the solute molecule. We present results from a variety of methods including one and two color R2PI, UV-UV Hole-burning and Resonant-Ion Dip Infrared Spectroscopy (RIDIRS), to determine the conformations of water bound clusters of N-Acetyl Tryptophan Methylamide (NATMA) in the gas phase. Quantum chemical calculations are used to calculate the harmonic frequencies of NATMA water clusters, which are compared to the infrared spectra to make assignments of the hydrogen bonding topologies of these clusters. The effects of water and water bridges on the conformational preferences of NATMA will be discussed.