MODELING COMPETITIVE INTERACTIONS IN PROTEINS: VIBRATIONAL SPECTROSCOPY OF $Na^+(N-METHYLACETAMIDE)_1(H_2O)_{0-4}$ IN THE $3\mu m$ REGION

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To properly understand the preferred structures and biological properties of proteins, it is important to know how they interact with their aqueous environment. Competitive intra-peptide, peptide-water, ion-water, and ion-peptide interactions, including hydrogen bonding, play a key role in determining the structures and properties of proteins. The primary types of hydrogen bonding that occur are the intramolecular amide-amide $(N-H\cdots O=C')$ and the intermolecular amide-water $(O-H\cdots O=C'$ and $H-O\cdots H-N)$. N-methylacetamide (NMA), which contains both a carbonyl group and an amide group, is a common model for investigating these competitive interactions. An analysis of the infrared photo dissociation spectra of $Na^+(NMA)_1(H_2O)_{0-4}$ in the O-H, N-H, and C=O spectral regions is presented. Parallel *ab initio* calculations are used as a guide in identifying both the type and location of non-covalent interactions present. In larger clusters, where several structural isomers may be present in the molecular beam, *ab initio* calculations are also used to suggest assignments for the observed IR transitions. The results presented offer insight to the nature of ion-NMA interactions present in an aqueous environment.