COMPETITIVE INTERACTIONS IN ALKALI METAL ION - ACETONE - WATER CLUSTERS

TIMOTHY D. VADEN, JAMES M. LISY, *Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*.

Interactions between ions and carbonyl groups are of fundamental importance in many size-selective systems such as ionophores and potassium ion channels. As the selection process generally occurs in an aqueous environment, there is a competition between ion-carbonyl and ion-water interactions. By combining infrared laser predissociation spectroscopy with *ab initio* calculations, we have characterized the structures of $M^+(Acetone)_n(H_2O)_m$ cluster ions to examine these competing interactions. The IR spectra in the O-H stretch region were compared to spectra of the corresponding $M^+(H_2O)_{n+m}$ species. For the smaller clusters ($n + m \leq 4$), subtle but detectable shifts in the water symmetric and asymmetric O-H stretch transitions reflect the influence of the acetone carbonyl group(s) on the ion-water interaction. For larger clusters ($n + m > 4$), hydrogen-bonded O-H stretch transitions are observed, which provide structural information and insight into the nature of water-water interactions when ion-carbonyl interactions are present.