COMPETITION IN ALKALI METAL ION - PHENOL CLUSTERS: DISRUPTING THE INTERMOLECULAR HYDROGEN BONDS WITH CATION-π INTERACTIONS

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

Competing non-covalent interactions are of fundamental importance in ionic systems as interactions between ions and neutral molecules often must compete with strong intermolecular forces such as hydrogen bonding. We have investigated this competition in alkali metal ion - phenol clusters with infrared predissociation spectroscopy in the O-H stretch region and DFT calculations. Evaporatively cooled $M^+(\text{Phenol})_n$Ar cluster ions were characterized for M = Li, Na, K, and Cs, and n = 2 - 3. The IR spectroscopic results illustrate that the intermolecular hydrogen bonds in both the phenol dimer and phenol trimer are weakened by the alkali metal ions. The DFT calculations assist in identifying the observed structures and show that cation-π interactions between the ions and phenol molecules disrupt the phenol hydrogen bonds. For M = Li and Na, multiple hydrogen bonded configurations were identified in the IR spectra, and a theoretical analysis of the isomerization pathways between different configurations suggests that the rapid argon evaporative cooling process may lead to kinetically-favored structures.