MAGIC NUMBERS IN HYDRATED ALKALI METAL ION CLUSTERS: INFARED SPECTROSCOPY OF $K^+(H_2O)_n$ and $Cs^+(H_2O)_n$

JASON D. RODRIGUEZ, MATTHEW ACKERMAN, DOROTHY J. MILLER, JAMES M. LISY, *Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*.

The mass spectrum of protonated water has long been the subject of many experimental and theoretical studies to explain the presence of unusually stable, or "magic" clusters. Similar magic number clusters are also present in the mass spectra of $K^+(H_2O)_n$ and $Cs^+(H_2O)_n$. Recent computational studies have shown that the magic numbers of these cluster ions contain only three-coordinated DDA or DAA water molecules. Here D (donor) and A (acceptor) describe the nature of the hydrogen bonds associated with each water. We have used infared predissociation spectroscopy in the O-H stretch region to identify the spectroscopic features of DA and DAA waters in $K^+(H_2O)_n$ and $Cs^+(H_2O)_n$ for $n = 16 - 23$. In particular, we will address the presence or absence of spectroscopically resolvable DA and DAA waters in these species.