MAGIC NUMBERS IN ALKALI CATION WATER CLUSTERS: INFARED SPECTROSCOPY OF $Li^+(H_2O)_n$ and $Na^+(H_2O)_n$

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

The local environment of solvated alkali metal ions is an important subject in aqueous chemistry as well as in biology. However, an accurate depiction of this environment is challenging. It is at or exceeds the limits of current *ab initio* (MP2) methods. Thus more approximate model potentials (with or without polarizability) must be employed. An experimental approach to this problem is to look at hydrated alkali metal ion clusters in the gas-phase. We have used IR spectroscopy in the O-H stretch region to characterize the $M^+(H_2O)_n$ system, where M=Li, Na and $n = 16 - 23$, as these vibrational modes are sensitive to ion-water interactions as well as hydrogen bond formation. Additional work done in our lab on M=K and Cs show magic numbers in the mass spectrum while the mass spectra of M=Li and Na display no magic numbers. Using theoretical work recently published by Schulz and Hartke[a] we offer an explanation for this observation.

[a] F. Schulz, B. Hartke, Theor. Chem. Acc. 114, 357 (2005).