TEMPERATURE EFFECTS IN HYDRATED ALKALI METAL IONS

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The role of temperature or internal energy in solvated ions is the dominant factor in determining the structures of these species. The strong electrostatic interaction between the ion and the water molecules, allows for multiple hydrogen-bonded and non-hydrogen bonded structures to co-exist at various temperatures. This reflects the competition between these two non-covalent interactions. I will present examples from our laboratory involving the alkali metal ions: Li^+, Na^+, K^+ and Cs^+, and three to five water molecules. The cluster ions are prepared by ion impact on preformed neutral clusters, which are then stabilized by evaporative cooling. Evaporation of water produces warmer clusters, while evaporation of argon generates colder species. By combining tandem mass spectrometry with tunable infrared laser spectroscopy, the vibrational spectra of these species in the 3300-3800 cm^{-1} region are obtained. Structural assignments are supported by *ab initio* calculations. At warmer temperatures, structures with fewer hydrogen bonds are favored, reflecting the role of entropy in these systems.