TEMPERATURE DEPENDANT STRUCTURAL CONFORMATIONS OF HYDRATED ALKALINE METAL ION CLUSTERS

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A delicate balance of competing intermolecular interactions dictates preferred structural configurations of hydrated alkaline metal ion clusters. We are able to shift the balance of these interactions by controlling the dominant evaporative loss pathway during cluster formation. Evaporative cooling through the loss of water molecules gives rise to clusters whose internal energy distribution corresponds to temperatures of 250 K - 500 K. In this temperature regime entropic effects may influence which structural isomers are present, favoring ones in which the free energy of the system has been minimized. Also, at these temperatures, there are often multiple comparable minima on the potential energy surface, giving rise to multiple structural isomers. Incorporating significant amounts of argon into the nascent clusters shifts the predominant evaporative loss pathway to the loss of argon. The lower binding energy of argon leads to more evaporative steps, which results in a terminal temperature that is substantially lowered (100 K - 200 K) and fewer structural isomers are formed. We will present the IR predissociation spectra of $Cs^+(H_2O)_{n=2-4}Ar$ and $Cs^+(H_2O)_{n=2-4}$ in the OH stretch region and discuss the structural differences induced by the presence of argon as reflected in the vibrational spectra.