UNRAVELING SPECTRAL SIGNATURES OF ION/WATER INTERACTIONS

ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

Complexation of a positively charged metal ion or a proton by even a single water molecule leads to large effects on the frequencies and intensities of the intermolecular vibrations compared to an isolated water molecule. For example, in metal ion/water complexes the splitting of the OH stretch frequencies is substantially decreased and the intensity of the symmetric stretch, relative to the asymmetric stretch, has increased dramatically compared to an isolated water molecule. In this talk, we will discuss several theoretical and computational methods that can be used to investigate the origins of these changes. Both reduced dimensional calculations and methods based on Diffusion Monte Carlo will be presented.