A CLUSTER PERSPECTIVE: THE HYDRATED PROTON

JEFFREY M. HEADRICK, ERIC G. DIKEN, and MARK A. JOHNSON, *Sterling Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, Connecticut 06520*.

Capturing the dynamics of proton transfer in water has been one of the most enduring puzzles in aqueous chemistry. Two models are typically invoked to address the nature of the excess proton, the pyramidal Eigen ($H_9O_4{}^+$) and symmetrically solvated Zundel ($H_2O \cdots H^+ \cdots OH_2$) accommodation motifs. These two motifs can be easily characterized in small protonated water clusters, $H^+{\cdot}(H_2O)_{n\leq 8}$, which form quasi planar structures that develop into 5 membered rings at n = 7. However, when cluster size becomes large (e.g. n $\geq$ 20) clathrate structures begin to form, and the proton defect signature becomes difficult to detect. In this talk, we report OH stretching spectra of large $NH_4{}^+{\cdot}(H_2O)_n$ clusters in order to elucidate vibrational signatures specific to a cluster possessing a pyramidal excess proton accommodation motif. With this information we hope to make a direct comparison to bands observed in the larger $H^+{\cdot}(H_2O)_n$ clusters.