A CLUSTER PERSPECTIVE: THE HYDRATED PROTON

JEFFREY M. HEADRICK, ERIC G. DIKEN, MARK A. JOHNSON, *Sterling Chemistry Laboratoy, Yale University, P.O. Box 208107, New Haven, CT, 06520-8107*.

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_3O^+) and symmetrically solvated Zundel ($H_2O \cdots H^+ \cdots OH_2$) accommodation motifs. Until now, spectral signatures of these two complexes could only be inferred from aqueous analyses in the bulk (via FTIR) or from the behavior of spectator OH stretches far from the excess charge. In this poster we report the infrared spectrum of $H^+ \cdot (H_2O)_{2-8}$ in the critical 1000 to 3900 cm^{-1} range and track the spectral signatures associated with motion of the hydrated proton as a function of solvent molecules. These studies are made possible by recent advances in non-linear laser technology that access the low energy range by parametric conversion in $AgGaSe_2$. Our main conclusion from these observations is that the solvated Eigen structure ($H_9O_4{}^+$) is actually a rare event, and that the preferred motif is mostly charge localization onto a single hydrogen atom.