INFRARED SPECTROSCOPY OF PROTONATED BENZENE-WATER NANOCLUSTERS: HYDRONIUM, ZUNDEL AND EIGEN AT A HYDROPHOBIC INTERFACE

T. C. CHENG, B. BANDYOPADHYAY, and M. A. DUNCAN, *University of Georgia, Dept. of Chemistry, 1001 Cedar St, Athens, GA 30602*.

Mixed protonated nanocluster cations of benzene and water are produced in a pulsed discharge/supersonic expansion source, mass-selected in a time-of-flight spectrometer, and studied with infrared laser photodissociation spectroscopy. Small cluster ions with strong bonding are studied via the method of ”tagging” with argon atoms, while larger clusters dissociation by the elimination of neutral benzene molecules. Vibrational patterns in these systems are studied with computational chemistry, and they are also compared to the known IR spectra of protonated water or protonated benzene clusters. Vibrations assigned to shared proton motions, π-hydrogen bonds, free-OH stretches, hydrogen bonded O-H stretches, and free C-H stretches are measured for clusters containing 1-4 benzene or water molecules. In each system, the structures detected are those for protonated water clusters solvated by neutral benzene, rather than protonated benzene ions solvated by water. Binding at the hydrophobic surface of benzene induces significant shifts on the vibrations of zundel and eigen ions at positions once and twice removed from the point of contact, illustrating the importance of inductive interactions in these systems.