INFRARED SPECTROSCOPY OF LARGER BENZENE-$(H_2O)_n$ HYDROGEN-BONDED CLUSTERS: EVIDENCE OF 3-DIMENSIONAL NETWORKS

C. J. GRUENLOH, C. A. ARRINGTON, J. R. CARNEY, R. N. PRIBBLE, and T. S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-1393*; S. Y. FREDERICKS and K. D. JORDAN, *Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260*.

One color resonant two-photon ionization time-of-flight mass spectroscopy (R2PI-TOFMS), ultraviolet hole-burning, and resonant ion-dip infrared spectroscopy (RIDIRS) have been used to assign and characterize size-selected benzene-$(H_2O)_n$ clusters formed in a supersonic molecular beam. The double resonance technique of RIDIRS utilizes a combination of a Nd:YAG-pumped OPO system and R2PI-TOFMS, and thus affords both wavelength and mass selectivity in recording the OH stretch spectrum (2900 to 3800 cm^{-1}) of a chosen cluster. The OH stretch is a powerful probe of hydrogen bonding since its vibrational frequency and infrared intensity sensitively depend on the number, type, and strength of hydrogen bonds in which each OH group participates. The hydrogen-bonding topology of each cluster is obtained with the assignment of OH stretch vibrations and a comparison to $ab\ initio$ calculations. The benzene-$(H_2O)_6$ cluster exists as a "cage" type water sub-cluster to which benzene is π-hydrogen bound to one of the free OH groups. A similar 3-dimensional network occurs in benzene-$(H_2O)_7$. Furthermore, several weaker transitions present in the electronic spectroscopy are tentatively assigned to other benzene-$(H_2O)_7$ conformers.