

THE SPECTROSCOPY OF INDOLE DERIVATIVES AND THEIR SMALL WATER CLUSTERS

JOEL CARNEY, and T. S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-1393.*

A spectroscopic summary of indole, 1-methylindole, and 3-methylindole will be presented. One color R2PI-TOFMS, IR-UV hole-burning, and resonant ion-dip infrared (RIDIR) spectroscopies along with density functional theory (DFT) calculations have been used to assign and characterize the hydrogen-bonding topologies of selected gas-phase clusters. The double resonance technique of RIDIRS utilizes the combination of an infrared OPO system and R2PI-TOFMS, thus affording both wavelength and mass selectivity in recording the IR spectrum (2800 to 3800 cm^{-1}) of a chosen cluster. The frequencies and intensities of the CH, OH, and NH stretch fundamentals provide sensitive probes of cluster size and conformation that can be used with IR-UV hole-burning and DFT calculations to firmly assign vibronic features to a given cluster size. This discussion will highlight two conformations of 1-methylindole-(water)₃, the topic of internal rotation in 3-methylindole-(water)₁, and a CH stretch summary.