THE SPECTROSCOPY OF INDOLE DERIVATIVES AND THEIR SMALL WATER CLUSTERS

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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.