INFRARED SPECTROSCOPY OF INDOLE, 1-METHYLINDOLE, 3-METHYLINDOLE, AND THEIR SMALL WATER CLUSTERS

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One color R2PI-TOFMS, IR-UV hole-burning, and resonant ion-dip (RIDIR) spectroscopies along with density functional theory calculations have been used to assign and characterize the hydrogen-bonding topologies of water-containing clusters with indole, 1-methylindole, and 3-methylindole. 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 (2900 to 3800 cm^{-1}) of a chosen cluster. The frequencies and intensities of the 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. The N-H hydrogen-bonding site on indole serves as the point of attachment for water molecules, which form H-bonded bridges to the indole π cloud. In 1-methylindole, the loss of this site results in the formation of π H-bonded water clusters. The implications of these different H-bonding motifs for the photophysics of indole and its derivatives will be discussed.