SOLVATION OF MELATONIN: THE ULTRAVIOLET AND INFRARED SPECTROSCOPY OF MELATONIN-WATER CLUSTERS

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The sequential solvation of melatonin in a molecular beam has been investigated using the techniques of 1-color and 2-color resonant two-photon ionization (R2PI), resonant ion-dip infrared spectroscopy (RIDIRS), and UV-UV holeburning spectroscopy. Melatonin presents f our distinct hydrogen bonding sites for water, which can be probed in the XH stretching region of the infrared (2800-3800 cm^{-1}), where X=C, N, and O. Water clusters of melatonin are observed both red and blue-shifted of the conformer origins in the R2PI spectra. The RIDIR spectra along with density functional theory calculations lead to assignments for the structures of several of the melatonin-(water)$_n$ clusters. Implications for the solvation of a model peptide will be discussed, along with the dynamics associated with the monomer orientations upon water cluster formation.