SHEDDING LIGHT ON THE MOLECULE OF DARKNESS: THE ULTRAVIOLET AND INFRARED SPECTROSCOPY OF MELATONIN

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Melatonin (N-acetyl-5-methoxytryptamine) is a neural hormone involved in biochemical regulation of the internal clock and sleep cycles. Melatonin is an indole derivative with a flexible peptide-like side chain attached at the C3 position with close structural similarities to tryptamine and tryptophan. Using a combination of 1-color and 2-color resonant two-photon ionization (R2PI), resonant ion-dip infrared spectroscopy (RIDIRS), and UV-UV holeburning spectroscopy, the conformational preferences of melatonin in a molecular beam have been determined. Two major conformers and one minor conformer have been identified in the R2PI spectra and characterized with RIDIRS in the CH and NH stretching region. Structural assignments of the three conformers are made using the infrared spectra in concert with the results of electrostatic force field conformational searching and quantum mechanical calculations. This work builds on previous studies of conformationally flexible molecules in the gas phase such as tryptamine and model peptides such as N-benzylformamide and N-acetyltryptophan derivatives.