CONFORMATIONAL ANALYSIS OF SEROTONIN-$(H_2O)_1$ AND $(H_2O)_2$ CLUSTERS

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Serotonin (5-hydroxytryptamine) has many functions in the human body. Previous studies of serotonin have determined the inherent conformational preferences of the isolated molecule, and mapped out the energy thresholds to conformational isomerization between particular conformational isomers. Since biological processes occur in aqueous solution, it is of interest to understand how the conformational preferences of serotonin are changed by its interactions with water. Since both the flexible side chains of serotonin (OH and ethylamine) have good H-bonding sites, we anticipate a significant interplay between the ways in which water binds to serotonin and the conformations that are thereby stabilized. While there are eight observed conformations of serotonin monomer, UV-UV hole-burning spectroscopy was used to prove the presence of three conformations of SERO-$(H_2O)_1$ and one conformation of SERO-$(H_2O)_2$. Resonant ion-dip infrared spectroscopy in the OH and CH stretch regions provides powerful diagnostics of the H-bonding present and its effect on serotonin conformation. In particular, one of the SERO-$(H_2O)_1$ conformers and the SERO-$(H_2O)_2$ conformer possess a water bridge between the amino group on the ethylamine side chain and the 5-OH group on the indole ring. The corresponding spectra for the remaining two conformers of SERO-$(H_2O)_1$ are nearly identical to that found in the tryptamine-H_2O complex, in which water binds as H-bond donor to the most stable conformation of serotonin. The two conformers differ in the orientation of the 5-OH group (*syn* or *anti*), producing a 5 cm^{-1} shift in the absorption frequency of the 5-OH stretch transition.