CONFORMATIONAL PROPERTIES, SPECTROSCOPY AND STRUCTURE OF ISATIN-(WATER)$_{n=1-3}$ CLUSTERS

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The structure, stability and vibrational characteristics of *Isatin-(Water)*$_n$ clusters with n=1=3 have been investigated using second order Moller-Plesset (MP2) perturbation tehory and Density Functional Theory (with B3LYP) methods employing the basis set 6-31+G(d). The vertical excitation energies for these complexes have been also computed using the time-dependent density functional theory. The three stable conformational isomers, each for *Isatin-(Water)*$_1$ and *Isatin-(Water)*$_2$ clusters were obtained. It is shown that in the most stable isomer of *Isatin-(Water)*$_1$ cluster hydrogen bond between amide hydrogen and oxygen of water is found stronger as compared to the H-bond in *Indole-(Water)*$_1$ cluster. For a particular position of complexation of water, between the carbonyl oxygen's, results an unusual increase in the dipole moment due to an electronic charge displacement from the N atom to the C atom of the neighboring carbonyl bond. This causes a large separation between the effective charges forming the dipole. The complexes involving this position of water are expected to show a small charge transfer character. The experimentally observed electronic absorption peaks are reasonably reproduced by the TD-DFT calculations and it is found that the longest wavelength absorption peak of isatin at 406 nm is significantly red shifted after addition of a water molecule.