DFT STUDIES ON THE SPECTRA AND STRUCTURE OF ISATIN AND ITS 5R SUBSTITUTED DERIVATIVES

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Density Functional Theory calculations for the geometric and energetic properties, rotational constants, harmonic vibrational frequencies of isatin and its various 5-R substituted (R=F, Cl, Br and NO_2) derivatives have been carried out regarding their monomeric and dimeric forms, invoking different basis sets. With all the basis sets, the dimeric conformations of each isatins are predicted to be more stable than monomeric conformation. The predicted shift in NH-stretching mode due to intermolecular hydrogen bonding, towards lower wave number side, is found to be in better agreement with the observed IR frequencies. Effects of 5R substitutions (R = NO_2, F, Cl, Br, and I) on the vibrational spectra in the region 4000-200 cm^{-1} and on the structure of isatin are investigated. The carbonyl stretching modes are less affected after substitutions, however the frequency of a strong C=C stretching mode decreases significantly from fluoroisatin to iodoisatin and the corresponding intensities increase towards iodoisatin. Vertical excitation energies for the monomer as well as dimer of isatin and its derivatives have also been computed using the time-dependent DFT calculations, which agree well with the experimental values.