An experimental and first-principles density functional theory study on the charge transfer complexes of iodine with homologous series of donors

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The formation of charge transfer (CT) complexes is effectively explained through stabilization of the highest occupied orbital of a donor molecule and destabilization of the lowest unoccupied orbital of an acceptor molecule in the molecular orbital diagram. Extensive density functional theory (DFT) calculations have been carried out to indicate the variation in structure, stability and charge transfer of CT complexes formed by homologous series of donors. The formation and structure of CT complexes of iodine with aromatic compounds are deduced. The excitation energy of CT complexes is also calculated by time-dependent DFT.

Keywords: Absorption spectra, aromatic compounds, charge transfer complexes, excitation energy, iodine.

with a homologous series of donors. The molecular orbital (MO) diagram is the best tool to understand the excitation and electronic properties of CT complexes. The first-principles density functional theory (DFT) calculation is performed to obtain the structural variations in CT complexes. Here, we report in detail the structure and interactions of CT complexes formed by iodine with *n*-donors like oxygen, sulphur, and nitrogen donors, and π-donors like aromatic hydrocarbons.

Experimental and theoretical methods

Absorption spectra were recorded using a UV spectrometer (Labman, India) in a quartz cell from 190 to 1100 nm with a resolution of 1 nm. The calculations were based on first-principles DFT, as implemented in the QUANTUM