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4-(Diethylamino) salicylaldehyde based fluorescent Salen ligand with red-shifted emission - A facile synthesis and DFT investigation

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Abstract

4-(Diethylamino) salicylaldehyde based Salen ligands were synthesized and studied using density functional theory (DFT) employing B3LYP/6-31G(d) method. These dyes exhibited intramolecular charge transfer (ICT) which were examined for their photophysical properties. They show red to deep red absorption and emission respectively in the range of 562-575 nm and 596-635 nm and exhibited positive solvatochromism which is supported by linear and multi-linear regression analysis. Oscillator strengths and transition state dipole moments are studied to understand charge transfer (CT) characteristics. These deep red emissive fluorophores showed aggregation-caused quenching (ACQ). The spectral variations were analyzed by linear solvation energy relationships proposed by Kamlet-Taft and Catalan which indicated that solvent polarizability/dipolarity influences more compared to solvent acidity or basicity. Bathochromic shift in emission and increase in dipole moment in the excited state signify ICT character. The calculated electronic spectra of dyes are elucidated on the basis of TD-DFT calculations. Spectroscopic and computational methods were used to obtain linear polarizability, hyperpolarizability of the dyes and have better NLO properties than urea. Molecular Electrostatic Potential (MEP), NBO, HOMO-LUMO analysis, global chemical reactivity descriptors are studied at same level DFT.

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