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A very rare fluorescent chemosensor of zinc(II) exhibiting AIEE, ESIPT and TICT: Spectroscopic, crystallographic and theoretical exploration

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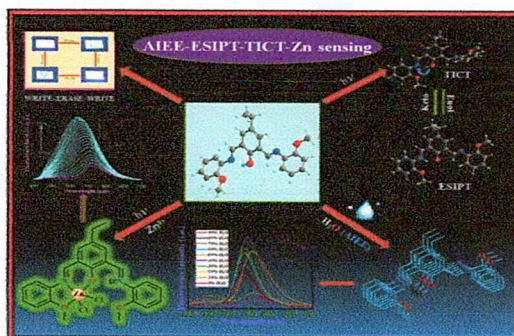
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HIGHLIGHTS

- HL is the 1:2 condensation product of 2,6-diformyl-4-ethylphenol and *o*-anisidine.
- HL is a fluorescent turn on Zn^{II} sensor which exhibits AIEE, ESIPT and TICT.
- Crystal structures of HL and its both Zn^{II} and Cd^{II} complexes are determined.
- HL is applied in inkless writing with the "write – erase – write" facility.
- DFT calculations in both ground and excited states have been done.

GRAPHICAL ABSTRACT



ARTICLE INFO

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ABSTRACT

The basic systems in this study are HL (1; 1:2 condensation product of 2,6-diformyl-4-ethylphenol and *o*-anisidine) and its Zn^{II} and Cd^{II} complexes of composition [Zn^{II}(LH)Cl₂].CH₃OH (2) and [Cd^{II}(LH)Cl₂] (3), all of which are synthesized and characterized by CHN elemental analyses, single crystal X-ray crystallography, powder X-ray diffraction (PXRD) and fourier transform infrared (FT-IR) spectrum. It has been established from the following experimental and theoretical studies that 1 is a fluorescent turn on sensor of Zn^{II} ion and it exhibits all of excited state intramolecular proton transfer (ESIPT), photoinduced electron transfer (PET), twisted intramolecular charge transfer (TICT) and aggregation induced enhanced emission (AIEE): (i) Detailed absorption and emission (steady state / time resolved) studies in various single solvents, in solvent mixtures, with pH variation, with various single metal ions, with mixtures of metal ions, on varying temperature and on varying viscosity; (ii) dynamic light scattering (DLS) and scanning electron microscopy (SEM) in solvent mixtures; (iii) density functional theory (DFT) and time dependent density functional theory (TD-DFT) calculations in ground and excited states of 1–3. It is shown that 1 can be efficaciously applied in inkless writing with the "write – erase – write" facility. The mechanisms/reasons of the observed properties have been addressed. The difference in fluorescence

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