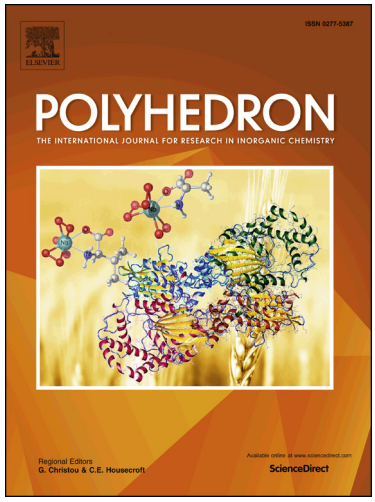

Experimental and theoretical studies on photoluminescent Zn(II) host complex with an open book structure: Implication on potential bioactivity and comparison with its ligand and Zn(II), Pd(II) siblings

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Experimental and theoretical studies on photoluminescent Zn(II) host complex with an open book structure: Implication on potential bioactivity and comparison with its ligand and Zn(II), Pd(II) siblings

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Abstract

A novel inclusion Zn(II) complex with water guest molecule is synthesized from 6,6′-diethoxy-2,2′-[2,2-dimethylpropane-1,3-diylbis(nitrilomethylidyne)]-diphenol salen-type Schiff base (H_2L) and is characterized through single crystal XRD studies, IR, UV-Vis methods. Thermal profile is studied using TG-DTG–DSC method. Single crystal XRD analysis reveals a rare open book structure for the complex and an interesting star-like supramolecular assembly. The emission properties of the complex is compared with that of the ligand, pseudo-inclusion and inclusion compounds from Zn(II) and Pd(II) ions prepared from the same ligand. Hirshfeld surface for the compounds were mapped with various functions and further quantification of intermolecular interactions was made through the generation of 2D finger print plots. To dissect the nucleophilic and electrophilic regions on the molecular surface, ESP plots of the compounds are generated. Further DFT calculations are done at B3LYP/def2-TZVP level of theory to optimize the geometry of the compounds and to compare frontier orbitals and charge distribution among the compounds. Molecular docking of the compounds with B-DNA dodecamer and Human Serum Albumin (HSA) is performed to gain an insight on the structure-activity relationship of these compounds.

Keywords: Zn(II), Salen-type; Hirshfeld; DFT studies; Molecular docking

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