Experimental and theoretical analysis of a rare nitrato bridged 3d-4f complex containing $LaZn_2$ core synthesized from a Zn(II) metalloligand

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Abstract

A trinulcear Zn_2La Schiff base complex was synthesized using slow-solvent evaporation technique from a Zn(II) mononuclear metalloligand by 2:1 addition with $La(NO_3)_3$ salt. Single crystal XRD analysis revealed a rare nitrato bridged trinuclear entity which is seldom seen in these class of ligand systems. Qualitative and quantitative analysis of intermolecular interactions/short contacts were done using Hirshfeld surface and 2D finger print analysis. The thermally stable, blue luminescent compound exhibits internal heavy atom effect thereby quenching the emission intensity of the ligand. DFT calculations were performed on the compound to analyze frontier orbitals and also ESP plots were used to monitor nucleophilic/electrophilic regions on the compound and its implications on hydrogen bonding. A comparison of the bond orders and atomic charges on the trinuclear compound and the Zn(II) metalloligand precursor was performed to substantiate the formation of the trinuclear product through ligand exchange.

Keywords: 3d-4f; Salen-type; Hirshfeld; DFT studies; La(III); Crystal structures.

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