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Title:	Heterometallic Zn(II)-K(I) complex with salen-type Schiff-base ligand: Synthesis, crystal structure, solid-state photoluminescent property and theoretical study
Authors:	Das, Sourav (/jspui/browse?type=author&value=Das%2C+Sourav)
Keywords:	Schiff base Zn(II) K(I) Fluorescence
Issue Date:	2019
Publisher:	Elsevier
Citation:	Journal of Molecular Structure, 1185, pp. 112-120.
Abstract:	<p>A novel tetranuclear heterometallic complex, $[\text{KZn}(\text{3-MeOsalm})_2(\mu_1,1\text{-NCS})]_2(\mu_1,1\text{-NCS})_2$ [3-MeOsalm = N, N'-propylene bis(3-methoxysalicylideneimine)] has been synthesized by the reaction of $\text{Zn}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ with the multidentate Schiff-base ligand, N, N'-bis(2-hydroxy-3-methoxybenzylidene)-propane-1,2-diamine (H_2LOMe) in the presence of KSCN. 1 is characterized by elemental analysis, powder X-ray diffraction and different spectroscopic techniques along with single crystal X-ray crystallography. Crystal structure of 1 completely divulges a very intricate heterometallic environment of Zn(II) which is a centrosymmetric penta-coordinated distorted square pyramidal molecule possessing a basic tetranuclear structural core $[\text{KZn}(\text{OAr})_2(\mu_1,1\text{-NCS})]_2$ that consisting mainly two Zn atoms and two K atoms bridged by four $\mu_2\text{-OAr}$ (O1, O1^*, O2 and O2^*), and two $[\mu_1,1\text{-NCS}]$- groups. In the asymmetric unit of the binding action $\mu_2\text{-OAr}$- from one fully deprotonated $[\text{LOMe}]_2$- enable to construct the four membered heterometallic $\text{ZnK}(\text{O})_2$ core. Complex 1 structure was optimized with the aid of density functional theory at B3LYP level hybrid functional and GAUSSIAN 16 programming package in presence of 6-31 + g(d, p) basis set. ESP study of Schiff base ligand further supported that polymerization is more favorable with potential border line Zn(II) metal ion. Hirshfeld surface and 2D fingerprint plots have been explored in 1 to find out different types of non-covalent supramolecular interactions. The solution and solid-state luminescent property of the title complex 1 was reported. Fluorescence life time study further indicates that excited state stabilities of 1 are smaller than Schiff base ligand. Finally, experimental UV-Vis electronic transitions of 1 were compared with those obtained theoretically from TD-DFT level of calculations.</p>
Description:	Only IISERM authors are available in the record.
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