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Title:	Dicyanamide-interlaced assembly of Zn(II)-schiff-base complexes derived from salicylaldimino type compartmental ligands: Syntheses, crystal structures, FMO, ESP, TD-DFT, fluorescence lifetime, in vitro antibacterial and anti-biofilm properties
Authors:	Das, Dhiraj (/jspui/browse?type=author&value=Das%2C+Dhiraj)
Keywords:	Schiff base Dicyanamide Tetranuclear Zn(II) TD-DFT
Issue Date:	2019
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Citation:	Inorganica Chimica Acta, 489, pp.244-254.
Abstract:	Two new dicyanamide-interlaced tetranuclear Zn(II)-Schiff-base complexes [Zn ₂ (LOMe)(μ-dca-κN1κN5)(μ-dca-κN1)] ₂ (1) and [Zn ₂ (LOEt)(μ-dca-κN1κN5)(μ-dca-κN1)] ₂ (2) were synthesized by using salicylaldimino type Schiff bases (H ₂ LOMe) and (H ₂ LOEt) respectively. Schiff base ligands and the complexes were characterized by elemental analyses, powder X-ray diffraction, FT-IR, FT-Raman, ¹ H NMR, ¹³ C NMR, UV-Vis, TGA and fluorescence spectroscopy. Dicyanamide modulated complexes were structurally characterized by single crystal X-ray diffraction studies. X-ray crystal structure divulges that the two complexes are isostructural. In both the complexes, the Zn ₁ metal centers fulfill 5-coordinated distorted square pyramidal geometry having ZnN ₃ O ₂ chromospheres where Schiff bases are mainly trapped in their complete deprotonated dianionic forms [L] ₂ ⁻ , whereas Zn ₂ metal center attained distorted octahedral geometry. In both complexes two asymmetric units are connected by double μ _{1,5} -dicyanamide ion thus forming Zn ₄ -nuclear metal complex. B3LYP/def2-TZVP level of theory (DFT) successfully applied in both complexes. The complexes (1–2) exhibit intraligand (π → π*) fluorescence in DMSO solvent with lifetimes in the range 0.66–0.82 ns. In vitro antibacterial, membrane damage assay and anti-biofilm properties of both complexes are evaluated against some important Gram-positive and Gram-negative bacterial strains. Finally, the UV-Vis experimental spectral findings are well rationalized with the electronic distribution of HOMO-LUMO through TD-DFT level of calculations.
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