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Title:	Syntheses, crystal structures and photo physical aspects of azido-bridged tetranuclear cadmium (II) complexes: DFT/TD-DFT, thermal, antibacterial and anti-biofilm properties
Authors:	Das, Dhiraj (/jspui/browse?type=author&value=Das%2C+Dhiraj)
Keywords:	Antimicrobial Azide Cd(II) Coordination compounds
Issue Date:	2019
Publisher:	Elsevier
Citation:	Journal of Molecular Structure, 1179, pp.694-708.
Abstract:	<p>In this work we have reported two novel tetranuclear Cd(II) complexes viz. [Cd₄(LOMe)₂(μ_{1,1}-N₃)₃(μ_{1,3}-N₃)_n] (1) and [Cd₄(LOEt)₂(μ_{1,1}-N₃)₃(OAc)]₂ (2) where (H₂LOMe) and (H₂LOEt) are two important less explored salen-type Schiff base ligands. Both of the complexes have been characterized by using routine spectroscopic techniques, elemental analyses (C, H and N), X-ray powder diffraction pattern (PXRD) and thermal analysis by TGA along with single x-ray crystallography. The complete structural study discloses that in both cases the fully deprotonated ligand [LOMe]₂⁻ or [LOEt]₂⁻ utilized all potential coordination sites to accommodate four Cd(II) ions. Complex 1 is a one-dimensional polymer with azide (N₃) linkage having both (μ_{1,1} end on) and (μ_{1,3} end-to-end) azido bridging but complex 2 is a discrete octanuclear ensemble where two [Cd₄(O₄(N₂)₂)₂ units bridged to each other showing μ_{1,1} end on end on azide bridging. Exploration of photo physical properties in DMSO solvent reveals that Cd(II) complexes enhance appreciably the fluorescence behavior over free Schiff base ligands (H₂LOMe) and (H₂LOEt). DFT calculations performed at B3LYP/def2-TZVP level of theory reveal both the energetics and composition of FMOs in these complexes and also show electrophilic and nucleophilic areas via molecular electrostatic maps [ESP] concept. The antibacterial, membrane damage assay and anti-biofilm properties of complexes 1 and 2 were investigated very carefully against some important Gram-positive and Gram-negative bacterial strains.</p>
Description:	Only IISERM authors are available in the record.
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