Title:	Synthesis, characterizations and single crystal structure of di-nuclear azido-bridged Cd(II) coordination polymer with Schiff base precursor (H2LpentOMe): DFT, fluorescence, solvatochromism and in vitro antimicrobial assay
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Keywords:	Azide Antibacterial Cd(II) DFT Schiff base
Issue Date:	2019
Publisher:	Elsevier
Citation:	Inorganica Chimica Acta, 496.
Abstract:	A di-nuclear azido-bridged Cd(II) 1-D coordination polymer [Cd2(H2LpentOMe)(μ1,1-N3)2]n (1) has been successfully synthesized using less explored bi-compartmental Schiff base ligand (H2LpentOMe) and characterized by elemental analysis, FT-IR, FT-Raman, UV–Visible, SEM-EDAX, powder X-ray diffraction and fluorescence spectroscopy. Solid-state X-ray single crystal study revealed two different geometrical environment of Cd metal centres with distorted square pyramidal (Cd1) and distorted pentagonal bipyramid (Cd2). Overall, small-sized azide ions in asymmetric unit act as μ1,1 bridging mode. Geometry is optimized in gas phase using ORCA 3.0.3 and B3LYP level TZVP basis set to explain frontier molecular orbitals (FMO), molecular electrostatic potential (MEP) and global reactivity. The HOMO-LUMO energy gap (3.434 Ev) suggests that chemical reactivity of complex 1 is low but fairly stable. Moreover, molecular electrostatic potential map was drawn to identify reactive regions in terms of electrophilic and nucleophilic. The steady state and time-resolved fluorescence properties have been explored in DCM and solid-state condition at room temperature. Complex 1 exhibit bi and tri-exponential decay in DCM as well as solid-state. The fluorescence behaviours are predominantly intra-ligand in nature (π → π*) with lifetimes in the range (1.16–1.11 ns). Solvatochromism has been reported to show solvent dependent absorption and fluorescence spectral changes. Fascinatingly, red shifted solvatochromism was observed upon increasing solvent polarity. Finally, concentration dependent antimicrobial activity was investigated against two standard bacterial strains (Staphylococcus aureus (ATCC 25923) and Methicillin-resistant Staphylococcus aureus (MRSA) where 250 μg/ml concentration of complex 1 is sufficient to show the antimicrobial effect.
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