Title:	Syntheses, X-ray crystal structures of two new Zn(II)-dicyanamide complexes derived from H2vanen-type compartmental ligands: Investigation of thermal, photoluminescence, in vitro cytotoxic effect and DFT-TDDFT studies
Authors:	Das, Dhiraj (/jspui/browse?type=author&value=Das%2C+Dhiraj)
Keywords:	Schiff base Zn(II) Dicyanamide DFT Cytotoxic Photoluminescence
Issue Date:	2019
Publisher:	Elsevier
Citation:	Inorganica Chimica Acta, 492, pp.221-234.
Abstract:	Two new dicyanamide modulated zinc metal complexes [Zn4(LOMe)2(μ1-dca)2(μ1,5-dca)2] (1) and [Zn3(LOEt)2(H2O)(μ1-dca)(μ1,5-dca)] (2) have been synthesized using H2vanen-type compartmental ligands. Schiff base ligands and the complexes were characterized by means of elemental analyses, FT-IR, FT-Raman, UV–Visible, powder X-ray diffraction, TGA and fluorescence spectroscopy. Dicyanamide modulated Zn4/Zn3-nuclear metal complexes were structurally characterized by single crystal X-ray diffraction studies. In 1, the asymmetric Zn2-nuclear unit was ensembled with one fully deprotonated Schiff base ligand [LOMe]2− along with two dicyanamide ions where two structurally independent Zn(II) metal centers are found in the X-ray crystal structure. Single X-ray crystal structure confirmed the environment of Zn1 is distorted square pyramidal whereas Zn2 acquires distorted tetrahedral geometry. Unlike 1, in 2 three independent zinc metal centers have been identified as square pyramidal (Zn1), distorted trigonal bipyramidal (Zn2) and distorted tetrahedral (Zn3). 1 and 2 geometry were optimized using hybrid B3LYP functional with DGDZVP basis set to explain frontier molecular orbitals, molecular electrostatic potential and Hirshfeld surface (dnorm surfaces and 2D fingerprint plots). The electronic UV–Vis properties were determined by TD-DFT approach. The steady state and time-resolved fluorescence properties have been explored in DMSO solution. 1 and 2 exhibit bi-exponential decay and intra-ligand (π → π*) fluorescence behaviors with lifetimes in the range (2.45–5.71 ns). In addition, complexes solid-state and different solvent-dependent absorption and fluorescence spectra have been reported. Finally, the cytotoxic effect of the investigated dicyanamide complexes against breast cancer cell line (MCF7) shows promising results which makes them prospective complexes for anticancer medicament studies.
Description:	Only IISERM authors are available in the record.
URI:	https://www.sciencedirect.com/science/article/pii/S0020169319302956 (https://www.sciencedirect.com/science/article/pii/S0020169319302956) http://hdl.handle.net/123456789/1992 (http://hdl.handle.net/123456789/1992)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/1992/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/1992?mode=full)

(/jspui/handle/123456789/1992/statistics)