



# Library Indian Institute of Science Education and Research Mohali



**DSpace@IISERMohali (/jspui/)**

**/ Publications of IISER Mohali (/jspui/handle/123456789/4)**

**/ Research Articles (/jspui/handle/123456789/9)**


Please use this identifier to cite or link to this item: <http://hdl.handle.net/123456789/1693>

Title:	Nitrato, Pseudohalo-Linked Zn(II)/Cd(II) Schiff-Base Complexes with 1,3-Diimine Spacer Group: Syntheses, Crystal Structures, DFT, TD-DFT and Fluorescence Studies
Authors:	Das, Dhiraj (/jspui/browse?type=author&value=Das%2C+Dhiraj)
Keywords:	Azide Cd(II)/Zn(II) Complex DFT study Fluorescence TD-DFT
Issue Date:	2018
Publisher:	Wiley-Blackwell
Citation:	Chemistry Select, 3(43), pp. 12371-12382
Abstract:	Self assemblies of (N2O4) salen-type bi-compartmental ligand (H2L <sup>Me</sup> ) [N,N'-Bis(3-methoxysalicylideneimino)-1,3-diaminopropane] afforded two series of complexes, a trinuclear nitrate [Cd3(L <sup>Me</sup> )2(NO3)2] (1) and a dinuclear (η <sup>1</sup> -N3) [Zn2(L <sup>Me</sup> )(η <sup>1</sup> -N3)2(CH3OH)2] (2). Elemental analysis, UV-visible and Fourier transform Infrared spectroscopic methods were employed successfully to characterize the complexes. Single-crystal X-ray studies reveal that complex 1 consists of planar trinuclear Cd(II)3 core coordinated by two fully deprotonated dianionic ligands [L <sup>1</sup> ] <sup>2-</sup> and nitrato (NO <sub>3</sub> <sup>-</sup> ) bridging but complex 2 is a centrosymmetric hexacoordinated Zn(II) double end-on azide (η <sup>1</sup> -N3) with methanol as co-ligands. Both complexes satisfied a common 4-membered M(II)2(μ <sub>2</sub> -O)2 basic structural core. Fluorescence properties in DMSO solvent reveal that complexes enhance appreciably the fluorescence behavior over free salen-type ligand (H2L <sup>Me</sup> ). Complexes are optimized using Density functional theory calculated at B3LYP/TZVP level of theory to obtain insights into optimized structure, Frontier molecular orbital, Electrostatic potential maps, charge analyses gives an insight into the electronic structure and charge/potential distribution in the molecule etc. which substantiate the experimentally observed supramolecular interactions. Existing different non-covalent supramolecular interactions have been explained by means of Hirshfeld surface and 2D fingerprint plot analysis. Further theoretical explanations for the observed experimental electronic spectra of both complexes were explained by using Time-dependent density functional theory level of calculations.
Description:	Only IISERM authors are available in the record.
URI:	<a href="https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/slct.201802996">https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/slct.201802996</a> ( <a href="https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/slct.201802996">https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/slct.201802996</a> ) <a href="http://hdl.handle.net/123456789/1693">http://hdl.handle.net/123456789/1693</a> ( <a href="http://hdl.handle.net/123456789/1693">http://hdl.handle.net/123456789/1693</a> )
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/1693/1/Need%20to%20add%20pdf.odt)		8.04 kB	OpenDocument Text	<a href="#">View/Open (/jspui/bitstream/123456789/1693/1/Need%20to%20add%20pdf.odt)</a>

Show full item record (</jspui/handle/123456789/1693?mode=full>)

 (</jspui/handle/123456789/1693/statistics>)

Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.