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Title:	Mononuclear Ni(II) and dinuclear Cd(II) complexes of 4-phenyl-2H-1,2,4-triazole-3-thione and Mn(II) catalyzed disulphide bond formation in 3,3'-dithiobis (4-phenyl-1,2,4-triazole): Syntheses, structural characterization, thermal analysis and DFT calculation
Authors:	Singh, Sanjay (/jspui/browse?type=author&value=Singh%2C+Sanjay)
Keywords:	Photo luminescent properties Thermal behavior DFT calculation 1,2,4-Triazole
Issue Date:	2014
Publisher:	Elsevier
Citation:	Inorganica Chimica Acta, 421, pp.519-530.
Abstract:	New complexes [Ni(phtt)2(en)2] (2) and [Cd2(μ-phtt)2(phtt)2(bpy)2] (3) have been synthesized by the reactions of M(NO3)2·xH2O and 4-phenyl-2H-1,2,4-triazole-3-thione (Hphtt) in the presence of ethylenediamine/bipyridy. Mn(NO3)2·4H2O yielded a new compound 3,3'-dithiobis (4-phenyl-1,2,4-triazole) (1, dbpht) by aerial oxidation of Mn(II) which oxidized the ligand. The compounds have been characterized by various physicochemical methods. In complex 2, the nickel centre is bonded through the triazole ring nitrogen whereas in complex 3, cadmium is bonded through the thiolato sulfur forming a dimeric structure via thiolato bridging. Complexes are stabilized by various types of inter and intramolecular hydrogen bonding. The DFT results of optimized molecular geometry of all compounds are presented and compared with the experimental X-ray diffraction data. Thermogravimetric analyses of the complexes have been investigated which indicate for NiO and CdS as the final residue. Photoluminescence properties indicate that complex 2 is nonfluorescent and complex 3 has characteristic fluorescence emissions which make it a desirable target for photophysical studies and electronics applications.
Description:	Only IISERM authors are available in the record.
URI:	<a href="https://www.sciencedirect.com/science/article/pii/S0020169314004071?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S0020169314004071?via%3Dihub</a> ( <a href="https://www.sciencedirect.com/science/article/pii/S0020169314004071?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S0020169314004071?via%3Dihub</a> ) <a href="http://hdl.handle.net/123456789/2820">http://hdl.handle.net/123456789/2820</a> ( <a href="http://hdl.handle.net/123456789/2820">http://hdl.handle.net/123456789/2820</a> )
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