



# 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/123456789/2965>


Title:	Manganese(II) and zinc(II) complexes of 4-phenyl(2-methoxybenzoyl)-3-thiosemicarbazide: Synthesis, spectral, structural characterization, thermal behavior and DFT study
Authors:	Singh, Sanjay (/jspui/browse?type=author&value=Singh%2C+Sanjay)
Keywords:	DFT Thiosemicarbazide Mn(II) and Zn(II) complexes Crystal structure Supramolecular architecture TGA
Issue Date:	2014
Publisher:	Elsevier
Citation:	Polyhedron,73, pp.98-109.
Abstract:	The ligand 4-phenyl(2-methoxybenzoyl)-3-thiosemicarbazide (Hpmt), forms isostructural [Mn(pmt) <sub>2</sub> (o-phen)] (1) and [Zn(pmt) <sub>2</sub> (o-phen)] (2) complexes containing o-phen as coligand which have been characterized by analytical, spectroscopic (IR, UV-Vis, NMR), magnetic susceptibility, TGA and single crystal X-ray data. Both complexes crystallize in monoclinic systems with the space group P2 <sub>1</sub> /n. The complexes have distorted octahedral geometry around the metal center. The ligand in the complexes is coordinated through the deprotonated hydrazinic nitrogen and carbonyl oxygen. The hydrazinic nitrogen coordinates with a shorter M-N distance than the o-phen nitrogen and bond lengths in the chelate ring systems are intermediate between single and double bond distances, suggesting considerable delocalization of charge. There is a good agreement between the geometrical parameters obtained by X-ray crystallography to those generated by DFT method. The thermal degradations of complexes 1 and 2 have been investigated by thermogravimetric analyses which indicate that the final residues left are Mn(NCO) <sub>2</sub> and Zn(NCSNH) <sub>2</sub> . The small HOMO-LUMO energy gap suggests low excitation energy for the complexes.
Description:	Only IISERM authors are available in the record.
URI:	<a href="https://www.sciencedirect.com/science/article/pii/S0277538714001053?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S0277538714001053?via%3Dihub</a> ( <a href="https://www.sciencedirect.com/science/article/pii/S0277538714001053?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S0277538714001053?via%3Dihub</a> ) <a href="http://hdl.handle.net/123456789/2965">http://hdl.handle.net/123456789/2965</a> ( <a href="http://hdl.handle.net/123456789/2965">http://hdl.handle.net/123456789/2965</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/123456789/2965/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text

[View/Open \(/jspui/bitstream/123456789/2965/1/Need%20to%20add%20pdf.odt\)](#)

Show full item record (</jspui/handle/123456789/2965?mode=full>)

 (</jspui/handle/123456789/2965/statistics>)

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