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Syntheses and characterization of mononuclear Zn(II), Cd(II) and Hg(II) complexes of 2-[(3, 5-Dibromo-2-hydroxy-benzylidene)-amino]-2-hydroxymethyl-propane-1,3-diol: Photoluminescence properties and DFT study

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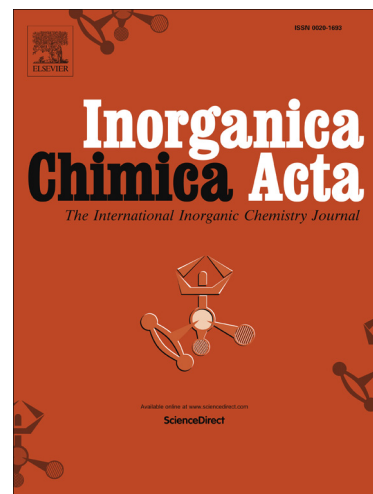
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Syntheses and characterization of mononuclear Zn(II), Cd(II) and Hg(II) complexes of 2-[(3, 5-Dibromo-2-hydroxy-benzylidene)-amino]-2-hydroxymethyl-propane-1,3-diol: Photoluminescence properties and DFT study

Sourav Chatterjee,^a Ishani Majumder,^b Aratrika Chakraborty^b, Madhulata Shukla^{*,c}, Tanmay Chattopadhyay^{*,a}

^a Department of Chemistry, Panchakot Mahavidyalaya, Sarbari, Purulia, Pin-723121, India,
E-mail: tanmayc2003@gmail.com

^b Department of Chemistry, University of Calcutta, 92 A. P. C. Road, Kolkata-700009, India.

^c Department of Chemistry, Faculty of Science, Banaras Hindu University, Varanasi, 221005, India.
E-mail address: madhu1.shukla@gmail.com.

Abstract

A new Schiff-base ligand **HL** ((2-[(3, 5-Dibromo-2-hydroxy-benzylidene)-amino]-2-hydroxymethyl-propane-1,3-diol)) was obtained by the 1: 1 condensation of 1, 3-dibromo salicylaldehyde and (tris hydroxy methyl) amino methane. Then three new complexes, [**Zn(L)**]₂, [**Cd(L)**]₂ and [**Hg(L)**]₂, have been prepared by the reaction of zinc(II), cadmium(II) and mercury(II) chlorides with the ligand and characterized by routine physicochemical techniques. Complex **1** has further been characterized by single crystal X-ray structural analyses. The ligands, as well as all three complexes, are highly fluorescent. For the ligand, the emission band is attributed to a $\pi \rightarrow \pi^*$ transition, whereas for the complexes the emissions may be assigned to ligand-to-metal charge transfers (LMCT). DFT calculation of all the three complexes has also been done.

Key Words: Schiff base, Zinc complex, Cadmium complex, Mercury complex, Photoluminescence and DFT study

1. Introduction

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