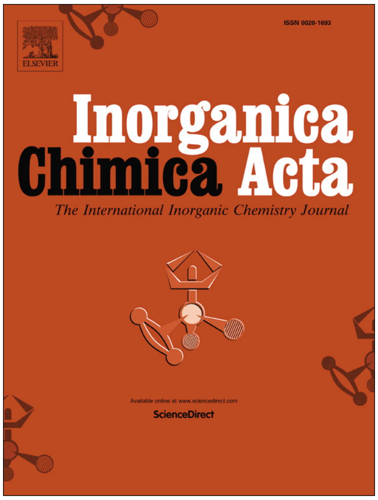

Research paper

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Isostructural zinc and cadmium silanethiolates with bridging biimidazole co-ligands – enhanced luminescence of zinc complex

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Abstract

Two dinuclear complexes of zinc and cadmium with silanethiolate and bridging biimidazole ligands are characterized by X-ray diffraction, FT-IR, UV-Vis and emission spectroscopies. Despite their identical ligand composition and isostructurality, the complexes **1** (Zn) and **2** (Cd) exhibit different electronic structures and entirely different character of frontier HOMO orbitals as indicated by DFT calculations. UV-Vis spectroscopy confirms the presence of distinct electronic transitions in zinc complex and luminescence studies prove its exceptionally strong emission properties.

Keywords

Zinc; Cadmium; Silanethiolates; Biimidazole; Crystal structure; Luminescence

Introduction

The design of hybrid inorganic-organic coordination compounds is a subject of constant research, mainly because of the possibility to combine properties of both classes of chemicals [1]. Much attention has been attracted by biimidazole ligands due to a number of potential application areas, e.g. in the field of catalysis, pharmaceutics, functionalized materials [2]. This class of N-donors can also serve as building blocks of supramolecular frameworks [3]. Moreover, biimidazole ligands were used to construct biomimetic models of multi-histidine metal binding sites [4].

Planar conformation of biimidazole molecule allows electronic interactions between two covalently bound aromatic rings and optimum delocalization of π electrons [5]. Consequently, biimidazoles in the neutral form usually act as chelating bidentate ligands [1-6]. However, the