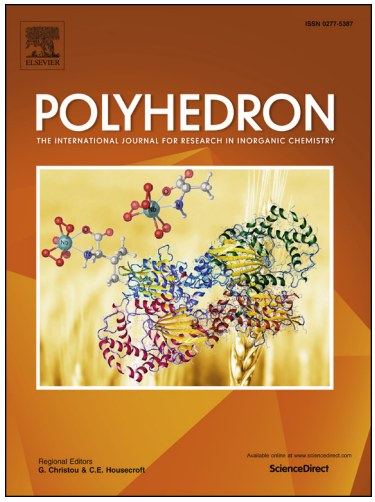

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Organic solvents-soluble zinc (II) and cadmium (II) complexes based on 2-aryl substituted-8-hydroxyquinoline: Synthesis, crystal structures, photoluminescence, thermal and theoretical studies

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Abstract

Two novel C-2 position modified 8-hydroxyquinoline ligands, (*E*)-2-[(4-tert-butylphenyl)ethenyl]-8-hydroxyquinoline (**L_1**) and (*E*)-2-[(2-chloro-3,4-dimethoxyphenyl)ethenyl]-8-hydroxyquinoline (**L_2**) as well as their zinc (II) and cadmium (II) complexes, namely $Zn_2(L_1)_4$, $Cd_3(L_1)_6$, $Zn_3(L_2)_6$ and $Cd_3(L_2)_6$ were designed and synthesized. Thanks to the introduction of aromatic tert-butyl and methoxy, ligands **L_1** and **L_2** are highly soluble and complexes are having good solubility in dimethyl sulfoxide (DMSO) and chloroform. X-ray structural analysis indicate four complexes were in *P21/c*, *P2/c*, *P-1*, *C2/c* space group, respectively, and exhibit a monoclinic crystal system except $Zn_3(L_2)_6$, which hold a triclinic crystal system. Structural formulea and coordinating behavior of these complexes were also investigated by NMR, UV–vis and fluorescence spectroscopic titrations in solution, revealing four complexes were well coordinated. Solid state photoluminescence studies reveal they emit strong yellow-orange luminescence at 568-612 nm with 5.47-11.79 ns lifetime. Thermogravimetric and theoretical electronic structure analysis indicate that four complexes appear to be promising candidates for the application as yellow luminescent materials.

Keywords: Soluble; 2-aryl substituted; 8-hydroxyquinoline; Photoluminescence; TD-DFT.

1. Introduction

8-hydroxyquinoline, a monoprotic bidentate chelating agent, was found highly sensitive and efficient to bind and precipitate metal ions in the field of gravimetric analysis by tuning pH of the media [1-2]. Yet have come to the fore in constructing light-emitting metal complexes since the representative tris-(8-hydroxyquinoline) aluminum (AlQ_3) developed serving as the emitting and electron transport material in multi-layered organic light emitting diodes (OLEDs) by Tang and VanSlyke [3]. The groundbreaking applications of 8-hydroxyquinoline based metal complexes in organic optoelectronic filed attract increased attention because of their remarkable thermal stability,