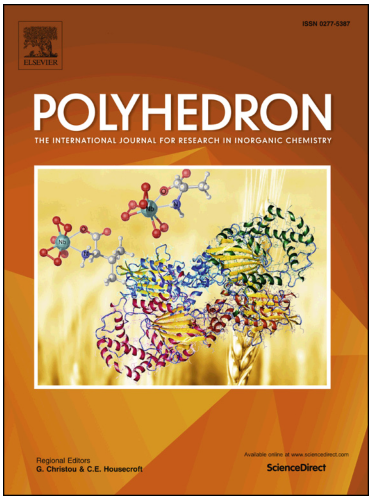

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Molecular structures and fluorescence property of Zn(II), Cd(II) complexes of 3-pyridyl-5-aryl-(1*H*)-1,2,4-triazoles

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ABSTRACT

The reaction of two 3-pyridyl-5-aryl substituted 1,2,4-triazole ligands (**trz-1** and **trz-2**) with $M(NO_3)_2$ and MCl_2 ($M = Zn^{II}/Cd^{II}$) afforded the metal complexes [Zn(**trz-1**)Cl_2], [Cd(**trz-1**)$_2(NO_3)_2$] and [M^{II}(**trz-2**)$_2](NO_3)_2\cdot H_2O$ (M = Zn, Cd). The reaction of $Cd(NO_3)_2$, **trz-2** and NaNCS in a 1:1:1 molar ratio resulted in the formation of the complex [Cd(**trz-2**)$_2(NCS)_2$]. These complexes have been characterized by spectroscopic analyses and X-ray crystallography. The crystal structures of the complexes show the presence of classical as well as non-classical C–H···O, C–H···F and C–H···S hydrogen bonds, along with a strong π···π interaction between the triazole moieties. The complexes exhibit strong fluorescence emissions both in the solid state and in DMSO solution. Further, the intraligand charge transfer origin of the emission in these complexes has been confirmed by DFT and TD-DFT studies.

Keywords: 1,2,4-Triazole, Fluorescence, Non-classical hydrogen bond, Intraligand charge transfer, TD-DFT.

1. Introduction

Triazoles are nitrogen rich heterocycles which can be considered as a structural combination of pyrazole and imidazole for the relative disposition of the three nitrogen atoms in the heterocyclic backbone [1]. Triazoles are broadly categorized into two classes, namely, 1,2,3-triazole and 1,2,4-triazole [2]. Multidentate 1,2,4-triazole based ligands offer versatile coordination chemistry as tuning of the substituents on the triazole ring leads to the formation of