Data in Brief 19 (2018) 2119–2125

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Data on a real-time tripodal colorimetric/fluorescence sensor for multiple target metal ions

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ARTICLE INFO

Article history:
Received 28 March 2018
Received in revised form
21 June 2018
Accepted 27 June 2018
Available online 2 July 2018

ABSTRACT

Currently considerable research both in life and in environmental sciences is dedicated to chemosensors able to detect metals of biological interest such as zinc and iron or other toxic and carcinogenic, as cadmium, mercury, chromium, lead. Recently, a new chemosensor strategy of "single chemosensor for multiple metals" has emerged. For this scope, many fluorescent sensors for Cd(II) and Zn(II) have been designed and synthetized, as ligand systems or in polymeric matrices [1–3]. The data presented in this article include experimental data on the of a pyridyl/phenolic/benzothiazole functionalized colorimetric receptor (**BPAP**) and its selectively recognise Fe(III) and Fe(II) ions with visible, naked eye colour changes and fluorometric selectivity towards Zn^{2+} and Cd^{2+} ions in aqueous medium.

This article is submitted as a companion paper to Caruso et al. (2018) [4].

DOI of original article: https://doi.org/10.1016/j.dyepig.2018.03.055
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https://doi.org/10.1016/j.dib.2018.06.096

Specifications Table

Subject area	*Chemistry, Materials Science*
More specific subject area	*Electro-optic field sensors*
Type of data	*Crystal data and structure refinement, NMR spectrum, tables and figure*
How data was acquired	*NMR recorded in DMSO using Bruker Spectrometers operating at 400 MHz.* *UV-Visible and fluorescence spectra recorded with JASCO spectrometers.* *Single crystals X-ray structural analysis performed on a BrukerNoniusKappaCCD diffractometer equipped with Oxford Cryostream apparatus.*
Data format	*Raw data and their elaborations*
Experimental factors	*The data concerns structural information, UV/Vis calculation and some spectroscopic raw data*
Experimental features	*Elaboration of X-ray diffraction data and UV/Vis curves*
Data source location	*Naples, Italy*
Data accessibility	*Data is within this article*

Value of the data

- The data show some molecular structure of **BPAP** along **a** and **c** axes.
- The data report relevant structural data of **BPAP** and its zinc complex (lengths and angles).
- The data report Job's plot analysis for the binding Zn(II) and Cd(II) with ligand system.
- ^{1}H NMR and ^{13}C NMR of BPAP and BPAP metal complexes are reported.

1. Data

The data presented in this article are related to the research article entitled “A real-time tripodal colorimetric/fluorescence sensor for multiple target metal ions” [4]. Recently an impressive progress has been done toward the design and synthesis of novel sensitive ligands and fluorescent materials [5–8]. The data presented here include experimental data on the of a pyridyl/phenolic/benzothiazole functionalized colorimetric receptor (**BPAP**) and its selectively recognise Fe(III) and Fe(II) ions with visible, naked eye colour changes and fluorometric selectivity towards Zn^{2+} and Cd^{2+} ions in aqueous medium.

The following data are a necessary support for the identification of materials and properties of the ligand system and its complexes.

2. Experimental design, materials and methods

Structural analysis of single crystals of ligand and its Zinc complex has been performed on a BrukerNoniusKappaCCD diffractometer equipped with Oxford Cryostream apparatus (graphite monochromated MoK_α radiation, $\lambda = 0.71073$ Å, CCD rotation images, thick slices, φ and ω scans to fill asymmetric unit). Semiempirical absorption corrections (SADABS [9]) were applied. Both the two structures were solved by direct methods (SIR97 program [10]) and anisotropically refined by the full matrix least-squares method on F^2 against all independent measured reflections using SHELXL-2016 [11] and WinGX software [12]. Crystal data and structure refinement details are reported in Table 1. Relevant bond lengths and angle are reported in Table 2. The figures were generated using ORTEP-3 [13] and Mercury CSD 3.9 [14] programs. Molecular structure of **BPAP** along **a** axis is shown in Fig. 1. Molecular structure of the complex Zn-**BPAP** along **c** axis is shown in Fig. 2.