



Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

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

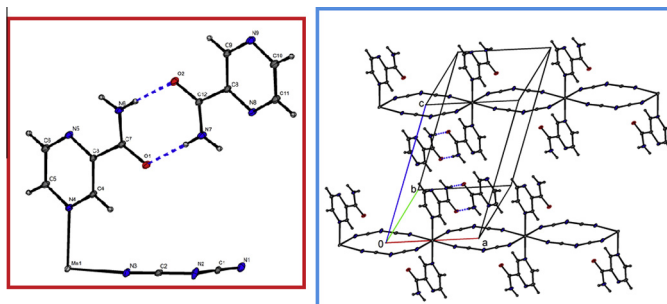
A novel one-dimensional manganese(II) coordination polymer containing both dicyanamide and pyrazinamide ligands: Synthesis, spectroscopic investigations, X-ray studies and evaluation of biological activities

Leila Tabrizi^a, Hossein Chiniforoshan^{a,*}, Patrick McArdle^b^a Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran^b School of Chemistry, National University of Ireland Galway, University Road, Galway, Ireland

HIGHLIGHTS

- A 1D coordination polymer of Mn(II) with ligands of dicyanamide (dca) and the pyrazinamide (PZA) was synthesized.
- The crystal structure of complex was determined.
- The complex evaluated for in vitro antibacterial and antitumor activities.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:

Received 18 September 2014

Received in revised form 6 December 2014

Accepted 17 December 2014

Available online 25 December 2014

Keywords:

Manganese(II)

Dicyanamide

Pyrazinamide

Antitumor activity

Antibacterial activity

ABSTRACT

A novel 1D coordination polymer $\{[\text{Mn}(\mu_{1,5}\text{-dca})_2(\text{PZA})_2](\text{PZA})_2\}_n$, **1**, has been synthesized and characterized by single crystal X-ray crystallography. The coordination mode of dicyanamide (dca) and pyrazinamide (PZA) ligands was inferred by IR spectroscopy. The compound **1** was evaluated for in vitro antimycobacterial and antitumor activities. It demonstrated better in vitro activity against *Mycobacterium tuberculosis* than pyrazinamide and its MIC value was determined. Complex **1** was also screened for its in vitro antitumor activity towards LM3 and LP07 murine cancer cell lines. In addition, the antibacterial activity of complex **1** has been tested against Gram(+) and Gram(−) bacteria and it has shown promising broad range anti-bacterial activity.

© 2014 Elsevier B.V. All rights reserved.

Introduction

The crystal engineering of novel coordination polymers is presently one of the major active fields in coordination chemistry and supramolecular and materials chemistry. These compounds attract considerable attention not only for their fascinating architectures

and topologies, but also due to the various practical applications in fields, ranging from molecular magnetism and adsorption science and gas storage to photoluminescence and catalysis [1–7].

There has been extensive interest in the coordination chemistry of manganese involving nitrogen and oxygen donor ligands due to the increasing identification of role of this metal in biological systems [8–11].

Pyrazinamide (PZA), chemical formula $\text{C}_5\text{H}_5\text{N}_3\text{O}$ is a member of the pyrazine family and it is known as a very useful

* Corresponding author. Tel.: +98 3113913261; fax: +98 3113912350.

E-mail address: Chinif@cc.iut.ac.ir (H. Chiniforoshan).

antimycobacterial agent, with a well established function in tuberculosis treatment, where it is able to shorten tuberculosis therapy from 9–12 to 6 months [12]. The appearance of strains resistant to PZA represents an important public health difficulty, where both primary and secondary line treatment schemes include PZA. Furthermore, molecular complexes having PZA as a ligand have been shown to have improved antimycobacterial properties [13]. Well known bioactive metal complexes include silver(I) sulfadiazine as an antimicrobial and antifungal agent and the anti-cancer drug cisplatin. Other metal complexes of for example Ga(III), Al(III), and Fe(III) have also been found useful in the treatment of malaria and many complexes of isoniazid and its hydrazone, ethambutol and pyrazinamide with Cu(II) or Ni(II) or macrocyclic compounds with V(IV), As(III), Fe(III), Bi(III), and In(III) have also been demonstrated to have antitubercular activity. Nevertheless, it is also well known that free heavy metal ions are highly toxic to mycobacteria, which can resist them, possibly by an extrusion mechanism [14–24].

PZA can coordinate through the pyrazine ring nitrogens and the C=O or $-\text{NH}_2$ groups. The strong hydrogen bonding properties of PZA and related carboxyamides, together with their ability to act as ligands in diverse complexes with transition metals, made them a potent tool for the synthesis of different distinct supramolecular complexes and highly organized coordination polymers [25–34].

Among the various types of anionic-bridging ligands, dicyanamide has been widely used because it is a versatile ligand with three nitrogen donor atoms and it may act as a uni-, bi-, and tridentate ligand. The variety of its coordination mode allows the preparation of large variety of architectures with one-, two-, and three-dimensional networks [35–46].

In this report, we have synthesized a novel 1D compound of manganese(II) with dca and PZA, which has the formula $\{[\text{Mn}(\mu_{1,5}\text{-dca})_2(\text{PZA})_2](\text{PZA})_2\}_n$, **1**, and has evaluated its antimycobacterial and antitumor activities against TB bacillus and murine tumor cell lines (LPO7 and LM3), respectively, as well as antibacterial assays. The details of synthesis, spectroscopic characterizations and X-ray structure of this complex are described below.

Experimental

Materials

All chemicals and solvents were purchased from Merck or Sigma-Aldrich and were used without any further purification. Pyrazinamide was obtained from the Abidi Pharmaceutical Company.

Physical measurements

Fourier transform infrared spectra were recorded on a FT-IR JASCO 680-PLUS spectrometer in the $4000\text{--}400\text{ cm}^{-1}$ region using KBr pellets. Elemental analysis was performed by using a Leco, CHNS-932 elemental analyzer.

Synthesis of $\{[\text{Mn}(\mu_{1,5}\text{-dca})_2(\text{PZA})_2](\text{PZA})_2\}_n$, **1**

An aqueous solution (10 cm^3) of MnCl_2 (125.8 mg, 1.0 mmol) and $\text{NaN}(\text{CN})_2$ (178.06 mg, 2.0 mmol) was stirred for 10 min, and an aqueous solution (50 cm^3) of PZA (492.4 mg, 4.0 mmol) was added dropwise. After filtration, the filtrate was then left to evaporate slowly. Colorless single crystals were obtained after several weeks. Yield: 75% (509 mg).

Elemental analysis result was in good agreement with the $\text{C}_{24}\text{H}_{20}\text{MnN}_{18}\text{O}_4$ stoichiometry for **1**. Found (calc.%): C, 42.36 (42.42);

N, 37.04 (37.11); H, 2.98 (3.06). IR data on KBr (ν , cm^{-1}) pellets: $\nu(\text{NH}_2)$: 3414 (s); $\nu(\text{aromatic C-H})$: 3069 (w); $\nu_s + \nu_{\text{as}}(\text{C}\equiv\text{N})$: 2322 (s); $\nu_{\text{as}}(\text{C}=\text{N})$: 2244 (s); $\nu_s(\text{C}=\text{N})$: 2176 (s); $\nu(\text{C}=\text{O})$: 1710 (vs); $\nu(\text{C}=\text{N})$: 1576 (s), (C=C): 1420 (s); $\nu_a(\text{C-N})(\text{dca})$: 1383; $\nu(\text{Ring breathing})$: 1088.

Crystal structure determination

Relevant results from data collection and structure solution are summarized in Table 1. Crystal of **1** was grown by slow evaporation from methanol solution. An Oxford Diffraction Xcalibur system was used to collect X-ray diffraction data. The crystal structure was solved by direct methods (Shelxt2014) and refined by full matrix least squares using Shelxl2014 within the Oscale package [47,48]. Non-hydrogen atoms were refined anisotropically.

Table 1
Crystallographic data for **1**.

1	
Empirical formula	$\text{C}_{24}\text{H}_{20}\text{MnN}_{18}\text{O}_4$
Formula weight	679.52
T/K	298.4(3)
Crystal system	Triclinic
Space group	$P\bar{1}$
$a/\text{\AA}$	7.5441(4)
$b/\text{\AA}$	7.6044(4)
$c/\text{\AA}$	14.6407(10)
$\alpha/^\circ$	75.622(6)
$\beta/^\circ$	78.758(5)
$\gamma/^\circ$	62.349(6)
$V/\text{\AA}^3$	717.57(9)
Z	1
μ (mm^{-1})	0.528
$D_{\text{calc}}/\text{Mg m}^{-3}$	1.572
$F(000)$	347
Θ Range/ $^\circ$	3.062–25.347
Independent reflections	2393 [$R(\text{int}) = 0.0325$]
Data/restraints/parameters	2393/159/214
Goodness-of-fit on F^2	1.073
Final R indices	$R1 = 0.0375$, $wR2 = 0.0954$
R indices (all data)	$R1 = 0.0458$, $wR2 = 0.0991$
Largest difference peak and hole ($e\text{\AA}^{-3}$)	1.150, -0.219

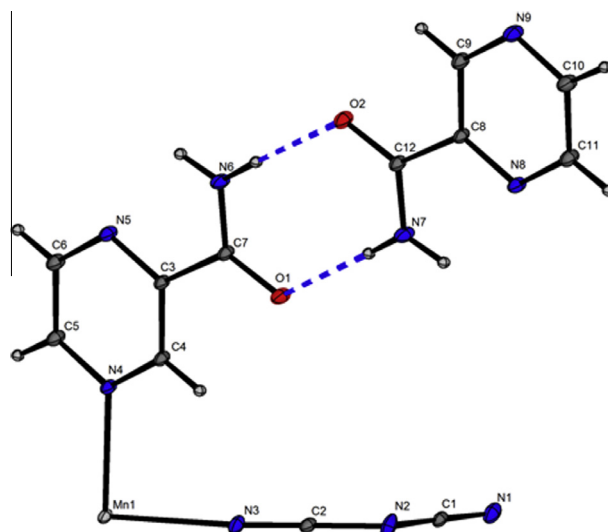


Fig. 1. ORTEP drawing with the atom-labeling scheme of the structural unit of complex **1**.

Download English Version:

<https://daneshyari.com/en/article/1232713>

Download Persian Version:

<https://daneshyari.com/article/1232713>

[Daneshyari.com](https://daneshyari.com)