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Structural Characterization of Zinc Coordination Polymer of Isonicotinoylhydrazone

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Abstract

The synthesis, structural elucidation, and crystallographic analysis of a novel hydrazone-based coordination polymer of zinc are presented. The compound was synthesized via the reaction of isonicotinoylhydrazide with an appropriate aldehyde derivative, followed by complexation with a zinc(II) salt under solvothermal conditions. Single-crystal X-ray diffraction studies revealed that the complex crystallizes in the monoclinic crystal system with the $P2_1/n$ space group. The asymmetric unit comprises one discrete coordination polymeric entity, and the unit cell accommodates four such molecules. The polymeric framework is stabilized by a network of weak intermolecular supramolecular interactions, including hydrogen bonding and π–π stacking, which govern the three-dimensional packing architecture. This study highlights the potential of hydrazone ligands in constructing metal-organic frameworks with defined geometries and packing arrangements, offering insights into their structural chemistry and possible functional applications in coordination-driven materials.

Keywords: Isonicotinoylhydrazide, Hydrazone, Crystal structure, Coordination polymer, Zinc complex, Supramolecular interactions

Introduction

Coordination polymers (CPs) are crystalline materials characterized by their highly ordered and extended architectures, composed of repeating coordination units that propagate in one, two, or three dimensions. These frameworks are constructed through the assembly of metal ions and organic ligands, which are connected via coordination bonds or, in some cases, through supramolecular interactions such as hydrogen bonding or π–π stacking interactions[^1,^2]. Among the various ligand systems employed, those containing both nitrogen atoms from pyridine rings and additional donor atoms like nitrogen or oxygen from acid hydrazide functionalities serve as versatile bifunctional coordinating agents. These ligands significantly enhance the potential for generating diverse CP structures and multimetallic complexes due to their ability to bind metal centers through multiple coordination sites[^3,^4].

The overall properties of coordination polymers—including their chemical reactivity, electronic behavior, and structural topology—are intricately governed by the specific nature of their metal-ligand interactions and spatial arrangement. These characteristics, in turn, directly influence their functional attributes such as electrical conductivity, luminescence, and magnetic responses[^5]. Moreover, CPs have attracted significant attention for their application potential in areas like heterogeneous catalysis, photocatalysis, and chemical sensing, owing to their tunable porosity, active metal centers, and high surface area[^6–^9].

Materials and Methods

Isonicotinoylhydrazide and formyl compounds were procured from Nice Chemicals and used without further purification. All organic solvents employed in the study were utilized as received.

Crystallographic data for the synthesized compound (DMN-INH) were collected using a CCD diffractometer equipped with monochromated MoKα radiation ($\lambda = 0.71073$ Å). Data acquisition and unit cell refinements were performed using the *APEX2* software suite, while *SAINT* and *XPREP* were utilized for data reduction and preliminary structure analysis.

Structure solution and refinement were carried out using *SIR92* and *SHELXL*, respectively. Molecular graphics and visual representations of the crystal structure were generated using *ORTEP3*.

Synthesis of the Metal Complex

A solution containing 10 mmol of isonicotinoylhydrazone dissolved in 15 mL of ethanol was prepared. To this solution, 10 mmol of zinc nitrate hexahydrate was added. The reaction mixture was then refluxed for 5 hours under constant stirring. Upon completion of the reaction, the resulting precipitate was filtered, washed, and dried under vacuum. The yield of the isolated complex was approximately 75%, with a melting point of 240°C.

Single crystals suitable for X-ray diffraction studies were obtained by slow crystallization of the complex from an acetic acid–methanol solvent mixture.

Results and Discussions

The reported zinc coordination polymer was found to be stable and insoluble in non-polar organic solvents, and was formulated by single-crystal X-ray analysis.

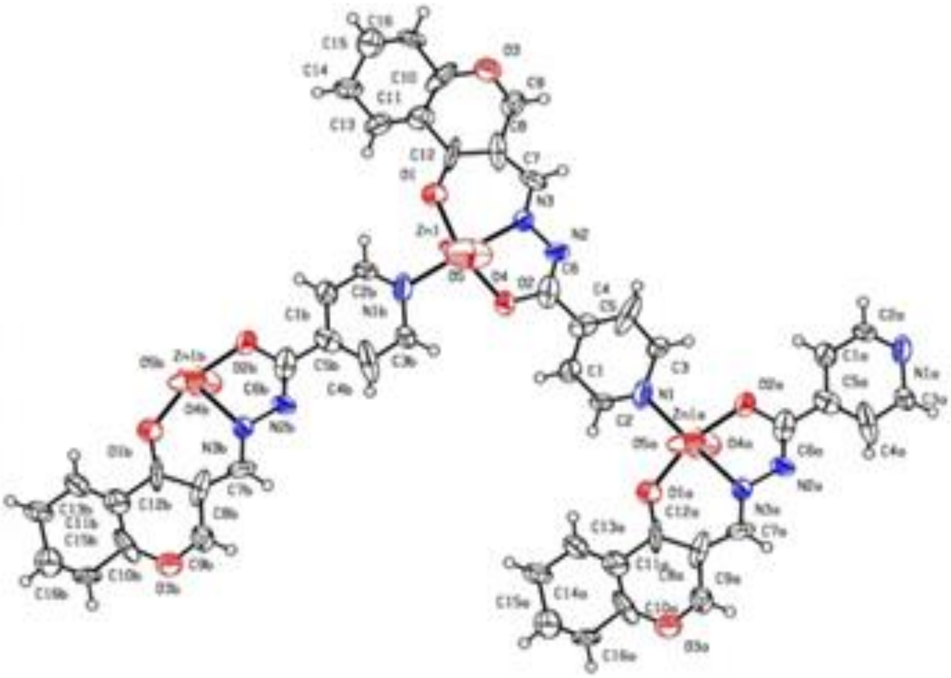

Fig. 1. ORTEP diagram

Table 1.: Structural details and refinement parameter

Empirical Formula	$C_{16}H_{10}N_3O_5Zn$
Formula Weight	389.64
Temperature	293K
Wavelength	0.71073Å
Crystal System	Monoclinic
Space Group	P21/n
Unit Cell Dimensions	a=9.3133(7) Å; alpha=90^{o}
	b=15.0916(11)Å; beta=97.810(3)^{o}
	c=18.4344(15)Å; gamma=90^{o}
Volume	2567.0(3)
Z, Calculated Density	4, 1.008
Absorption Coefficient	0.977
F(000)	788
Crystal size	0.35×0.35×0.30
Completeness to Theta=28.36	94.80%

Table 2.: Important bond lengths [Å]

Zn-O(1)	1.998	O(1)-C(12)	1.35(4)
Zn-O(2)	2.019(19)	N(2)-C(6)	1.24
Zn-N(1)	2.04(2)	N(2)-N(3)	1.41(2)
Zn-O(4)	2.13(3)	N(3)-C(7)	1.27
Zn-O(5)	2.150(17)	N(1)-C(2)	1.25(3)
Zn-N(3)	2.156(16)	N(1)-C(3)	1.52
O(3)-C(9)	1.29	N(1)-Zn	2.04(2)
O(3)-C(10)	1.41	C(6)-O(2)	1.36

Conclusion

2D zinc-coordination polymer was easily obtained by reacting isonicotinoylhydrazone and zincnitratehexahydrate under solvothermal method. Ethanol was used in the synthetic step. Good yield of isolated compound was obtained, and single-crystal x-ray diffraction revealed its polymeric nature.

Conflict of Interests

No conflicting financial interests exist for the authors.

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