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*NOTE*

# Hydrothermal Synthesis and Crystal Structure of a New 3D Zn(II) Coordination Polymer

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One new zinc compound $[Zn(L)(H_2O)_3]_n$ (**1**) ($H_2L$ = 5-hydroxyisophthalic acid) has been successfully synthesized. Compound shows a one-dimensional framework. The 3D supramolecular structure is formed *via* hydrogen bonding connection.

**Key Words: Coordination polymer, Crystal structure, Zinc(II).**

Metal organic frameworks (MOFs) have received much attention in the field of crystal engineering and supramolecular chemistry because of their diverse structures and promising applications in functional materials such as luminescent materials, gas adsorption and magnetism[1-4]. Hydrogen bonds are well suited for the design of polymeric arrangement and crystal engineering because of their important directional interactions and because they can interlink 1-D or 2-D structures into higher-dimensionality systems[5,6].

**Physical measurements:** All reagent and solvents employed were commercially available and used as received without further purification.

**Preparation of compound:** A mixture of 5-hydroxyisophthalic acid (1 mmol), $Zn(OAc)_2{\cdot}2H_2O$ (1 mmol) and distilled water (15 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 160 ºC for 96 h, followed by slow cooling to room temperature. Yellow crystals of the compound formed (Fig. 1).

**X-Crystallography:** Diffraction intensity data of the single crystal of the five compounds were collected on a Bruker SMART APEXII CCD diffractometer equipped with a graphite monochromated Mo-$K_\alpha$ radiation ($\lambda$ = 0.71073 Å) by using a $\omega$-scan mode. All the structures were solved by direct methods and refined by full-matrix least-squares methods on $F^2$ using the program SHEXL 97[7]. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement. The crystallographic data and experimental details of structural analyses for coordination polymers are summarized in Table-1. Selected bond and angle parameters are listed in Table-2. CCDC: 862872.

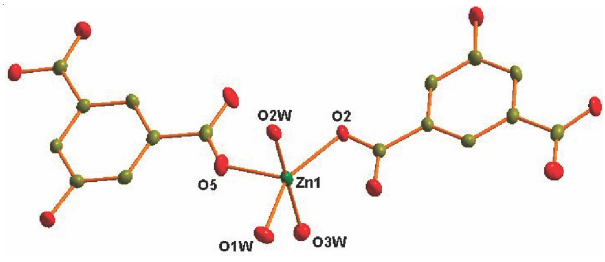


Fig. 1. Molecular structure of $[Zn(L)(H_2O)_3]_n$ at 30 % probability displacement ellipsoids

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

| | | | |
|---|---|---|---|
| Empirical formula | $C_8H_{10}O_8Zn$ | Z, Calculated density(mg/m$^3$) | 8,2.154 |
| Formula weight | 299.55 | Absorption coefficient(mm$^{-1}$) | 2.459 |
| Crystal system space group | Orthorhombic, Pccn | $F_{(000)}$ | 1344 |
| Unit cell dimensions | a = 18.325(5) Å, b = 7.397(5) Å, c = 15.081(5) Å | Limiting indices | $-23 \le h \le 21$, $-9 \le k \le 8$, $-19 \le l \le 19$ |
| Volume (Å$^3$) | 2044.2(16) | Largest diff. peak and hole (e/Å$^3$) | 0.782 and -0.670 |
| $\theta$ range for data collection | 2.22-27.52 | Goodness-of-fit on $F^2$ | 1.063 |
| Final R indices [I > 2$\sigma$ (I)] | $R_1$ = 0.0285 $wR_2$ = 0.0746 | R indices (all data) | $R_1$ = 0.0380, $wR_2$ = 0.0792 |

TABLE-2
SELECTED BOND LENGTHS (Å)
AND ANGLES (°) FOR Zn(II) COMPLEX

| | | | |
|---|---|---|---|
| Zn1-O5 | 1.9895 (19) | Zn1-O3W | 2.096 (2) |
| Zn1-O2 | 2.0348 (18) | Zn1-O2W | 2.139 (2) |
| Zn1-O1W | 2.043 (2) | – | – |
| O5-Zn1-O2 | 116.76 (7) | O2-Zn1-O3W | 95.35 (7) |
| O5-Zn1-O1W | 96.17 (8) | O1W-Zn1-O3W | 85.52 (8) |
| O2-Zn1-O1W | 147.01 (8) | O5-Zn1-O2W | 94.68 (8) |
| O5-Zn1-O3W | 90.96 (9) | O2-Zn1-O2W | 88.78 (7) |

Symmetry codes: (i).

**Structure description:** X-Ray diffraction analysis of $[Zn(L)(H_2O)_3]_n$ revealed that the fundamental building unit consists of one Zn(II) ions, two L and three coordinated water molecules. Each Zn(II) atom is five-coordinated by five oxygen atoms, showing a trigonal bipyramidal geometry. Each L anion adopts a monodentate coordination mode to link adjacent Zn atoms to form a 1D chain. The 1D chains are further assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 3D framework (Fig. 2).

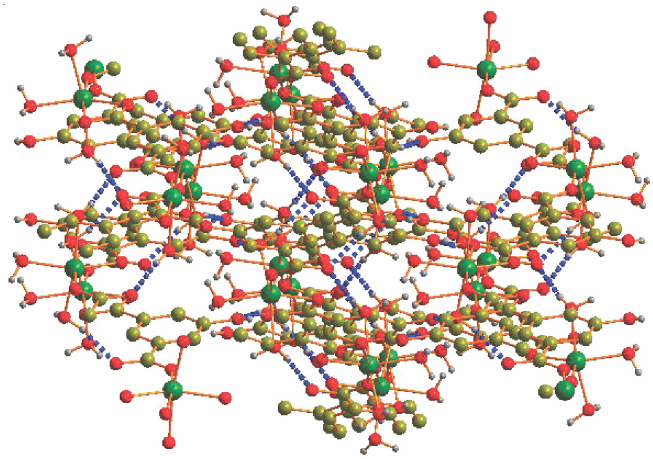

Fig. 2. 3D structure formed *via* hydrogen bonding interactions

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