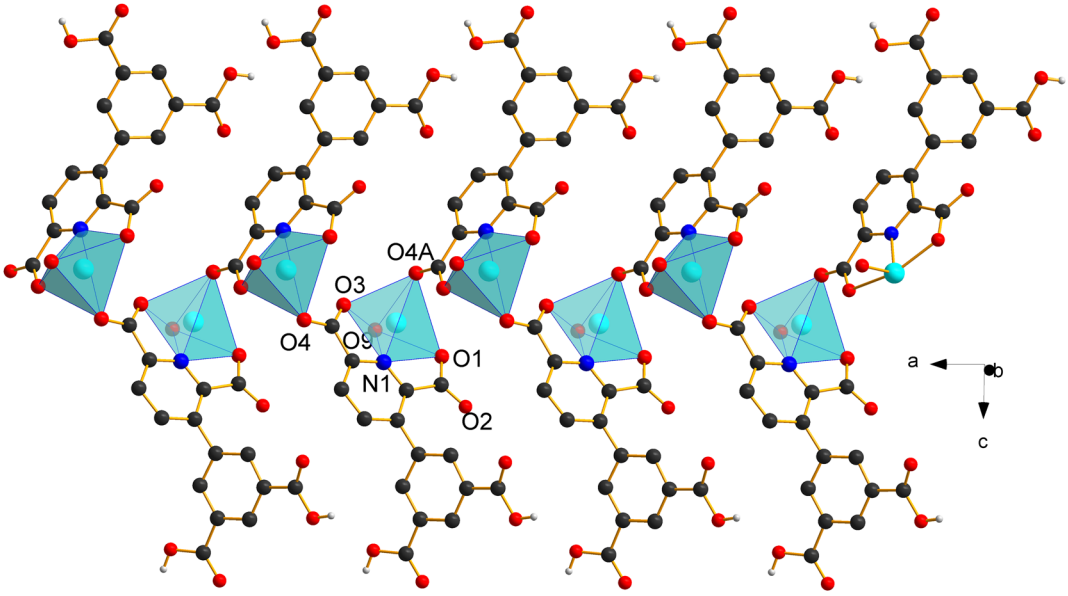
Yuan Gao and Shi Xie*

Crystal structure of catena-poly[monoaqua (u^2-(3-(3,5-dicarboxyphenyl)pyridine-2,6-dicarboxylic-k^4O:O′:O″:N)zinc(II))] monohydrate, $C_{15}H_{11}NO_{10}Zn$



https://doi.org/10.1515/ncrs-2025-0279
Received June 21, 2025; accepted August 21, 2025;
published online September 3, 2025

Abstract

$C_{15}H_{11}NO_{10}Zn$, orthorhombic, $P2_12_12_1$ (no. 19), a = 7.566(3) Å, b = 8.326(4) Å, c = 24.734(11) Å, V = 1558.0(12) Å^3, Z = 4, $R_{gt}(F)$ = 0.0311, w$R_{ref}(F^2)$ = 0.0810, T = 293 K.

CCDC no.: 2466128

1 Source of materials

A mixture of 10 mL DMF (N, N–dimethylformamide), 0.2 mmol $Zn(NO_3)_3$. $6H_2O$, 0.3 mmol 3-(3,5-dicarboxyphenyl) pyridine-2,6-dicarboxylic acid (DPPDA) was sealed in a 23 mL Teflon lined stainless steel container, and then heated at 373 K for 48 h. Finally, colorless block crystals were collected with a yield of about 50 % (calculated based on Zn) (Table 1).

2 Experimental details

The data were collected and processed using CrysAlis^{PRO}.[1] And the structure was solved by Direct Methods using Olex2 software[2] and refined with the SHELXL.[3] The hydrogen atom positions were fixed geometrically at the calculated distances and allowed to ride on the parent atoms. The U_{iso} of the H-atoms were set to 1.2 times U_{eq} of the parent atoms with C–H = 0.93 Å (aromatic) or 1.5 times in the case of hydroxyl groups and water molecules.

Over the past few decades, the design and preparation of coordination polymers (CPs) has attracted widespread attention due to their potential applications in fields such as fluorescent sensing, gas storage/separation and catalysis.[4–7] Many CPs constructed from aromatic carboxylate linkers have been extensively studied, particularly rigid aromatic carboxylate

***Corresponding author: Shi Xie**, Shenyang Institute of Science and Technology, No. 30 Quanyun Second West Road, Hunnan District, Shenyang, Liaoning Province, 110167, China,
E-mail: 15940418284@163.com. https://orcid.org/0009-0002-3121-0265
Yuan Gao, Shenyang Institute of Science and Technology, No. 30 Quanyun Second West Road, Hunnan District, Shenyang, Liaoning Province, 110167, China

Table 1: Data collection and handling.

Crystal:	Colorless prism
Size:	0.20 × 0.20 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.64 mm^{-1}
Diffractometer, scan mode:	Bruker P4, φ and ω scans
θ_{max}, completeness:	27.4°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	15,842, 3,553, 0.059
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3,453
$N(param)_{refined}$:	246
Programs:	Bruker,[1] Olex2,[2] Shelx[3]

linkers used to construct CPs, which can enhance their structural stability and light absorption.[8,9] The Zn(II) complex crystallizes in the orthorhombic system and $P2_12_12_1$ space group. The asymmetric unit contains one Zn(II) ion, one DPPDA dianion, one coordinated water molecule and one isolated water molecule. The Zn(II) ion locates in the center of a slightly distorted square pyramidal geometry, the apex oxygen atom of which is derived from the coordinated water molecule, and the square base of which is composed of three oxygen atoms (O1, O3, O4A, A = $-1/2 + x, 1/2 - y, 1 - z$) from two DPPDA dianion and one nitrogen atom (N1) from pyridine ring of DPPDA ligand. And the Zn–O/N bond distances range from 1.982(3) to 2.236(3) Å, which are within the normal range.[10–12] The coordination mode of DPPDA ligand is k^1–O, k^1–O, k^1–O, k^1–(N)-u_2 coordination mode. The two carboxylic groups substituted the benzene ring are not coordinated and are still in their original state. The O4 atom of the deprotonated carboxyl group connect the Zn (II) centers into an infinite one-dimensional helical chain structure with the distance of Zn–Zn is 5.013 Å along *a* axis. The lattice water molecules connect to the main chain via the O–H···O hydrogen bonds between carboxyl oxygen and coordinated water.

References

1. BRUKER. Saint, Apex2 and Sadabs; Bruker AXS Inc.: Madison, Wisconsin, USA, 2009.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. Olex2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.
3. Sheldrick, G. M. Crystal Structure Refinement with Shelxl. *ActaCrystallogr* **2015**, *C71*, 3–8.
4. Wang, S. J.; Song, W.; Liu, Y.; Li, Q.; You, L. X.; Xiong, G.; Ding, F.; Sun, Y. G. A Terbium Coordination Polymer Based on Mixed Rigid and Flexible Organic Ligands as a Luminescent Sensor for the Convenient Visual Detection of Ascorbic Acid. *Dyes Pigments* **2024**, *231*, 112403.
5. Fan, W. D.; Zhang, X. R.; Kang, Z. X.; Liu, X. P.; Sun, D. F. Isoreticular Chemistry Within Metal-Organic Frameworks for Gas Storage and Separation. *Coord. Chem. Rev.* **2021**, *443* (15), 213968.
6. Xiong, G.; Chen, X. L.; You, L. X.; Ren, B. Y.; Ding, F.; Dragutan, I.; Dragutan, V.; Sun, Y. G. La–Metal–Organic Framework Incorporating Fe_3O_4 Nanoparticles, Post-Synthetically Modified with Schiff Base and Pd. A Highly Active, Magnetically Recoverable, Recyclable Catalyst for C–C cross-couplings at Low Pd Loadings. *J. Catal.* **2018**, *361*, 116–125.
7. Kirchon, A.; Feng, L.; Drake, H. F.; Joseph, E. A.; Zhou, H. C. From Fundamentals to Applications: A Toolbox for Robust and Multifunctional MOF Materials. *Chem. Soc. Rev.* **2018**, *47*, 8611–8638.
8. Wang, K. C.; Li, Y. P.; Xie, L. H.; Li, X. Y.; Li, J. R. Construction and Application of Base-Stable MOFs: A Critical Review. *Chem. Soc. Rev.* **2022**, *51*, 6417–6441.
9. Xiong G., Qin X. Y., Shi P. F., Hou Y. L., Cui J. Z., Z. Bin. New Strategy to Construct Single-Ion Magnets: A Unique Dy@Zn_6clustCr exhibEting Slow SagneMic RelaxRtion. Chem. Commun., **2014**, *50*, 4255–4257.
10. Song, J.; Wu, M.; Zhou, Y. L.; Jin, L. X.; Gao, Y. H.; Dai, H. P. The Effect of Ligand/Metal-Ligand Ratio on the Structural Architectures of Five Different 1D Zinc(II) Coordination Polymers with Pyridyl Derivative Ligands. *J. Mol. Struct.* **2024**, *1307*, 137955.
11. Ghosh, T. K.; Rao, G. R. Design and Synthesis of Mixed-Ligand Architectured Zn-Based Coordination Polymers for Energy Storage. *Dalton Trans.* **2023**, *52*, 5943–5955.
12. Liu, X.; Du, L.; Wang, Y.; Li, R.; Feng, X.; Ding, Y. Synthesis, Crystal Structures and Properties of Two Nickel (II) Complexes with Different Nitrogen-Heterocyclic Polycarboxylate Ligand. *J. Mol. Struct.* **2019**, *1186*, 224.