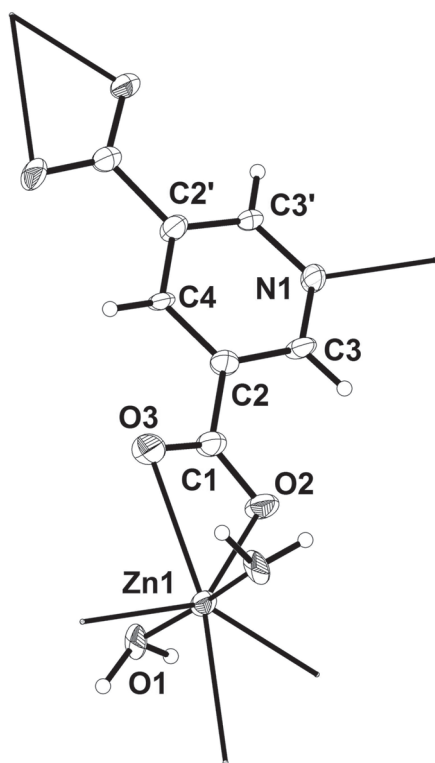


Dong-Mi Li*, Xue-Li Xu and Shi-Hui Li

Crystal structure of poly[aqua-(μ_3 -pyridine-3,5-dicarboxylato- $\kappa^5 O, O':O'', O''', N$)zinc(II)], $C_7H_7NO_6Zn$



A part of the 2D polymeric structure of the title compound is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.41 × 0.35 × 0.28 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	29.2 cm $^{-1}$
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
2 $\theta_{\max}$, completeness:	51°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3027, 791, 0.072
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 612
$N(\text{param})_{\text{refined}}$:	71
Programs:	Bruker programs [1], SHELX [2]

Source of materials

A mixture of $Zn(OAc)_2 \cdot 2H_2O$ (22 mg, 0.1 mmol), pyridine-3,5-dicarboxylic acid (0.1 mmol, 232 mg) and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 433 K for 47 h, followed by slow cooling to room temperature. Colourless crystals of the title compound formed.

Experimental details

C-bound hydrogen atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(H)$ set to $1.2U_{\text{eq}}(C)$.

Comment

The design and synthesis of coordination polymers (CPs) results from their potential applications in gas storage, molecular sieves, catalysis, drug delivery, nonlinear optics, and molecular sensing, but also because of their topologies [3–5]. Over the past decades, numerous CPs have been constructed, and crystal engineering has reached a level that some CPs with specific topologies can be designed by the judicious selection of metal ions and organic ligands [6–8]. However, it still remains a challenge to predict the structure and property of coordination polymers because of many factors involved in

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Abstract

$C_7H_7NO_6Zn$, monoclinic, $C2/c$ (no. 15), $a = 10.009(10)$ Å, $b = 11.907(12)$ Å, $c = 7.328(7)$ Å, $\beta = 105.050(12)^\circ$, $V = 843.3(15)$ Å 3 , $Z = 2$, $R_{\text{gt}}(F) = 0.0681$, $wR_{\text{ref}}(F^2) = 0.1757$, $T = 296(2)$ K.

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*Corresponding author: Dong-Mi Li, College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, Henan Province, P.R. China, e-mail: shihui471022@126.com

Xue-Li Xu: School of Biological and Chemical Engineering, Nanyang Institute of Technology, Nanyang 473004, Henan Province, P.R. China

Shi-Hui Li: College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, Henan Province, P.R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Zn1	0.5000	0.65492(9)	0.7500	0.0223(5)
N1	0.0000	0.3402(6)	0.7500	0.0229(18)
O1	0.5329(6)	0.6660(4)	1.0397(7)	0.0286(13)
H1A	0.5951	0.7174	1.0877	0.043*
H1B	0.5627	0.6018	1.0944	0.043*
O2	0.3574(5)	0.5235(4)	0.7503(7)	0.0290(12)
O3	0.2390(6)	0.6799(4)	0.6998(9)	0.0350(14)
C1	0.2447(7)	0.5766(6)	0.7268(10)	0.0247(17)
C2	0.1159(7)	0.5148(6)	0.7359(9)	0.0208(16)
C3	0.1107(6)	0.3983(6)	0.7325(10)	0.0201(16)
H3	0.1874	0.3589	0.7175	0.024*
C4	0.0000	0.5731(8)	0.7500	0.019(2)
H4	0.0000	0.6512	0.7500	0.023*

the formation such as the bonding capabilities of the metal ions (node) and ligands (linker), supramolecular interaction, and many other factors [9, 10]. One strategy is to perform reactions with mixed-ligands such as polycarboxylate and N-containing ligands, and a great number of novel intriguing structures are obtained [11], which indicates that the introduction of N-containing auxiliary ligands into a metal-polycarboxylate system often leads to structural diversity.

The asymmetric unit of the title structure contains one half of a Zn(II) ion, one half pyridine-3,5-dicarboxylate ligand as a bridging ligand to construct a new coordination polymer and one water molecule. The zinc atom is seven-coordinated by four oxygen atoms from pyridine-3,5-dicarboxylate ligands. The Zn—O(1) bond length is 2.066(6) Å, the Zn—O(2) bond length is 2.119(5) Å, respectively, which is in the typical range [12]. The coordinations result in a 2D-network. In addition, there are intermolecular hydrogen bonds between coordinated water molecules with adjacent pyridine-3,5-dicarboxylate anions: d(O(1)⋯O(2)A) = 2.791(7) Å, d(O(1)⋯O(3)B) = 2.782(8) Å. Symmetry codes: A: $-x + 1, -y + 1, -z + 2$; B: $x + 1/2, -y + 3/2, z + 1/2$. These interactions result in an infinite three dimensional architecture.

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