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The crystal structure of catena-poly[aqua- μ_2 -2-nitro-benzene-1,3-dicarboxylato- $\kappa^2 O, O'$ -(1,10-phenanthroline- $\kappa^2 N, N'$)-zinc(II)], $C_{20}H_{13}N_3O_7Zn$

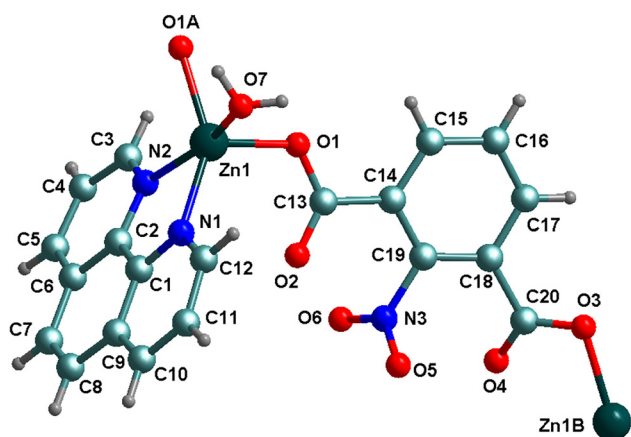


Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.26 × 0.18 × 0.12 mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	2.36 mm ⁻¹
Diffraction, scan mode:	Rigaku Synergy, ω scans
$\theta_{\max}$, completeness:	70.0°, 100 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12843, 3420, 0.020
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3,268
$N(\text{param})_{\text{refined}}$:	287
Programs:	Rigaku ¹ , Olex2 ² , SHELX ^{3,4}

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Abstract

$C_{20}H_{13}N_3O_7Zn$, orthorhombic, *Pbca* (no. 61), $a = 7.28990(10)$ Å, $b = 19.6852(2)$ Å, $c = 25.3532(3)$ Å, $V = 3638.26(8)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0328$, $wR_{\text{ref}}(F^2) = 0.0924$, $T = 297(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of materials

2-Nitro-benzene-1,3-dicarboxylic acid (0.1 mmol, 0.0211 g), 1,10-phenanthroline (0.1 mmol, 0.0198 mg), $ZnCl_2$ (0.1 mmol, 0.0136 g) and NaOH (0.2 mmol, 0.008 g) was added to 10.0 mL

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bi-distilled water and was stirred for 10 min to form a mixture, then was placed in a 23 mL Teflon-lined stainless steel autoclave. The autoclave was heated to 413 K for 3 days, and then cooled naturally to room temperature. A large number of colourless crystals were obtained, filtered off, washed with anhydrous ethanol, and dried in air, yield 46.3 % (based on 2-nitro-benzene-1,3-dicarboxylic acid).

2 Experimental details

The structure was solved by Direct Methods with the SHELXS-2018 program. All H-atoms from C and O atoms were positioned with idealized geometry and refined isotropically ($U_{\text{iso}}(H) = 1.2 U_{\text{eq}}(C)$ and $U_{\text{iso}}(H) = 1.5 U_{\text{eq}}(O)$) using a riding model with C–H = 0.930 Å and fixed distances of O–H = 0.842 and 0.847 Å, respectively.

3 Comment

Metal-organic coordination polymers offer innovative solutions to the limitations through their unique combination of metal ions and organic ligands for pharmacy, such as drug loadings, tumor therapy, drug delivery and detection of drugs, and so on. Zinc-organic coordination polymers have been increasingly studied due to their low toxicity.⁵ To date, many 1,10-phenanthroline combining benzene-1,3-dicarboxylic acid^{6,7} and its derivatives based zinc-organic complexes have been reported, including 2-,^{8,9} 4-^{10,11} and 5-substituted^{11–28}

benzene-1,3-dicarboxylic acid. We herein report the crystal structure of the title zinc-organic coordination polymer, catena- $[\mu_2$ -2-nitro-benzene-1,3-dicarboxylato- κ^2O,O']-aqua-(1,10-phenanthroline- κ^2N,N')-zinc(II)].

As shown in the figure, the title compound crystallizes in an orthorhombic system, group *Pbca* (no. 61), with the formula of $C_{20}H_{13}N_3O_7Zn$. The asymmetric unit has a Zn(II) ion, a completely deprotonated μ_2 -2-nitro-benzene-1,3-dicarboxylate anion, a chelating 1,10-phenanthroline ligand and a terminal coordination water molecule. This coordination environment of Zn(II) is similar to the structure reported in reference 9. The Zn1 is five-coordinated (ZnN_2O_3) forming a distorted square pyramidal geometry, where two nitrogen atoms are from the 1,10-phenanthroline, two oxygen atoms come from two μ_2 -2-nitro-benzene-1,3-dicarboxylate anion, and the last oxygen atom belongs to the terminal coordination water molecule. A 1D chain-like structure is generated by the linkage of the μ_2 -2-nitro-benzene-1,3-dicarboxylate anion, which is further forming a three-dimensional supramolecular structure by the hydrogen bonds $O7-H7A\cdots O1$ and $O7-HB\cdots O3$. All bond lengths of the title compound are comparable with the reported results.^{5–29}

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