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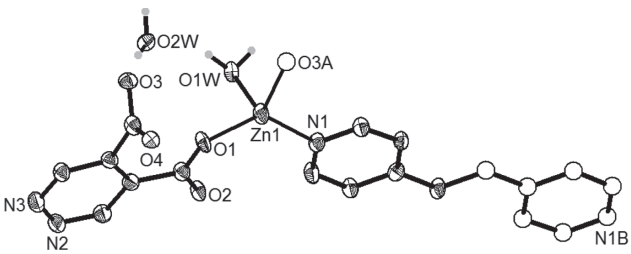
Crystal structure of *catena*-poly[diaqua-(μ_2-1,2-bis(4-pyridinyl)ethyane-κ^2 *N*:*N′*)-(μ_2–pyridazine-4,5-dicarboxylato-κ^2*O*:*O′*)]dizinc(II) dihydrate, $C_{12}H_{12}ZnN_3O_6$



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Abstract

$C_{12}H_{12}ZnN_3O_6$, monoclinic, $I2/a$ (no. 15), $a = 17.6153(6)$ Å, $b = 6.6922(2)$ Å, $c = 24.1330(9)$ Å, $\beta = 107.899(4)°$, $V = 2707.22(17)$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0262$, $wR_{ref}(F^2) = 0.0691$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The mixture of pyridazine-4,5-dicarboxylic acid (H_2pda, 0.05 mmol, 8 mg), 1,2-bis(4-pyridinyl)ethyane (bpa, 0.1 mmol, 18 mg), $Zn(OAc)_2{\cdot}2\,H_2O$ (0.2 mmol, 44 mg), H_2O (7.0 mL) was placed in a 23 mL Teflon lined stainless steel reactor. This reactor was placed in a oven and heated to 393 K under autogenous pressure for seventy-two hours, and then was cooled naturally to room temperature. Colorless block crystals of the titled compound were obtained.

Experimental details

All hydrogen atoms were modeled at their calculated positions and included *via* the riding model. The U_{iso} of the H-atoms were constrained to 1.2 times U_{eq} of their carbon atoms and 1.5 times U_{eq} for the hydrogen atoms at water.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.36 × 0.27 × 0.21 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	1.85 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	28.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12623, 2990, 0.024
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2649
$N(param)_{refined}$:	200
Programs:	CrysAlis^{PRO} [1], Olex2 [2], SHELX [3, 4]

Comment

The inherent properties of organic ligands play a critical role in the assemblies of coordination polymers with charming architectures and promising applications [5–7]. Multi-carboxylates with strong coordination abilities and flexible coordination modes have evoked a great deal of interests and proven themselves reliable building units [8–11]. N-heterocyclic ligands are beneficial for reconstructing the motifs and tailoring the properties of relevant coordination polymers [12, 13]. The N-heterocyclic carboxylates, such as pyridine carboxylates, imidazole carboxylates and pyrazine carboxylates, have been widely used to form coordination polymers [14–16]. For the present study we selected pyridazine-4,5-dicarboxylic acid (*H_2pda*) as one educt, though there are only few examples using it as organic ligand [17], and the 1,2-bis(4-pyridinyl)ethyane (*bpa*) ligand to moderate the coordination mode of the pda ligand.

The title compound displays one dimension chain structure. The asymmetric unit consists of one Zn(II) cation, one completely deprotonated pda dianion, one half bpa ligand, one coordinated water and one uncoordinated water molecule, as shown in the figure. Zn1 atom adopts a slightly distorted tetrahedral geometry by two oxygen atoms from two symmetry-related pda dianions, one terminal nitrogen atom from one bpa ligand and one oxygen atom from the coordinated water molecule. The Zn—O distances are in the range of 1.9202(13) Å to 2.0247(15) Å, and the Zn—N distance is 2.0090(14) Å. Neighboring Zn atoms are propagated by two

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.63100(2)	0.63049(3)	0.41066(2)	0.02465(9)
O1	0.73468(8)	0.7319(2)	0.41512(6)	0.0339(3)
O1W	0.64725(9)	0.3419(2)	0.39179(7)	0.0354(3)
H1WA	0.6106	0.2686	0.3970	0.053*
H1WB	0.6896	0.2956	0.4159	0.053*
O2	0.70458(9)	0.7320(3)	0.31858(6)	0.0485(5)
O3	0.88296(8)	0.5906(2)	0.51043(6)	0.0287(3)
O4	0.87462(9)	0.9204(2)	0.51396(6)	0.0340(3)
N1	0.52229(9)	0.6901(2)	0.35536(7)	0.0235(3)
N2	0.94376(10)	0.7942(3)	0.33066(7)	0.0303(4)
N3	0.99853(10)	0.8016(3)	0.38375(8)	0.0307(4)
C1	0.75177(11)	0.7434(3)	0.36771(8)	0.0247(4)
C2	0.83966(10)	0.7690(3)	0.37590(8)	0.0206(4)
C3	0.86753(11)	0.7799(3)	0.32773(8)	0.0260(4)
H3	0.8300	0.7769	0.2910	0.031*
C4	0.97581(11)	0.7933(3)	0.43098(9)	0.0281(4)
H4	1.0151	0.8000	0.4669	0.034*
C5	0.89624(10)	0.7751(3)	0.43045(8)	0.0205(4)
C6	0.88073(10)	0.7647(3)	0.48834(8)	0.0233(4)
C7	0.50787(11)	0.6948(3)	0.29740(8)	0.0295(4)
H7	0.5507	0.6868	0.2826	0.035*
C8	0.43166(11)	0.7110(3)	0.25912(8)	0.0303(5)
H8	0.4241	0.7133	0.2192	0.036*
C9	0.36624(10)	0.7238(3)	0.27955(8)	0.0230(4)
C10	0.38194(11)	0.7208(3)	0.33967(8)	0.0237(4)
H10	0.3403	0.7305	0.3557	0.028*
C11	0.45964(11)	0.7032(3)	0.37548(8)	0.0243(4)
H11	0.4689	0.7004	0.4155	0.029*
C12	0.28330(11)	0.7389(3)	0.23692(8)	0.0311(5)
H12A	0.2819	0.8525	0.2117	0.037*
H12B	0.2733	0.6201	0.2127	0.037*
O2W	0.79946(9)	0.2493(2)	0.44614(7)	0.0404(4)
H2WA	0.8274	0.3490	0.4623	0.061*
H2WB	0.8034	0.1598	0.4719	0.061*

μ_2-pda dianions to form one dinuclear unit with the Zn···Zn seperation of 5.0059(3) Å, wherein all $-COO^-$ groups display monodentate coordination modes. The dinuclear units are further bridged by μ_2-bpa ligands to generate a chain.

Four kinds of hydrogen-bonding interactions are observed among pda dianions, the coordinated water and the free water molecules. Their detailed data are listed as follows: O(1W)···N(3) #1 = 2.741(2) Å, O(1W)···O(2W) = 2.671(2) Å, O(2W)···O(3) = 2.896(2) Å, O(2W)···O(4) #2 = 2.819(2) Å. (symmetry codes: #1 $-1/2+x, 1-y, z$; #2 $x, -1+y, z$). The latter three hydrogen bonds extend the adjacent chain motifs to a layered structure. And the O(1W)···N(3) hydrogen bonds connect the layers to the three-dimensional supramolecular structure.

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