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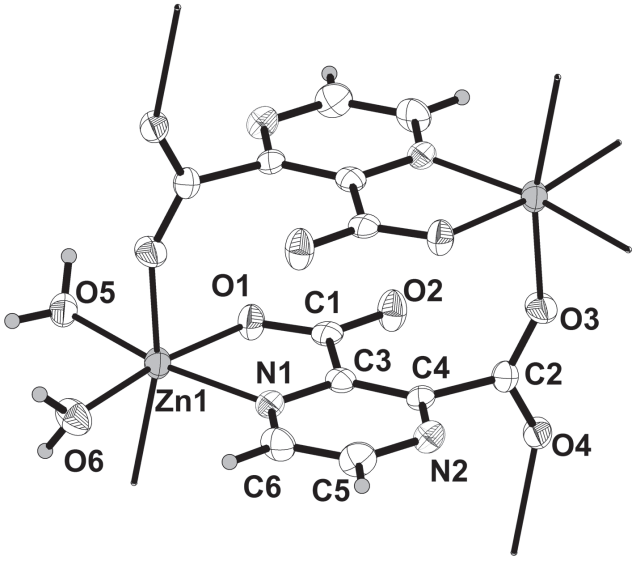
Crystal structure of *catena*-poly[diaqua(μ_3-pyrazine-2,3-dicarboxylato-κ^4*O,N:O′:O″*)zinc(II)] 1.25 hydrate, $C_6H_{8.5}N_2O_{7.25}Zn$



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Abstract

$C_6H_{8.5}N_2O_{7.25}Zn$, triclinic, $P\bar{1}$ (no. 2), $a = 6.4463(5)$ Å, $b = 8.4180(7)$ Å, $c = 9.8370(8)$ Å, $\alpha = 66.130(1)°$, $\beta = 79.537(1)°$, $\gamma = 81.153(2)°$, $V = 478.11(7)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0292$, $wR_{ref}(F^2) = 0.0782$, $T = 298$ K.

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A part of the polymeric title 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.

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Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	0.39 × 0.21 × 0.17 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	2.6 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	50°, >98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2410,1656, 0.021
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1486
$N(param)_{refined}$:	154
Programs:	Bruker programs [1], SHELX [2], DIAMOND [3], PLATON [4]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.28894(5)	0.78200(4)	0.20990(3)	0.02068(14)
N1	0.3025(4)	0.5054(3)	0.3352(3)	0.0195(5)
N2	0.2821(4)	0.1631(3)	0.5368(3)	0.0227(5)
O1	0.2511(3)	1.0530(2)	0.1242(2)	0.0243(5)
H1C	0.2788	1.1037	0.0296	0.029*
H1D	0.1274	1.0908	0.1515	0.029*
O2	0.3660(3)	0.7615(3)	0.0012(2)	0.0301(5)
H2C	0.4780	0.8143	−0.0337	0.036*
H2D	0.2941	0.7865	−0.0703	0.036*
O3	0.2344(3)	0.7712(2)	0.4266(2)	0.0232(5)
O4	0.1821(4)	0.5881(3)	0.6664(2)	0.0279(5)
O5	0.0316(3)	0.2140(3)	0.8200(2)	0.0249(5)
O6	0.3757(3)	0.1995(3)	0.8206(2)	0.0254(5)
O7	0.8652(3)	0.1530(3)	0.2348(2)	0.0307(5)
H7C	0.8485	0.2329	0.2688	0.037*
H7D	0.8206	0.0607	0.3046	0.037*
O8[a]	0.074(3)	0.478(3)	1.005(2)	0.094(6)
H8C[a]	0.0955	0.4921	0.9129	0.112*
H8D[a]	0.0163	0.3834	1.0555	0.112*
C1	0.2228(4)	0.6221(4)	0.5302(3)	0.0186(6)
C2	0.2156(4)	0.2362(3)	0.7541(3)	0.0181(6)
C3	0.2607(4)	0.4669(4)	0.4834(3)	0.0182(6)
C4	0.2537(4)	0.2948(3)	0.5846(3)	0.0177(6)
C5	0.3209(5)	0.2041(4)	0.3893(3)	0.0281(7)
H5	0.3397	0.1155	0.3536	0.034*
C6	0.3341(5)	0.3749(4)	0.2878(3)	0.0262(7)
H6	0.3652	0.3988	0.1857	0.031*

[a]Occupancy: 0.25.

Source of material

A mixture of pyrazine-2,3-dicarboxylic acid (0.1 mmol), $Zn(NO_3)_2{\cdot}H_2O$(0.1 mmol), H_2O (10 mL) and methanol 2 mL was stirred for 20 min and then sealed in a 25 mL Teflon-lined stainless steel autoclave and heated at 170° for 72 h. White block crystals of the title compound were obtained, which were washed with water and dried in air with a 72% yield.

Experimental details

The H atoms of the solvent water molecule were located from the difference Fourier map and then allowed to ride on their parent O atom in the final cycles of refinement with d(O—H) = 0.850 Å and U_{iso}(H) = 1.5 U_{eq}(O).

Discussion

In this paper, we choose the pyrazine-2,3-dicarboxylate (PDC) a ligands to synthesized a new compound. This compound crystallizes in the P-1 space group, and possesses an extended one-dimensional framework. Each Zn(II) is coordinated by five O and one N atoms. Two oxygen atoms come from two individual H_2O molecules, one O atom and the N atom come from one PDC ligand, the remaining two O atoms are from two adjacent PDC ligands, as shown in the figure. The Zn^{2+}, 2 H_2O and 1 PDC ligand form a plane, two Zn—O bonds spread out combining the other two planes and extending to a one-dimensional chain.

The analogous monohydrate of the title compound is known for decades [5]. The structure is similar to the structure reported in this manuscript. Results indicate that especially the number of water molecules is not the same.

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