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Crystal structure of *catena*-poly[*diaqua*-(μ_2 -oxalyl dihydrazide- $\kappa^4N,O:N',O'$)-bis(μ_2 -pyridine-2,3-dicarboxylato- κ^3N,O,O')dicadmium(II)] hexahydrate, $C_{16}H_{28}O_{18}N_6Cd_2$

Table 1: Data collection and handling.

Crystal:	Colorless cubic
Size:	0.30 × 0.26 × 0.20 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.63 mm ⁻¹
Diffractometer, scan mode:	SMART, ω
θ_{max} , completeness:	27.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	15249, 3170, 0.019
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 3031
$N(param)_{refined}$:	211
Programs:	Bruker [1], SHELX [2, 3], Diamond [4]

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

Atom	x	y	z	U_{iso}^*/U_{eq}
Cd1	0.47737(2)	0.33223(2)	0.22026(2)	0.02556(4)
O1	0.74684(17)	0.3045(2)	0.12440(10)	0.0375(3)
O2	1.04804(17)	0.21930(19)	0.14435(10)	0.0369(3)
O3	1.33967(18)	0.1366(2)	0.35142(13)	0.0508(4)
O4	1.18734(17)	0.42134(18)	0.29185(11)	0.0374(3)
O5	0.54645(18)	0.05893(17)	0.12996(10)	0.0355(3)
O6	0.4351(2)	0.6349(2)	0.22289(16)	0.0535(4)
N1	0.71370(18)	0.2643(2)	0.34752(11)	0.0269(3)
N3	0.29412(19)	0.38984(19)	0.05065(11)	0.0279(3)
H3A	0.1763	0.4189	0.0669	0.034*
H3B	0.3049	0.4836	0.0098	0.034*
N2	0.35370(18)	0.23267(18)	−0.00989(11)	0.0258(3)
H2	0.3116	0.2367	−0.0761	0.031*
C1	0.8743(2)	0.2640(2)	0.30759(12)	0.0224(3)
C2	1.0171(2)	0.2588(2)	0.37760(13)	0.0252(3)
C3	0.9906(3)	0.2525(3)	0.49158(15)	0.0390(4)
H3	1.0833	0.2495	0.5405	0.047*
C4	0.8267(3)	0.2507(3)	0.53152(15)	0.0460(5)
H4	0.8078	0.2454	0.6075	0.055*
C5	0.6910(2)	0.2570(3)	0.45720(14)	0.0375(4)
H5	0.5801	0.2562	0.4842	0.045*
C6	0.8920(2)	0.2636(2)	0.18233(13)	0.0249(3)
C7	1.1944(2)	0.2694(2)	0.33610(13)	0.0294(3)
C8	0.4749(2)	0.0795(2)	0.03664(12)	0.0247(3)
O7	0.1648(2)	0.8640(2)	0.08232(13)	0.0457(3)
O8	0.3776(2)	0.2109(2)	0.65727(14)	0.0489(4)
O9	0.0870(2)	0.2870(2)	0.81199(15)	0.0555(4)
H9A	0.0144	0.3986	0.8050	0.067*
H9B	0.032(4)	0.234(4)	0.835(2)	0.067*
H8B	0.453(4)	0.109(4)	0.653(2)	0.067*
H8A	0.310(4)	0.203(4)	0.698(2)	0.067*

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Abstract

$C_{16}H_{28}O_{18}N_6Cd_2$, triclinic, $P\bar{1}$ (no. 2), $a = 7.8375(3)$ Å, $b = 7.8877(4)$ Å, $c = 12.0841(6)$ Å, $\alpha = 85.956(2)^\circ$, $\beta = 89.833(2)^\circ$, $\gamma = 68.269(1)^\circ$, $V = 692.00(6)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0159$, $wR_{ref}(F^2) = 0.0395$, $T = 293(2)$ K.

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A part of the molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H6A	0.492(4)	0.677(4)	0.254(2)	0.067*
H6B	0.365(4)	0.709(4)	0.182(2)	0.067*
H7A	0.134(4)	0.972(4)	0.089(2)	0.067*
H7B	0.176(4)	0.842(4)	0.021(2)	0.067*

Source of material

Chemicals were purchased from commercial source. The solvent used in the synthesis is deionized water. IR spectra were measured on a Nicolet 170SX spectrophotometer in the 4000–400 cm^{−1} region.

A mixture of 2,3-pyridinedicarboxylic acid (0.5 mmol, 83.5 mg), NaOH (1 mmol, 40 mg) and H₂O (5 mL) was placed in a high pressure resistant glass bottle (20 mL), the bottle was sealed and heated at 353 K for 30 min. A solution of oxalyl dihydrazide [5] (0.5 mmol, 59 mg), Cd (CH₃COO)₂ · 2H₂O (1 mmol, 266 mg) and H₂O (5 mL) was added and the solution stayed for one night at room temperature. Colorless cubic crystals were obtained (yield 56% based on Cd). IR (cm^{−1}, KBr): 3304 (s), 2979 (w), 1687 (w), 1575 (vs), 1388 (vs), 1110 (m), 1009 (w), 853 (m), 708 (s), 523 (m).

Experimental details

H atoms were positioned geometrically and treated as riding, with C–H = 0.93 Å and with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Comment

Research focused on coordination polymers due to their versatile architecture and potential applications for luminescent properties, magnetic interactions, catalytic ability, and so on [6–8]. It is critical to choose ligands to synthesize novel complexes. 2,3-Pyridinedicarboxylic acid ligand has been widely used to construct a series of metal complexes for its multiple coordination function [9–11].

The structure of the complex is as shown in the figure. The complex crystallizes in the triclinic system and *P*1 space group. The central Cd (II) ion is seven-coordinated by three O atoms and one N atom from two deprotonated 2,3-pyridinedicarboxylic acid ligands (pda^{2−}) (N1, O1, O3A and O4A, where symmetry code A is −1 + *x*, +*y*, +*z*), one oxalyl dihydrazide ligand (N3, O5) and one water molecule (O6). The distance of Cd–O ranges from 2.2891(16) to 2.6319(18) Å, which is in good agreement with the reported [12]. Each pda^{2−} ion bridges two Cd (II) ions along *a*-axis to form a one-dimensional chain structure. Two adjacent Cd (II) ions were connected by oxalic hydrazine ligand along *b*-axis, forming a

ladder shaped one-dimensional chain. A closed ring is formed by two pda^{2−} ions, two oxalyl dihydrazide ligands and four Cd (II) ions. Each one-dimensional chain is connected to each other through O–H ··· O and N–H ··· O hydrogen bonds.

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