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Crystal structure of poly[diaqua-(μ_2 -2,5-dihydroxyterephthalato- $\kappa^2 O:O'$)(μ_2 -bis(4-pyridylformyl)piperazine- $\kappa^2 N:N'$)cadmium(II)] dihydrate, $C_{24}H_{28}CdN_4O_{12}$

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Abstract

$C_{24}H_{28}CdN_4O_{12}$, monoclinic, $P2_1/c$ (no. 14), $a = 11.0801(4)$ Å, $b = 8.3925(3)$ Å, $c = 13.9503(5)$ Å, $\beta = 102.810(3)^\circ$, $Z = 2$, $V = 1353.89(8)$ Å³, $R_{gt}(F) = 0.0273$, $wR_{ref}(F^2) = 0.0633$, $T = 291$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Cd(OAc)_2 \cdot 2H_2O$ (26.7 mg, 0.1 mmol), 2,5-dihydroxy-1,4-benzenedicarboxylic acid (18.9 mg, 0.1 mmol), bis(4-pyridylformyl)piperazine (29.6 mg, 0.1 mmol) and 8 mL distilled water in a 25 mL Teflon-lined autoclave was kept under autogenous pressure at 353 K for four days. After cooling down to room temperature

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.31 \times 0.28 \times 0.25$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.88 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.0° , 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	15330, 2347, 0.030
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2117
$N(\text{param})_{\text{refined}}$:	192
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], Olex2 [4]

naturally, colourless crystals were collected by filtration and washed with distilled water in 32% yield.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Coordination polymers (CPs), have attracted interests due to their potential applications in gas storage, molecular recognition, catalysis, chromism, and magnetism [5–9]. The structures of CPs based on central metal ions and organic ligands are difficult to predict. Some factors, such as temperature, solvent, pH value, counterion, metal-to-ligand ratio, etc., have unpredictable impacts in the self-assembly [10, 11]. From the point of view of structural chemistry, the 2,5-dihydroxy-1,4-benzenedicarboxylate ligand (H_2L) is a good organic linker which may exhibits versatile coordination modes, and useful as a riding ligand [12, 13]. In this work, we report a CP based on Zn(II) ions, H_2L and the flexible bis(4-pyridylformyl)piperazine (bpfp) ligand.

The asymmetric unit of the crystal structure consists of one crystallographically independent Cd(II) centre, one

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7491 (2)	0.4829 (3)	0.9432 (2)	0.0360 (6)
C2	0.8789 (2)	0.4912 (3)	0.97427 (19)	0.0297 (6)
C3	0.9429 (2)	0.5212 (3)	0.90396 (19)	0.0333 (6)
H3A	0.9043	0.5352	0.8388	0.040*
C4	1.0618 (2)	0.5307 (3)	0.92805 (19)	0.0327 (6)
C5	0.4463 (2)	0.5671 (4)	0.76476 (19)	0.0399 (6)
H5	0.5068	0.6390	0.7835	0.048*
C6	0.3837 (2)	0.5714 (4)	0.66906 (19)	0.0408 (6)
H6	0.4019	0.6441	0.6244	0.049*
C7	0.2938 (2)	0.4659 (3)	0.64093 (19)	0.0342 (6)
C8	0.2718 (2)	0.3588 (4)	0.7092 (2)	0.0433 (7)
H8	0.2122	0.2851	0.6921	0.052*
C9	0.3389 (2)	0.3622 (3)	0.8028 (2)	0.0408 (7)
H9	0.3236	0.2888	0.8482	0.049*
C10	0.2275 (2)	0.4610 (3)	0.53671 (19)	0.0373 (6)
C11	0.0487 (3)	0.5070 (4)	0.4145 (2)	0.0471 (8)
H11A	0.0921	0.4557	0.3718	0.057*
H11B	0.0288	0.6138	0.3899	0.057*
C12	−0.0584 (2)	0.4150 (4)	0.41435 (19)	0.0443 (7)
H12A	−0.1081	0.4163	0.3490	0.053*
H12B	−0.0387	0.3051	0.4321	0.053*
Cd1	0.5000	0.5000	1.0000	0.02992 (11)
N1	0.42504 (18)	0.4659 (3)	0.83182 (15)	0.0348 (5)
N2	0.1196 (2)	0.5149 (3)	0.51529 (17)	0.0452 (6)
O1	0.69512 (15)	0.4641 (3)	1.01165 (15)	0.0491 (5)
O2	0.70226 (18)	0.4950 (3)	0.85630 (16)	0.0602 (7)
O3	1.11681 (17)	0.5634 (3)	0.85459 (15)	0.0595 (6)
H3	1.1863	0.5732	0.8777	0.089*
O4	0.49253 (16)	0.2294 (2)	1.02284 (14)	0.0468 (5)
H4A	0.4257	0.2014	1.0295	0.070*
H4B	0.5364	0.2033	1.0775	0.070*
O5	0.6671 (3)	0.3802 (4)	0.66682 (19)	0.0835 (8)
H5A	0.7024	0.4475	0.6386	0.125*
H5B	0.6757	0.4148	0.7252	0.125*
O6	0.27584 (16)	0.4099 (3)	0.47317 (13)	0.0506 (5)

half of a bpf ligand [14–16], one half of a L^{2-} ligand, one coordinated water molecule and one solvent water molecule (see the figure). The Cd(II) centre is in a distorted octahedral geometry with the CdO_4N_2 coordination. The Cd–O/N distances associated with central Cd(II) centres are in the range of 2.297(2)–2.335 (2) $\text{\AA}$ and the bond angles about the Cd(II) centers range from 78.02(7) to 180.0°. In the title compound, L^{2-} anions and bpf ligands link Cd(II) centers to a two-dimensional structure.

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