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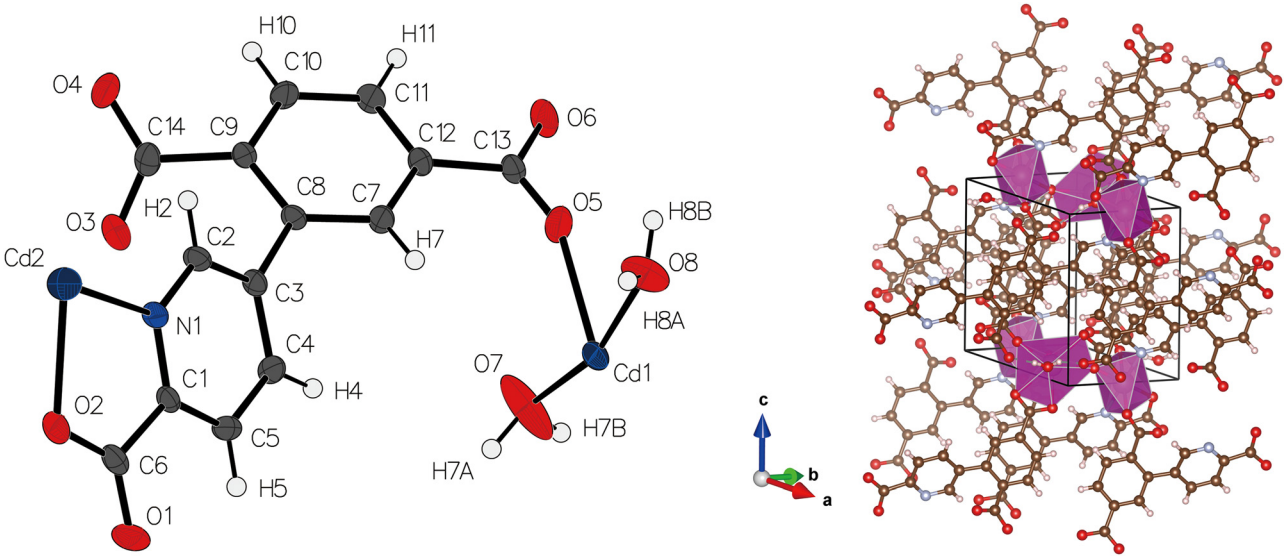
The crystal structure of poly[2-(4-carboxypyridin-3-yl)terephthalpoly[diaqua-(μ_4-2-(6-carboxylatopyridin-3-yl)terephthalato-κ^5O,N:O′:O″,O‴)]) cadmium(II)] dihydrate, $C_{28}H_{20}Cd_3N_2O_{16}$



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Abstract

$C_{28}H_{20}Cd_3N_2O_{16}$, triclinic, $P\bar{1}$ (no. 2), a = 7.3205(3) Å, b = 9.9488(5) Å, c = 10.0326(5) Å, α = 104.473(4)°, β = 91.566(4)°, γ = 90.191(4)°, V = 707.19(6) Å^3, Z = 1, $R_{gt}(F)$ = 0.0239, w$R_{ref}(F^2)$ = 0.0576, T = 293 K.

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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 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.32 × 0.28 × 0.26 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	2.32 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	29.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6111, 3206, 0.015
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2917
$N(param)_{refined}$:	227
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

1 Source of materials

The chemical reagents: 2-(4-carboxypyridin-3-yl) terephthalic acid, cadmium nitrate tetrahydrate ($Cd(NO_3)_2{\cdot}4H_2O$), acetonitrile (CH_3CN) were purchased from Shanghai Macklin Biochemical Technology Co., Ltd with no further purification. The 2-(4-carboxypyridin-3-yl) terephthalic acid (14 mg, 0.05 mm), $Cd(NO_3)_2{\cdot}4H_2O$ (31 mg, 0.1 mm) were dissolved in the mixture solutions of acetonitrile (3 mL) and water (2 mL). Then stir at room temperature for 10 min.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0940 (3)	0.4318 (3)	0.2724 (3)	0.0175 (5)
C2	0.2692 (4)	0.6214 (3)	0.2582 (3)	0.0194 (5)
H2	0.302528	0.684919	0.208919	0.023*
C3	0.3514 (3)	0.6319 (3)	0.3870 (2)	0.0171 (5)
C4	0.2911 (4)	0.5415 (3)	0.4621 (3)	0.0204 (5)
H4	0.336041	0.549351	0.551374	0.024*
C5	0.1628 (4)	0.4390 (3)	0.4028 (3)	0.0210 (5)
H5	0.124017	0.375977	0.450990	0.025*
C6	−0.0412 (4)	0.3199 (3)	0.1996 (3)	0.0217 (6)
C7	0.4969 (3)	0.8183 (3)	0.5723 (3)	0.0192 (5)
H7	0.397189	0.811924	0.626032	0.023*
C8	0.5022 (3)	0.7345 (3)	0.4389 (2)	0.0167 (5)
C9	0.6528 (4)	0.7459 (3)	0.3580 (2)	0.0187 (5)
C10	0.7876 (4)	0.8444 (3)	0.4106 (3)	0.0287 (7)
H10	0.883254	0.856034	0.355282	0.034*
C11	0.7822 (4)	0.9254 (3)	0.5439 (3)	0.0296 (7)
H11	0.875288	0.989615	0.578254	0.035*
C12	0.6381 (4)	0.9114 (3)	0.6269 (3)	0.0191 (5)
C13	0.6419 (4)	0.9916 (3)	0.7749 (3)	0.0204 (5)
C14	0.6901 (4)	0.6401 (3)	0.2244 (3)	0.0223 (6)
Cd1	0.29264 (3)	0.87593 (2)	0.94522 (2)	0.02201 (7)
Cd2	0.000000	0.500000	0.000000	0.03131 (9)
N1	0.1443 (3)	0.5241 (2)	0.2023 (2)	0.0181 (4)
O1	−0.1091 (3)	0.2416 (2)	0.2636 (2)	0.0337 (5)
O2	−0.0824 (3)	0.3120 (2)	0.07412 (19)	0.0261 (4)
O3	0.6478 (3)	0.5183 (2)	0.2199 (2)	0.0360 (5)
O4	0.7713 (3)	0.6788 (2)	0.13037 (19)	0.0313 (5)
O5	0.5130 (3)	0.9818 (2)	0.8502 (2)	0.0389 (6)
O6	0.7772 (3)	1.0687 (2)	0.8214 (2)	0.0307 (5)
O7	0.4973 (4)	0.7071 (3)	0.9364 (3)	0.0705 (10)
H7A	0.446366	0.625006	0.900417	0.106*
H7B	0.537080	0.700424	1.018843	0.106*
O8	0.1340 (3)	1.0595 (2)	0.9144 (3)	0.0409 (6)
H8A	0.035703	1.048823	0.865643	0.061*
H8B	0.184426	1.131230	0.899465	0.061*

After this, the mixture was transferred into a high-pressure stainless-steel reactor lined with Teflon, and heated at 150 °C for 72 h. After natural cooling to room temperature, yellow block crystals were obtained.

2 Experimental details

A Bruker D8 diffractometer equipped with MoKα radiation (λ = 0.71073 Å) was utilized for data collection. The intensity data obtained were processed and reduced using the Bruker SAINT software [1]. For the refinement process, all hydrogen atom positions were assumed to be in idealized positions and treated as riding atoms. The U_{iso} values for the hydrogen atoms were set to 1.2 times the U_{eq} of the parent atoms. The structure solution was achieved using ShelXT [2], and the refinement was performed using ShelXL [3] incorporated in the Olex2 software [4].

3 Comment

Coordination polymers, also known as metal-organic frameworks (MOFs), have emerged as a significant area of research in materials science and chemistry [5–8]. Their unique structural and chemical properties make them highly versatile and attractive for various applications. Researching coordination polymers provides insights into fundamental principles of coordination chemistry, supramolecular chemistry, and crystal engineering [7, 9–12]. The exploration of their structural diversity, tunable porosity, functional properties, and sustainable nature paves the way for creating innovative materials with tailored properties and applications. Here in, we supplied a novel coordination polymer belonging to a group of structures which are reported in the literature [13, 14].

In this study, we present the crystal structure analysis of the title compound. The coordination geometry around Cd atoms is distorted octahedrally and decahedrally, with two kinds of Cd atoms in the asymmetric unit. The Cd atoms are coordinated to oxygen and nitrogen atoms from neighboring ligands.

The crystal structure also reveals the presence of hydrogen bonding interactions between H atoms and oxygen atoms.

The detailed structural information presented in this study can contribute to the understanding of the physical and chemical properties of this compound and its potential applications in various fields.

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