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Crystal structure of *catena-poly*[dichlorido-(μ_2 -4-(pyridin-4-yl)-isophthalate- $\kappa^2 O, O'$)cadmium(II)] monohydrate, $C_{13}H_{11}NO_5Cl_2Cd$

Table 1: Data collection and handling.

Crystal:	Colourless blocks
Wavelength:	Size $0.32 \times 0.28 \times 0.17$ mm
μ :	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
Diffractometer, scan mode:	18.3 cm^{-1}
$2\theta_{\max}$, completeness:	Bruker SMART, φ and ω
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	51° , $>99\%$
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	5246 , 2675 , 0.015
$N(\text{param})_{\text{refined}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2558
Programs:	200
	SHELX [7], Bruker programs [8]

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Abstract

$C_{13}H_{11}N_1O_5Cl_2Cd$, monoclinic, $P2_1$ (no. 4), $a = 8.036(4) \text{ \AA}$, $b = 7.113(3) \text{ \AA}$, $c = 13.556(6) \text{ \AA}$, $\beta = 104.725(5)^\circ$, $V = 749.5(6) \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.0220$, $wR_{\text{ref}}(F^2) = 0.0562$, $T = 296(2) \text{ K}$.

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A part of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Cd(NO_3)_2 \cdot 2H_2O$ (0.1 mmol, 0.0272 g), 4-(pyridin-4-yl)-isophthalic acid (0.1 mmol, 24.3 mg), HCl (2 mL) and

distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 423 K for 36 h, followed by slow cooling to room temperature. Colourless crystals of the title compound formed.

Experimental details

C-bound hydrogen atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(H)$ set to $1.2U_{\text{eq}}(C)$. The hydrogen atom of the hydroxyl group was allowed to rotate with a fixed angle around the C–O bond to best fit the experimental electron density (HFIX 147 in the SHELX program suite [7]), with $U_{\text{iso}}(H)$ set to $1.5U_{\text{eq}}(O)$.

Discussion

Research on coordination polymers have made considerable progress in the fields of supramolecular chemistry and crystal engineering, owing to their intriguing architectures and functional applications, such as gas storage [1], catalysis [2], magnetism [3] and luminescence [4]. Studies in this field have been focused on the rational design and synthesis of novel frameworks and the relationships between their structures and properties. Coordination complexes constructed from organic ligands and metal ions through self-assembly has been explored intensively [5]. However, it is still a great challenge in crystal engineering to obtain designed and predictable frameworks with potential properties assembled by coordination

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cd1	0.99467(4)	0.43390(11)	−0.00255(2)	0.02460(8)
Cl1	0.75581(9)	0.18015(19)	−0.03252(6)	0.02777(17)
Cl2	1.19557(9)	0.1829(2)	−0.06104(6)	0.02612(16)
O1	1.1010(4)	0.3366(4)	0.1666(2)	0.0342(8)
O2	1.1110(4)	0.0215(4)	0.1721(2)	0.0320(8)
O3	1.5942(3)	0.1882(8)	0.5466(2)	0.0490(7)
H3	1.6819	0.2136	0.5907	0.074*
O4	1.4660(4)	0.2674(6)	0.6679(2)	0.0580(10)
O5	0.8735(3)	0.1879(10)	0.70235(18)	0.0428(6)
H1W	0.8641	0.2895	0.7501	0.064*
H2W	0.8600	0.0742	0.7458	0.064*
N1	0.4859(5)	0.2248(8)	0.1467(3)	0.0552(14)
H1	0.3868	0.2268	0.1037	0.066*
C1	0.9718(5)	0.2223(5)	0.3567(3)	0.0292(10)
C2	1.1230(4)	0.1956(12)	0.3248(2)	0.0228(8)
C3	1.2828(4)	0.1922(9)	0.3967(2)	0.0279(7)
H3A	1.3827	0.1679	0.3762	0.034*
C4	1.2909(5)	0.2256(5)	0.4992(3)	0.0289(9)
C5	1.1400(5)	0.2580(6)	0.5290(3)	0.0370(10)
H5	1.1455	0.2817	0.5972	0.044*
C6	0.9827(5)	0.2555(6)	0.4587(3)	0.0345(9)
H6	0.8829	0.2763	0.4799	0.041*
C7	1.1111(4)	0.1822(8)	0.2122(2)	0.0232(6)
C8	1.4583(5)	0.2302(5)	0.5800(3)	0.0347(11)
C9	0.5768(6)	0.0643(9)	0.1585(4)	0.0511(14)
H9	0.5325	−0.0424	0.1214	0.061*
C10	0.7361(6)	0.0598(7)	0.2263(3)	0.0392(10)
H10	0.8011	−0.0499	0.2352	0.047*
C11	0.8000(4)	0.2214(6)	0.2818(3)	0.0295(10)
C12	0.6985(6)	0.3815(7)	0.2669(4)	0.0479(12)
H12	0.7376	0.4899	0.3038	0.058*
C13	0.5424(7)	0.3809(9)	0.1986(4)	0.0592(14)
H13	0.4752	0.4890	0.1880	0.071*

bonds and/or weak supramolecular interactions such as hydrogen bonds, π – π stacking, and host–guest ionic interactions, etc. [6].

This is not a hydride its a coordination polymer. The asymmetric unit of the title structure contains one Cd(II) ion, two chlorine ions, 4-(pyridin-4-yl)-isophthalate anion and one water molecule. The cadmium atom is six-coordinated by four chlorido ligands and two isophthalate ligands. The Cd–O bond lengths is 2.339(3) Å. The Cd1–Cl bond lengths are 2.5906(16) Å, 2.6597(15) Å, respectively. The bond angles of Cl–Cd–Cl are in the range of 88.12(6)° to 178.050(15)°. In addition, uncoordinated water molecules are connected to adjacent 4-(pyridin-4-yl)-isophthalate anions by hydrogen bonds ($d(O(5)–H(2W) \cdots O(1)\#3) = 3.043(7)$ Å, $d(O(5)–H(1W) \cdots O(2)\#4) = 2.905(7)$ Å, $d(O(3)–H(3) \cdots O(5)\#5) = 2.661(3)$ Å. Symmetry codes: #3 $-x+2, y-1/2, -z+1$; #4 $-x+2, y+1/2, -z+1$; #5 $x+1, y, z$. Finally, all these intermolecular bonds result in a 3D framework.

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