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Crystal structure of poly[tetraqua-bis(μ_4 -5-(4-carboxy-benzylamino)-isophthalato- $\kappa^4 O, O': O'': O'''$)-(μ_2 -4,4'-di(1*H*-imidazol-1-yl)-1,1'-biphenyl- $\kappa^2 N:N'$)dicadmium(II)], $C_{25}H_{22}N_3O_8Cd$

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Abstract

$C_{25}H_{22}N_3O_8Cd$, triclinic, $P\bar{1}$ (no. 2), $a = 10.2722(10)$ Å, $b = 10.6897(11)$ Å, $c = 12.5667(13)$ Å, $\alpha = 79.698(9)^\circ$, $\beta = 72.168(9)^\circ$, $\gamma = 63.166(10)^\circ$, $V = 1170.8(2)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0618$, $wR_{ref}(F^2) = 0.1078$, $T = 293(2)$ 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:	$0.41 \times 0.32 \times 0.25$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.99 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.5° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	19983, 4352, 0.105
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3318
$N(\text{param})_{\text{refined}}$:	345
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Source of material

A mixture of $Cd(NO_3)_2 \cdot 2H_2O$ (0.1 mmol, 0.0272 g), 4,4'-di(1*H*-imidazol-1-yl)-1,1'-biphenyl (0.1 mmol, 0.052 g) and 5-(4-carboxy-benzylamino)-isophthalic acid ($H_3C_{10}H_6N_2O_4$) (0.1 mmol, 0.0330 g), was dissolved in 10 mL H_2O . The solution was heated in a 23 mL autoclave under autogenous pressure at 393 K for 4 days. After cooling to room temperature colorless crystals formed.

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

Atom	x	y	z	U_{iso}^*/U_{eq}
Cd1	1.06754(5)	0.23551(4)	0.52852(4)	0.02989(16)
N1	1.0662(5)	0.0979(5)	0.6826(4)	0.0385(13)
N2	1.0702(5)	−0.0792(5)	0.8032(4)	0.0398(13)
N3	0.5216(5)	0.6026(5)	0.1933(4)	0.0481(15)
H3	0.5988	0.6196	0.1591	0.058*
O1	1.1972(5)	0.0459(5)	0.4081(4)	0.0473(13)
H1A	1.2994	0.0306	0.3686	0.071*
O2	0.9894(5)	0.4222(4)	0.6465(4)	0.0444(13)
H2A	0.9152	0.4936	0.6293	0.067*
O3	0.8813(4)	0.3797(4)	0.4415(3)	0.0363(10)
O4	0.8365(4)	0.1997(4)	0.5290(4)	0.0398(11)
O5	0.3318(5)	0.2059(5)	0.5408(4)	0.0532(13)
O6	0.2257(4)	0.3246(4)	0.4065(3)	0.0329(10)
O7	0.4773(6)	1.0270(5)	−0.3153(4)	0.0682(14)
H7	0.4433	1.0860	−0.3629	0.102*
O8	0.3431(6)	1.2056(5)	−0.2005(4)	0.0668(15)
C1	1.0854(8)	0.1208(8)	0.7773(6)	0.066(2)
H1	1.0948	0.1994	0.7890	0.079*
C2	1.0890(9)	0.0129(8)	0.8530(6)	0.069(2)
H2	1.1018	0.0033	0.9246	0.083*
C3	1.0536(7)	−0.0204(6)	0.7035(5)	0.0384(16)
H3A	1.0348	−0.0599	0.6530	0.046*
C4	1.0561(6)	−0.2050(6)	0.8546(5)	0.0373(15)
C5	1.1197(9)	−0.2732(8)	0.9403(7)	0.082(3)
H5	1.1787	−0.2420	0.9616	0.098*
C6	1.0979(8)	−0.3885(8)	0.9963(7)	0.078(3)
H6	1.1425	−0.4331	1.0550	0.093*
C7	1.0125(7)	−0.4389(6)	0.9679(5)	0.0398(16)
C8	0.9544(8)	−0.3711(7)	0.8785(5)	0.0512(19)
H8	0.8996	−0.4048	0.8544	0.061*
C9	0.9737(7)	−0.2544(6)	0.8226(5)	0.0433(17)
H9	0.9305	−0.2099	0.7632	0.052*
C10	0.8041(6)	0.3089(6)	0.4678(5)	0.0302(14)
C11	0.6707(6)	0.3577(5)	0.4182(5)	0.0256(13)
C12	0.5664(6)	0.3003(6)	0.4584(5)	0.0292(14)
H12	0.5772	0.2325	0.5169	0.035*
C13	0.4460(6)	0.3441(6)	0.4110(5)	0.0270(13)
C14	0.4306(6)	0.4439(6)	0.3242(5)	0.0304(14)
H14	0.3496	0.4722	0.2931	0.037*
C15	0.5332(6)	0.5040(6)	0.2815(5)	0.0307(14)
C16	0.6508(6)	0.4600(6)	0.3324(5)	0.0312(14)
H16	0.7184	0.5010	0.3077	0.037*
C17	0.3287(6)	0.2877(6)	0.4564(5)	0.0329(15)
C18	0.3872(7)	0.6771(7)	0.1567(6)	0.0545(19)
H18A	0.3054	0.7272	0.2186	0.065*
H18B	0.3615	0.6105	0.1344	0.065*
C19	0.4012(7)	0.7798(7)	0.0605(6)	0.0421(17)
C20	0.4872(8)	0.7359(7)	−0.0461(6)	0.058(2)
H20	0.5402	0.6402	−0.0575	0.070*
C21	0.4964(8)	0.8293(8)	−0.1355(6)	0.058(2)
H21	0.5551	0.7965	−0.2060	0.070*
C22	0.4193(7)	0.9711(7)	−0.1210(6)	0.0408(16)
C23	0.3364(7)	1.0173(7)	−0.0132(5)	0.0437(17)
H23	0.2869	1.1129	−0.0012	0.052*
C24	0.3276(7)	0.9219(7)	0.0751(5)	0.0460(17)
H24	0.2708	0.9542	0.1461	0.055*
C25	0.4091(8)	1.0816(8)	−0.2142(6)	0.0495(18)
H2B	1.049(6)	0.442(5)	0.643(4)	0.021(17)*
H1B	1.189(7)	−0.024(6)	0.431(5)	0.04(2)*

Experimental details

Hydrogen atoms were included by riding models. Their U_{iso} values were set to $1.2U_{eq}$ of the parent atoms.

Comment

Mixed ligands-MOFs and CPs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. N-containing ligands are electrically neutral, while carboxylate ligands are mainly negatively charged. Multicarboxylates like the 5-(4-carboxy-benzylamino)-isophthalic acid have been widely utilized to construct such networks [4–6]. On the other hand, 4,4'-bis(pyrid-4-yl)biphenyl serves as bridging ligand [7–10].

In the title complex, there are one Cd(II) ion, two coordinated water molecule, one H₂Cbic ligand, and one half of the 4,4'-bis(pyrid-4-yl)biphenyl ligand in the asymmetric unit. Cd1 is seven-coordinated by six O atoms from two H₃Cbic and two coordinated water molecules, and one N atom from the 4,4'-bis(pyrid-4-yl)biphenyl ligand (see the figure). The Cd–N bond lengths are 2.216(5) Å and the Cd–O ones are in the range of 2.290(4) to 2.640(4) Å. Cd(II) ions are linked by 4,4'-bis(pyrid-4-yl)biphenyl ligands and H₂Cbic ligands to form a 2-D layer. In the title complex, there are hydrogen bonds between water and carboxylate O atoms. An extended three-dimensional network of hydrogen bonds contributes to the stability of the structure.

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