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Crystal structure of *catena*-poly[tetraaqua-(μ_2 -4,4'-bipyridine- $k^2N:N'$)-bis(μ_2 -4'-methyl-[1,1'-biphenyl]-3,5-dicarboxylato- $k^4O,O':O'',O'''$) dicadmium(II)] dihydrate, $C_{20}H_{20}NO_7Cd$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.42 × 0.32 × 0.25 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.13 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9906, 3720, 0.065
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2947
$N(\text{param})_{\text{refined}}$:	264
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'-methyl-[1,1'-biphenyl]-3,5-dicarboxylic acid (0.1 mmol, 0.0256 g) (H_2mbdc), 4,4'-bipyridine (0.1 mmol, 0.0156 g), and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 443 K for 26 h, followed by slow cooling to room temperature. Colourless crystals of the compound formed.

Experimental details

Coordinates of hydrogen atoms were refined without any constraints or restraints. Their U_{iso} values were set to $1.2U_{\text{eq}}$ of the parent atoms.

Comment

In the last two decades, a large number of mixed ligands metal-organic frameworks (MOFs) and coordination polymers (CPs) have been reported in the literature. Mixed ligands–MOFs and CPs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. N-containing ligands normally coordinate as neutral tectons [4, 5]. Among organic aromatic multicarboxylates

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Abstract

$C_{20}H_{20}NO_7Cd$, triclinic, $P\bar{1}$ (no. 2), $a = 9.9506(8)$ Å, $b = 10.1867(11)$ Å, $c = 11.2774(11)$ Å, $\alpha = 110.528(9)^\circ$, $\beta = 93.830(7)^\circ$, $\gamma = 107.307(8)^\circ$, $V = 1003.18(17)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0775$, $wR_{\text{ref}}(F^2) = 0.2051$, $T = 293(2)$ K.

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

Atom	x	y	z	U _{iso} [*] /U _{eq}
C1	0.8023 (13)	−0.0773 (12)	0.1803 (11)	0.071 (2)
H1	0.7247	−0.1541	0.1824	0.085*
C2	0.8571 (13)	−0.0999 (13)	0.0681 (12)	0.076 (3)
H2	0.8168	−0.1905	−0.0021	0.091*
C3	0.9704 (11)	0.0106 (11)	0.0599 (10)	0.0494 (19)
C4	1.0190 (11)	0.1401 (11)	0.1639 (10)	0.0526 (19)
H4	1.0923	0.2209	0.1624	0.063*
C5	0.9589 (11)	0.1531 (11)	0.2744 (10)	0.0532 (19)
H5	0.9966	0.2434	0.3453	0.064*
C6	0.6993 (10)	0.3530 (10)	0.5359 (9)	0.0430 (14)
C7	0.6624 (10)	0.4918 (10)	0.5936 (9)	0.0432 (14)
C8	0.7056 (10)	0.6051 (10)	0.5503 (9)	0.0389 (14)
H8	0.7587	0.5965	0.4850	0.047*
C9	0.6700 (10)	0.7325 (10)	0.6039 (9)	0.0422 (15)
C10	0.5913 (10)	0.7447 (10)	0.7018 (9)	0.0429 (15)
H10	0.5678	0.8304	0.7374	0.052*
C11	0.5467 (10)	0.6319 (10)	0.7481 (9)	0.0411 (14)
C12	0.5856 (10)	0.5066 (10)	0.6939 (9)	0.0428 (14)
H12	0.5599	0.4311	0.7250	0.051*
C13	0.4547 (11)	0.6418 (11)	0.8476 (10)	0.0466 (15)
C14	0.4272 (12)	0.7655 (12)	0.9140 (11)	0.0623 (18)
H14	0.4736	0.8519	0.9012	0.075*
C15	0.3348 (12)	0.7736 (13)	1.0000 (11)	0.0660 (19)
H15	0.3195	0.8632	1.0406	0.079*
C16	0.2674 (12)	0.6564 (12)	1.0260 (11)	0.0580 (18)
C17	0.2869 (12)	0.5279 (13)	0.9586 (11)	0.0632 (18)
H17	0.2403	0.4426	0.9729	0.076*
C18	0.3759 (12)	0.5197 (12)	0.8675 (11)	0.0602 (17)
H18	0.3814	0.4273	0.8185	0.072*
C19	0.7116 (10)	0.8543 (10)	0.5566 (9)	0.0417 (15)
C20	0.1659 (13)	0.6633 (15)	1.1205 (12)	0.077 (3)
H20A	0.1270	0.7403	1.1254	0.115*
H20B	0.2171	0.6849	1.2042	0.115*
H20C	0.0894	0.5690	1.0918	0.115*
Cd1	0.76026 (7)	0.08605 (6)	0.46903 (6)	0.0344 (3)
N1	0.8543 (9)	0.0482 (8)	0.2853 (7)	0.0441 (19)
O1	0.0710 (9)	0.5222 (9)	0.6983 (8)	0.076 (2)
H1A	0.0790	0.5550	0.6384	0.114*
H1B	0.0505	0.4281	0.6661	0.114*
O2	0.5388 (7)	−0.0679 (7)	0.3311 (6)	0.0482 (16)
H2A	0.4823	−0.1439	0.3632	0.072*
H2B	0.4569	−0.0202	0.3498	0.072*
O3	0.9828 (7)	0.2177 (7)	0.5981 (7)	0.0528 (17)
H3A	0.9736	0.2631	0.6749	0.079*
H3B	1.0267	0.2876	0.5747	0.079*
O4	0.6516 (7)	0.2497 (6)	0.5741 (7)	0.0472 (16)
O5	0.7754 (8)	0.3414 (7)	0.4523 (7)	0.0521 (17)
O6	0.7745 (7)	0.8417 (7)	0.4609 (7)	0.0470 (16)
O7	0.6852 (7)	0.9726 (7)	0.6131 (7)	0.0453 (16)

like the 4'-methyl-[1,1'-biphenyl]-3,5-dicarboxylato can yield predetermined networks [6–10]. Additionally, 4,4'-bipyridine serves as bridging ligand [11–15].

In the title complex, there are one Cd(II) ion, two coordinated water molecules one mbdc ligand, and one half of the 4,4'-bipyridine ligand, and finally one uncoordinated water molecule in the asymmetric unit (see the Figure). The cadmium atom Cd1 is seven-coordinated by four O atoms from the mbdc ligands, two water ligands, and one N atom from the 4,4'-bipyridine ligand from the axial positions (see the Figure). The Cd–N bond length is 2.287(7) Å and the Cd–O ones are in the range of 2.283(6) to 2.634(6) Å.

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