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Crystal structure of poly[diaqua-(m₃-3',5'-dicarboxy-[1,1'-biphenyl]-3,4-dicarboxylato-K⁴O,O':O'':O''') cadmium(II)], C₁₆H₁₁O₁₀Cd

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.45 x 0.35 x 0.26 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.40 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.5°, >99 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9282, 3010, 0.036
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2521
$N(\text{param})_{\text{refined}}$:	247
Programs:	CrysAlis ^{PRO} [1], SHELX [2,3]

Source of material

A mixture of Cd(NO₃)₂·2H₂O (0.1 mmol, 0.0272 g), and 3,3',4,5'-biphenyl tetracarboxylic acid (H4btc) (0.1 mmol, 0.0330 g), was dissolved in 10 mL H₂O. Then the solution was heated in a 25 mL Teflon-lined autoclave under autogenous pressure at 443 K for 4 days. After cooling to room temperature, crystals were collected.

Experimental details

Coordinates of hydrogen atoms were positioned based on the molecular restrictions. Their U_{iso} values were set to 1.2 U_{eq} of the parent atoms.

Comment

In the last two decades, a large number of metal-organic frameworks (MOFs) have been reported. Organic aromatic multicarboxylates like the biphenyl-tetracates can yield predetermined networks and have been widely utilized to construct MOFs [4–8]. On the other hand, 3,3',4,5'-biphenyl tetracarboxylic acid serves as bridging ligand [9, 10].

In the title complex, there are one Cd(II), two water molecules and one H2btc ligand in the asymmetric unit.

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Abstract

C₁₆H₁₁O₁₀Cd, monoclinic, C2/c (no. 15), $a = 26.026(3)$ Å, $b = 6.3807(6)$ Å, $c = 19.738(5)$ Å, $\alpha = 90$, $\beta = 98.162(16)$, $\gamma = 90$, $V = 3244.5(10)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0359$, $wR_{\text{ref}}(F^2) = 0.0702$, $T = 293(2)$ 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.

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Cd1	0.71693 (2)	0.28960 (4)	0.41166 (2)	0.02573 (11)
O1	0.74533 (14)	0.4337 (7)	0.31824 (16)	0.0827 (14)
H11	0.742673	0.344302	0.285234	0.124*
H12	0.778199	0.456398	0.327242	0.124*
O2	0.75421 (12)	−0.0259 (4)	0.39677 (13)	0.0400 (8)
H21	0.730647	−0.120067	0.385414	0.060*
H22	0.770153	−0.070314	0.435515	0.060*
O3	0.69635 (11)	0.6598 (4)	0.47673 (14)	0.0364 (7)
O4	0.64513 (12)	0.4898 (4)	0.39848 (14)	0.0416 (8)
O5	0.38858 (11)	0.3694 (4)	0.39040 (13)	0.0361 (7)
H5	0.370225	0.266998	0.394513	0.054*
O6	0.32767 (11)	0.4328 (4)	0.30154 (13)	0.0382 (8)
O7	0.34180 (11)	1.1026 (4)	0.17462 (13)	0.0351 (7)
O8	0.41226 (12)	1.3050 (4)	0.20173 (14)	0.0334 (7)
H8	0.397 (2)	1.386 (8)	0.174 (3)	0.077 (19)*
O9	0.67154 (11)	0.9397 (4)	0.59051 (12)	0.0299 (7)
O10	0.70490 (10)	1.1428 (4)	0.51627 (12)	0.0224 (6)
C1	0.61267 (14)	0.8043 (5)	0.44149 (17)	0.0191 (8)
C2	0.56459 (15)	0.7792 (6)	0.40077 (17)	0.0236 (9)
H2A	0.558460	0.657899	0.374737	0.028*
C3	0.52559 (15)	0.9292 (5)	0.39780 (17)	0.0211 (9)
C4	0.53595 (15)	1.1127 (6)	0.43528 (18)	0.0257 (9)
H4	0.511099	1.218263	0.432415	0.031*
C5	0.58311 (15)	1.1392 (6)	0.47691 (18)	0.0240 (9)
H5A	0.589089	1.261300	0.502528	0.029*
C6	0.62161 (14)	0.9869 (5)	0.48111 (16)	0.0178 (8)
C7	0.47467 (14)	0.8905 (6)	0.35460 (17)	0.0213 (8)
C8	0.44744 (15)	0.7072 (6)	0.36300 (17)	0.0233 (9)
H8A	0.461445	0.609221	0.395326	0.028*
C9	0.39956 (15)	0.6676 (5)	0.32390 (17)	0.0215 (9)
C10	0.37941 (15)	0.8097 (5)	0.27365 (17)	0.0237 (9)
H10A	0.347839	0.782562	0.246650	0.028*
C11	0.40640 (15)	0.9915 (5)	0.26384 (17)	0.0208 (8)
C12	0.45358 (15)	1.0346 (6)	0.30515 (17)	0.0219 (9)
H12A	0.470881	1.159607	0.299606	0.026*
C13	0.65441 (15)	0.6435 (5)	0.43950 (17)	0.0212 (9)
C14	0.36838 (16)	0.4795 (6)	0.33680 (18)	0.0253 (9)
C15	0.38340 (16)	1.1384 (6)	0.20916 (18)	0.0247 (9)
C16	0.67032 (15)	1.0219 (5)	0.53241 (17)	0.0198 (9)

The cadmium atom is six-coordinated by two water ligands, and four oxygen atoms from four H2btc ligands. The Cd–O bond lengths are all in the expected ranges.

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