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Crystal structure of poly [aqua-(μ_2 -1,3-di(1*H*-imidazol-1-yl)propane- $\kappa^2 N:N'$)-(μ_3 -2,3,5,6-tetrafluoroterephthalato- $\kappa^3 O:O':O''$)cadmium(II)], $C_{17}H_{14}N_4O_5F_4Cd$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.20 × 0.18 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.21 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9653, 3400, 0.020
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3057
$N(\text{param})_{\text{refined}}$:	284
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Source of material

The mixture of 2,3,5,6-tetrafluoroterephthalic acid 23.8 mg (0.1 mmol), cadmium(II) nitrate tetrahydrate 30.8 mg (0.1 mmol), 1,3-di(1*H*-imidazol-1-yl)propane 20.1 mg (0.1 mmol), NaOH 12 mg (0.15 mmol) and 10 mL H₂O were placed in the autoclave lined with PTFE and heated at 130 °C for 24 h, then cooled up to room temperature over 24 h. The colorless crystals of the title compound were collected.

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [1]. The hydrogen atoms were placed at calculated positions and refined as riding atoms [2].

Comment

Mixed ligands–CPs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. Multicarboxylates like the 2,3,5,6-tetrafluoroterephthalate have been widely utilized to construct such networks [4–6]. Furthermore, 1,3-di(1*H*-imidazol-1-yl)propane serves as bridging ligand [7–10].

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Abstract

$C_{17}H_{14}N_4O_5F_4Cd$, monoclinic, $P2_1/c$ (no. 14), $a = 9.6671(7)$ Å, $b = 20.0783(13)$ Å, $c = 10.4225(7)$ Å, $\beta = 107.365(1)^\circ$, $V = 1930.8(2)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0250$, $wR_{\text{ref}}(F^2) = 0.0880$, $T = 293(2)$ 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}
C1	0.8393 (3)	0.26850 (13)	0.8784 (3)	0.0215 (6)
C2	0.9706 (3)	0.27903 (13)	1.0013 (3)	0.0209 (6)
C3	1.0260 (3)	0.22665 (12)	1.0872 (3)	0.0207 (6)
C4	1.1339 (3)	0.23586 (13)	1.2076 (3)	0.0215 (6)
C5	1.1952 (3)	0.29754 (15)	1.2465 (3)	0.0229 (6)
C6	1.1442 (3)	0.34946 (14)	1.1579 (3)	0.0287 (6)
C7	1.0358 (3)	0.34051 (14)	1.0382 (3)	0.0276 (6)
C8	1.3090 (3)	0.30588 (14)	1.3824 (3)	0.0224 (6)
C9	0.6045 (3)	0.41451 (14)	0.4308 (3)	0.0322 (7)
H9	0.543678	0.392383	0.356987	0.039*
C10	0.7421 (4)	0.43591 (16)	0.6263 (3)	0.0381 (8)
H10	0.796506	0.430876	0.715865	0.046*
C11	0.7307 (4)	0.49290 (16)	0.5547 (3)	0.0425 (8)
H11	0.773797	0.533680	0.584994	0.051*
C12	0.6052 (4)	0.52202 (16)	0.3105 (3)	0.0460 (9)
H12A	0.554108	0.560770	0.328624	0.055*
H12B	0.540575	0.498427	0.234980	0.055*
C13	0.7365 (4)	0.54431 (17)	0.2740 (3)	0.0495 (9)
H13A	0.792010	0.574116	0.343645	0.059*
H13B	0.704666	0.569677	0.191135	0.059*
C14	0.8362 (4)	0.48891 (17)	0.2555 (4)	0.0484 (9)
H14A	0.910958	0.508104	0.222202	0.058*
H14B	0.883464	0.469016	0.342359	0.058*
C15	0.7466 (3)	0.37288 (15)	0.1952 (3)	0.0341 (7)
H15	0.787266	0.355349	0.280774	0.041*
C16	0.6330 (5)	0.38299 (18)	−0.0126 (3)	0.0534 (10)
H16	0.578154	0.373056	−0.100115	0.064*
C17	0.6892 (5)	0.44307 (19)	0.0294 (3)	0.0539 (11)
H17	0.680472	0.481484	−0.022253	0.065*
Cd1	0.64479 (2)	0.27539 (2)	0.58565 (2)	0.02196 (11)
F1	0.97358 (18)	0.16466 (8)	1.05682 (16)	0.0324 (4)
F2	1.17822 (19)	0.18358 (8)	1.29022 (16)	0.0349 (4)
F3	1.2030 (2)	0.41102 (9)	1.18718 (19)	0.0532 (6)
F4	0.9910 (2)	0.39409 (9)	0.95832 (18)	0.0505 (5)
H1WA	0.4042 (10)	0.3088 (11)	0.6328 (17)	0.051 (11)*
N1	0.6619 (3)	0.38689 (12)	0.5476 (3)	0.0291 (5)
N2	0.6431 (3)	0.47824 (12)	0.4292 (3)	0.0345 (6)
N3	0.6682 (3)	0.33792 (14)	0.0924 (2)	0.0325 (6)
N4	0.7615 (3)	0.43665 (13)	0.1629 (2)	0.0383 (6)
O1	0.8475 (2)	0.28980 (11)	0.7688 (2)	0.0316 (5)
O2	0.7346 (2)	0.23819 (10)	0.89759 (19)	0.0263 (4)
O3	1.4280 (2)	0.27689 (9)	1.3955 (2)	0.0303 (5)
O4	1.2740 (2)	0.33901 (11)	1.46713 (19)	0.0338 (5)
O1W	0.4797 (2)	0.30118 (12)	0.69810 (19)	0.0343 (5)
H1WB	0.455524	0.270436	0.743212	0.051*

The asymmetric unit of the title structure contains one Cd(II) cation, one coordinated water molecule, one 1,3-di(1*H*-imidazol-1-yl)propane and one dianionic (2,3,5,6-tetrafluoroterephthalate) (see the Figure). Each Cd(II) is six-coordinated by three oxygen atoms from

three 2,3,5,6-tetrafluoroterephthalate, one oxygen atom from one coordinated water molecule and two nitrogen atoms from two 1,3-di(1*H*-imidazol-1-yl)propane ligands [Cd(1)–O(1W) 2.303(2) Å, Cd(1)–O(1) 2.310(2) Å, Cd(1)–O(2) 2.3845(19) Å, Cd(1)–O(3) 2.417(2) Å, Cd(1)–N(1) 2.288(2) Å, d(1)–N(3) 2.285(3) Å], exhibiting a distorted octahedral geometry. The bridging 2,3,5,6-tetrafluoroterephthalate and 1,3-di(1*H*-imidazol-1-yl)propaneligands link Cd cations to form a 2D layer.

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