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Crystal structure of *catena*-poly[diaqua-bis(μ_2-1,3-di(1*H*-imidazol-1-yl)propane-κ^2*N*:*N*′)cobalt(II)] tetrafluoroterephthalate, $C_{26}H_{28}N_8O_6F_4Co$

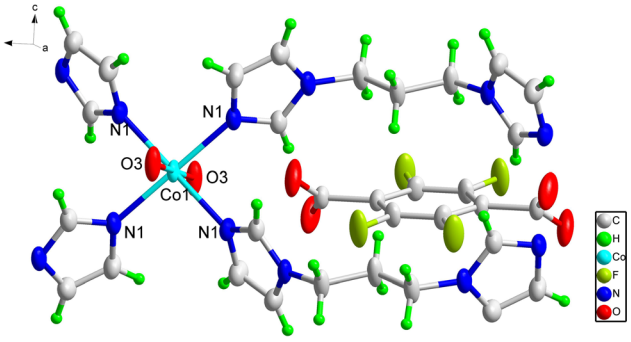

Table 1: Data collection and handling.

Crystal:	Pink
Size:	0.40 × 0.38 × 0.30 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.68 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3666, 1327, 0.017
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1202
$N(param)_{refined}$:	108
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3]

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Abstract

$C_{26}H_{28}N_8O_6F_4Co$, monoclinic, *C*2/*m* (no. 12), a = 15.7590(18) Å, b = 11.6981(15) Å, c = 9.1210(12) Å, β = 121.227(7)°, V = 1437.8(3) Å^3, Z = 2, $R_{gt}(F)$ = 0.0323, $wR_{ref}(F^2)$ = 0.0904, 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.

Source of material

The mixture of 2,3,5,6-tetrafluoroterephthalic acid 23.8 mg (0.1 mmol), cobalt(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 H_2O were placed in the autoclave, lined with polytetrafluoroethylene and heated at 120 °C for 24 h, then cooled up to room temperature over 24 h. The pink crystals of the title compound were collected.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	1.000000	0.500000	1.000000	0.0258 (2)
F1	0.92494 (13)	0.11177 (12)	0.6665 (2)	0.0558 (5)
N1	0.89139 (13)	0.36627 (14)	0.8878 (2)	0.0306 (4)
N2	0.80923 (13)	0.21109 (15)	0.8753 (2)	0.0326 (4)
O1	0.97290 (17)	0.29977 (15)	0.3624 (2)	0.0596 (6)
O2	0.9950 (2)	0.500000	1.2317 (3)	0.0474 (7)
H2	0.987234	0.441010	1.277920	0.057*
C1	0.88654 (16)	0.27921 (18)	0.9742 (3)	0.0321 (5)
H1	0.931409	0.266431	1.090119	0.039*
C2	0.81271 (18)	0.3515 (2)	0.7235 (3)	0.0411 (6)
H2A	0.796892	0.400178	0.632155	0.049*
C3	0.76181 (18)	0.2566 (2)	0.7137 (3)	0.0414 (6)
H3	0.705800	0.227740	0.616852	0.050*
C4	0.78273 (19)	0.10614 (19)	0.9300 (3)	0.0404 (6)
H4A	0.711229	0.102866	0.877530	0.049*
H4B	0.812093	0.107928	1.053401	0.049*
C5	0.8176 (3)	0.000000	0.8818 (5)	0.0418 (8)
H5A	0.791699	−0.000001	0.759389	0.050*
H5B	0.889490	0.000001	0.940684	0.050*
C6	1.000000	0.2533 (2)	0.500000	0.0293 (6)
C7	1.000000	0.1225 (2)	0.500000	0.0273 (6)
C8	0.96409 (16)	0.05881 (18)	0.5844 (3)	0.0307 (5)

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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.

Comment

Mixed ligands – CPs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. A large number of studies have been focused on photoluminescent, upconversion luminescent, and nonlinear optical CPs for applications in areas such as white-light emission, bioimaging, sensing, and photocatalysis. 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]. Meanwhile, the isomorphic structure has also been reported [11].

The unit cell of the title structure contains one Co(II) cation, two coordinated water molecules, two 1,3-di(1*H*-imidazol-1-yl)propane and one deprotonated dianionic 2,3,5,6-tetrafluoroterephthalate (see Figure 1). Each Co(II) ion is six-coordinated by two oxygen atoms from two coordinated water molecules, four nitrogen atom from four 1,3-di(1*H*-imidazol-1-yl)propane ligands, which exhibit distorted octahedral geometry. Each Co(II) bridged by four bidentate 1,3-di(1*H*-imidazol-1-yl)propane ligands to afford a 1D loop-like chain along the c axis with the neighboring Co(II)–Co(II) distances of 11.745 Å. Meanwhile, the deprotonated dianionic 2,3,5,6-tetrafluoroterephthalate anions aggregates in the title compound can be seen as intercalation of guests into void spaces in the adjacent 1D loop-like chain, which is further reinforced through strong intermolecular hydrogen bonds (O3W–H3–O1 = 2.757(6) Å, O4W–H4–O2 = 2.799(6) Å, C1–H1–O1 = 3.090(8) Å, C6–H6–O2 = 3.154(8) Å) to form an overall 3D supramolecular framework.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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