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Crystal structure of poly[di-µ₂-aqua]-diaqua-bis(µ₆-4,4′,4″-(benzene-1,3,5-triyltris(oxy))tribenzoato-κ⁶O¹:O²:O³:O⁵:O⁶)tricadmium(II)] dihydrate, C₅₄H₄₂Cd₃O₂₄

Abstract
C₅₄H₄₂Cd₃O₂₄, triclinic, P̅1 (no. 2), a = 7.9122(5) Å, b = 9.0693(6) Å, c = 18.6637(11) Å, β = 100.765(6)°, V = 1241.99(15) Å³, Z = 1, Rgt(F) = 0.0266, wRref(F²) = 0.0646, T = 293(2) K.

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A part of the title crystal 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.

Source of material
A mixture of 1,3,5-tris(4-carbonylphenyloxy)benzene (H₃TCPB, 0.004 mmol, 1.9 mg), Cd(NO₃)₂·4 H₂O (0.008 mmol, 2.5 mg), and 5 mL mixed solution of EtOH/H₂O (v/v = 1/4) was added to a glass tube, pumped to a near-vacuum, heated at 160 °C for 50 h, and cooled to 25 °C with a decreasing rate of 2 °C/h. Colorless block crystals of the title complex were obtained with the yield of ca. 48% (based on H₃TCPB).

Experimental details
H atoms bonded to C atoms from organic ligands were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, with Uiso(H) = 1.2 times Ueq(C).

Comment
The design and synthesis of coordination polymers (CPs) have gained great interests for their interesting modular structures and potential applications in the fields of fluorescent probes and magnetism [4–6]. The selection of suitable organic ligands plays an important role in the final structure and property of the as-prepared CPs. According to previous reports,
multicarboxylate ligands are widely used to build CPs with multi-dimensional architectures and interesting properties because of their rich coordination modes [7]. In this study, we choose the flexible multicarboxylate ligand 1,3,5-tris(4-carboxybenzoylphenoxy)benzene (H$_3$TCPB) to build targeted CPs because the flexible ligands have been shown to be capable of improve the performances of CPs in terms of adsorption and separation, sensing, and shape memory [8].

A single crystal X-ray diffraction study reveals that the title complex shows a three-dimensional framework structure. The asymmetric unit contains one and a half of crystallographically independent Cd$^{2+}$ ions, one TCPB$^{3-}$ ligand, one $\mu_2$-coordinated water molecule, one coordinated water molecule, and one lattice water molecule. The distorted octahedral coordination environment of Cd1 is shaped by four carboxylato oxygen atoms, one $\mu_2$-coordinated water molecule and one H$_2$O ligand; Cd2 is six-coordinated by four carboxylato oxygen atoms and two $\mu_2$-H$_2$O ligands, which also result in a distorted octahedral coordination environment.

The H$_3$TCPB ligand is completely deprotonated and adopts ($k^0$,$k^0$)$-$(k$^-$,$k^-$)-($k^1$,$k^1$)$-\mu_4$ coordination mode to form a 3D framework. The structure of the title complex is similar to the Mn(II)-based coordination polymer reported by Liu and Hu [9, 10].

### References


