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Poly[[diaqua(μ_6-1,3,5-benzenetricarboxylato)-tricadmium(II)] dihydrate]

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The title compound, $\{[Cd_3(C_9H_3O_6)_2(H_2O)_2]\cdot 2H_2O\}_n$, consists of a three-dimensional channel-like network. The asymmetric unit contains two crystallographically independent Cd^{II} ions, one of which shows a distorted trigonal prismatic coordination provided by six O atoms from one bidentate and three monodentate carboxylate groups, and one water molecule. The second independent Cd^{II} ion, which lies on an inversion centre, displays a distorted octahedral coordination environment provided by six O atoms from four monodentate carboxylate groups and two water molecules.

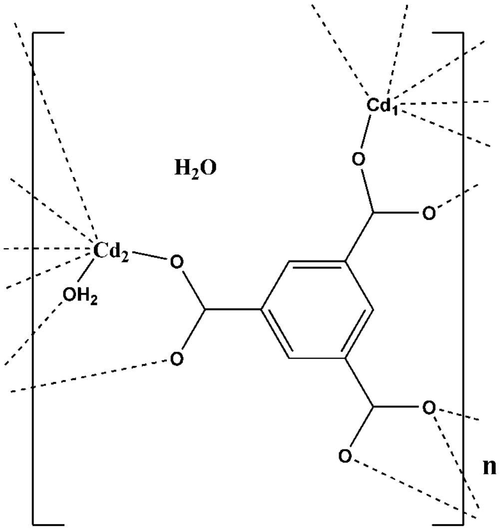
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.013 Å
R factor = 0.048
wR factor = 0.116
Data-to-parameter ratio = 10.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The construction of supramolecular networks is currently of great interest owing to their intriguing network topologies and potential functions as new classes of materials (Kepert *et al.*, 2000; Lu *et al.*, 2001). 1,3,5-Benzenetricarboxylate (btc) has a rigid benzene ring and three symmetrically distributed carboxylate groups, which have potentially diverse coordination modes. Thus, btc is usually adopted as a good spacer to build cavitary networks (Yaghi *et al.*, 1996; Chui *et al.*, 1999; Dai *et al.*, 2002; Prior *et al.*, 2003). We report here the synthesis and crystal structure of a novel three-dimensional polymeric network, formulated as $\{[Cd_3(btc)_2(H_2O)_2]\cdot 2H_2O\}_n$, (I).



(I)

Single-crystal X-ray diffraction analysis reveals that (I) crystallizes in the space group $P\overline{1}$ and consists of a three-dimensional channel-like network. The asymmetric unit contains Cd^{II} ions, btc ligands and water molecules in a 1.5:1:2 stoichiometric ratio (Fig. 1).

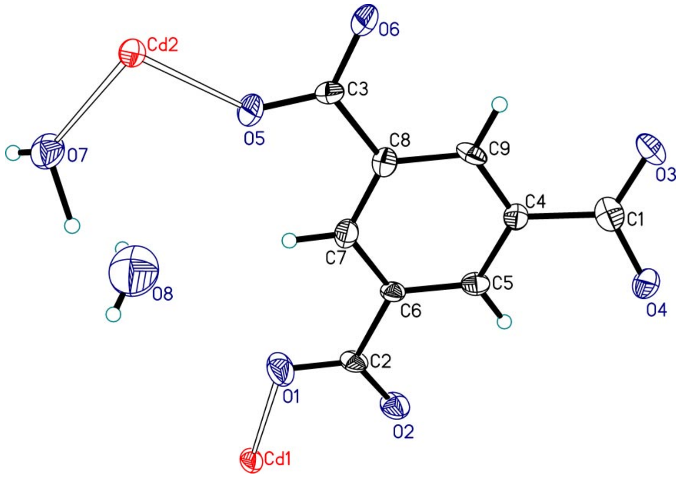


Figure 1
The asymmetric unit of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

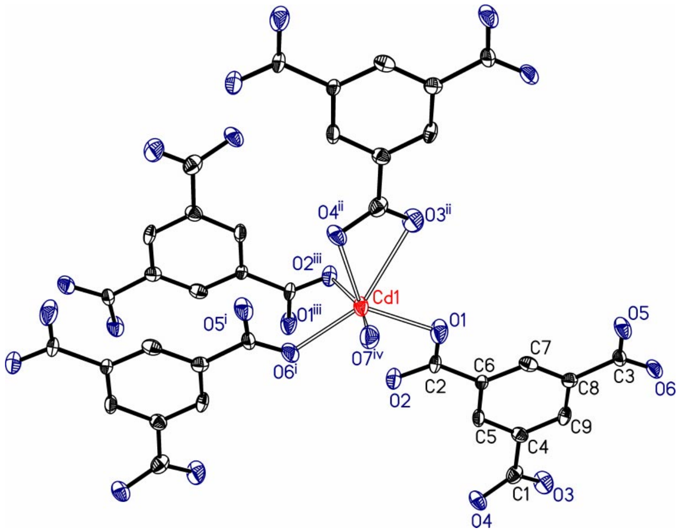


Figure 2
The coordination environment of the Cd1 ion. [Symmetry codes: (i) x, $1 + y$,$z - 1$;(ii)x,y,$z - 1$;(iii)$-x$,$1 - y$,$-1 - z$;(iv)$1 - x$,$-y$,$-1 - z$.]$-1 - z$.] $-1 - z$.] H atoms have been omitted.

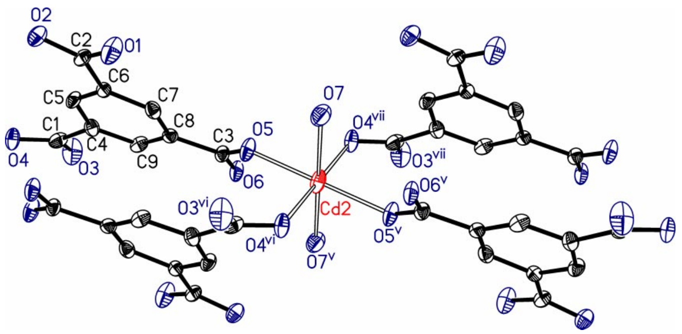


Figure 3
The coordination environment of the Cd2 ion. [Symmetry codes: (v) $1 - x$, $-1 - y$, $-z$; (vi) $1 - x$, $-y$, $-z$; (vii) x, $y - 1$, z.] H atoms have been omitted.

The Cd1 ion is coordinated by six O atoms from one bidentate and three monodentate carboxylate groups of btc ligands [Cd1—O = 2.193 (7)–2.628 (7) Å] and one water molecule [Cd1—O7 = 2.548 (8) Å], furnishing a trigonal prismatic geometry (Fig. 2). The Cd2 ion, an inversion centre, is coordinated by six O atoms from four monodentate btc carboxylate groups [Cd2—O = 2.159 (6)–2.311 (7) Å] and two water molecules [Cd2—O7 = 2.470 (8) Å] providing a distorted octahedral geometry (Fig. 3).

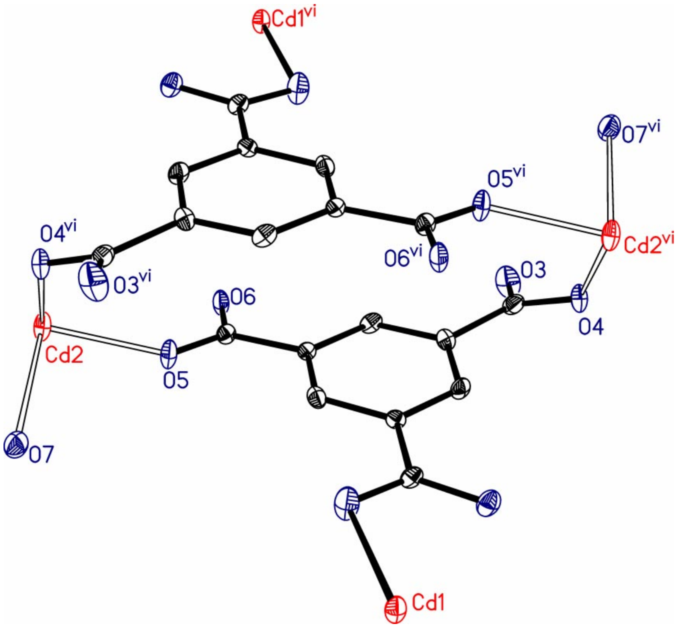
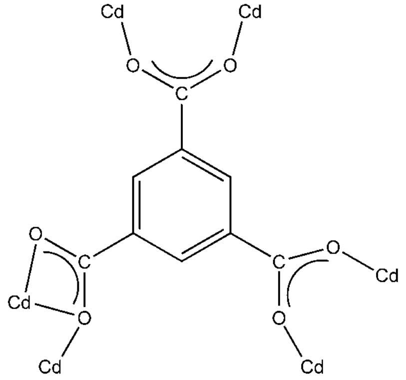


Figure 4
Perspective view of the dinuclear 16-membered ring. [Symmetry code: (vi) $1 - x$, $-y$, $-z$.] H atoms have been omitted.

The btc ligand adopts a bidentate–bidentate–tridentate coordination mode (see scheme below). Two symmetry-related Cd2 ions are linked by two btc ligands through atoms O4 and O5 from carboxylate groups to form a 16-membered dinuclear ring as building unit [$Cd2\cdots Cd2^{vi}$ = 9.529 (2) Å; symmetry code: (vi) $1 - x$, $-y$, $-z$], as shown in Fig. 4. The rings are further extended through the Cd^{II} ions and O atoms to form a three-dimensional channel-like network.



It is interesting that the three-dimensional network contains different channels along different directions. When viewed down the a axis, the three-dimensional network shows ellipsoidal channels (7.52 × 7.88 Å^2) (Fig. 5). The separation between the coordinated and the uncoordinated water O atoms is short [O7$\cdots$O8 = 2.628 (7) Å], indicating the existence of hydrogen bonds, which anchor the uncoordinated water molecules lying at the centre of the channels. However, the network displays rectangular channels (3.41 × 9.53 Å^2) when viewed down the *c* axis (Fig. 6). Uncoordinated water molecules are close to the inner backbone of the channels.

Experimental

The hydrothermal reaction of $Cd(NO_3)_2{\cdot}4H_2O$ (92 mg, 0.30 mmol), H_3btc (42 mg, 0.20 mmol) and water (10 ml) was carried out at 433 K for 3 d. After cooling to room temperature at a rate of 5 K h^{-1}, crystals of the title compound were collected by filtration and washed with distilled water (yield 41%, based on Cd). IR (KBr, ν cm^{-1}): 3392, 1618, 1562, 1439, 1369, 1109, 760, 731; Elemental analysis calculated for $C_{18}H_{14}Cd_3O_{16}$: C 26.25, H 1.71%; found: C 26.11, H 1.45%.

Crystal data

$[Cd_3(C_9H_3O_6)_2(H_2O)_2]{\cdot}2H_2O$
M_r = 823.50
Triclinic, $P\overline{1}$
a = 6.5573 (10) Å
b = 9.5294 (14) Å
c = 9.8799 (15) Å
α = 62.979 (2)°
β = 79.162 (2)°
γ = 78.385 (1)°
V = 535.40 (14) Å^3
Z = 1
D_x = 2.554 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1498 reflections
θ = 2.3–25.0°
μ = 3.04 mm^{-1}
T = 273 (2) K
Plate, colorless
0.22 × 0.14 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.616, T_{max} = 0.830
2767 measured reflections
1898 independent reflections
1510 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°
$h = -5 \rightarrow 7$
$k = -8 \rightarrow 11$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.116
S = 1.09
1898 reflections
181 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 7.0083P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.193 (7)	Cd2—O5^{v}	2.159 (6)
Cd1—O6^{i}	2.212 (6)	Cd2—O5	2.159 (6)
Cd1—O4^{ii}	2.273 (6)	Cd2—O4^{vi}	2.311 (7)
Cd1—O2^{iii}	2.330 (7)	Cd2—O4^{vii}	2.311 (7)
Cd1—O7^{iv}	2.548 (7)	Cd2—O7	2.475 (7)
Cd1—O3^{ii}	2.629 (7)	Cd2—O7^{v}	2.475 (7)
O6^{i}—Cd1—O2^{iii}	86.7 (2)	O4^{vi}—Cd2—O7	76.0 (2)
O1—Cd1—O7^{iv}	89.5 (3)	O4^{vii}—Cd2—O7	104.0 (2)
O6^{i}—Cd1—O7^{iv}	80.8 (2)	O5^{v}—Cd2—O7^{v}	89.0 (2)
O4^{ii}—Cd1—O3^{ii}	52.4 (2)	O5—Cd2—O7^{v}	91.0 (2)

Symmetry codes: (i) $x, 1+y, z-1$; (ii) $x, y, z-1$; (iii) $-x, 1-y, -1-z$; (iv) $1-x, -y, -1-z$; (v) $1-x, -1-y, -z$; (vi) $1-x, -y, -z$; (vii) $x, y-1, z$.

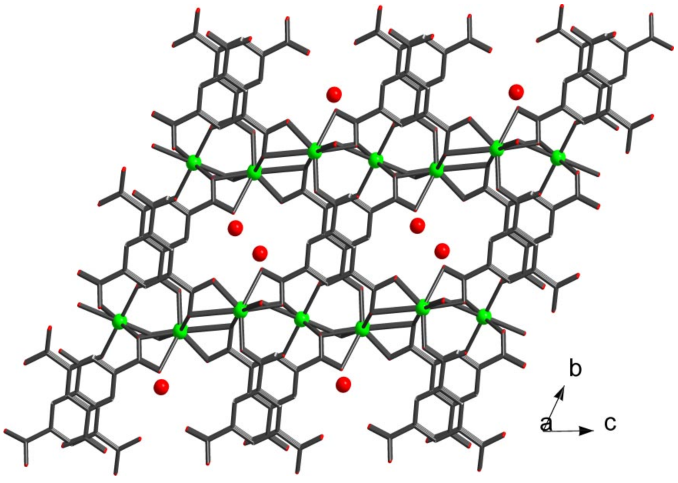


Figure 5
View of the three-dimensional network down the *a* axis. H atoms have been omitted.

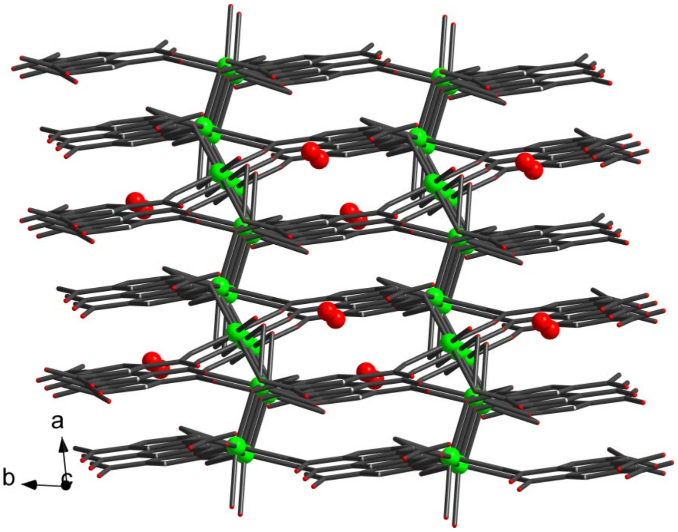


Figure 6
View of the three-dimensional network down the *c* axis. H atoms have been omitted.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O7—H7*C*$\cdots$O8	0.93 (5)	1.77 (7)	2.628 (12)	151 (10)

Water H atoms were located in a difference Fourier map and refined with isotropic displacement parameters. Other H atoms were introduced in idealized positions (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(H)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* ; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

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