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Polymeric diaquabis(μ_4-benzene-1,2,4-tricarboxylato)bis(2,2′-bipyridine)tricadmium(II)

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Key indicators

Single-crystal X-ray study
$T = 295$ K
Mean σ(C–C) = 0.005 Å
R factor = 0.023
wR factor = 0.091
Data-to-parameter ratio = 15.0

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

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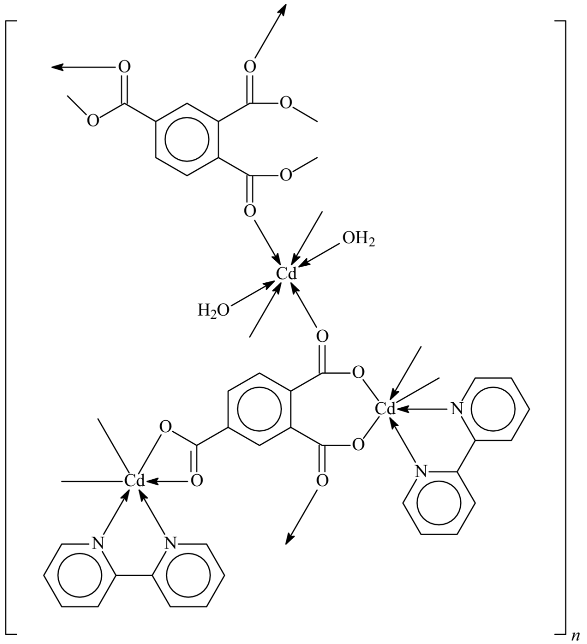
The benzene-1,2,4-tricarboxylate trianion in the polymeric title compound, $[Cd_3(C_9H_3O_6)_2(C_{10}H_8N_2)_2(H_2O)_2]_n$, uses the carboxylate groups in the 1,2-positions to chelate to a bipyridine-chelated Cd atom, which is simultaneously chelated by the 4-CO_2 group of an adjacent trianion. The O atoms of the 1,2-CO_2 groups that are not involved in chelation to the first Cd atom are each bonded to water-coordinated Cd atoms that lie on centres of inversion. The trianion links the Cd atoms to form a three-dimensional network structure, which is further consolidated by hydrogen bonds involving the water molecules.

Comment

The cadmium derivative of benzene-1,2,4,5-tetracarboxylic acid has previously been authenticated as the water-coordinated 1,10-phenanthroline complex (Shi *et al.*, 2001). The Cd atom is chelated by a carboxyl –CO_2 group, as well as by the heterocycle, and the six-coordinate geometry includes the O atoms of the carboxyl group of an adjacent tetrananion, as well as that of a water molecule, in a geometry described as a trigonal prism. The polymeric compound forms ribbons. The corresponding cadmium derivative of benzene-1,2,4-tricarboxylate, (I), exists as a polymeric three-dimensional network.



(I)

The benzene-1,2,4-tricarboxylate trianion of (I) uses the carboxyl –CO_2 groups in the 1,2-positions to chelate to a bipyridine-chelated Cd atom. This atom is also chelated by the

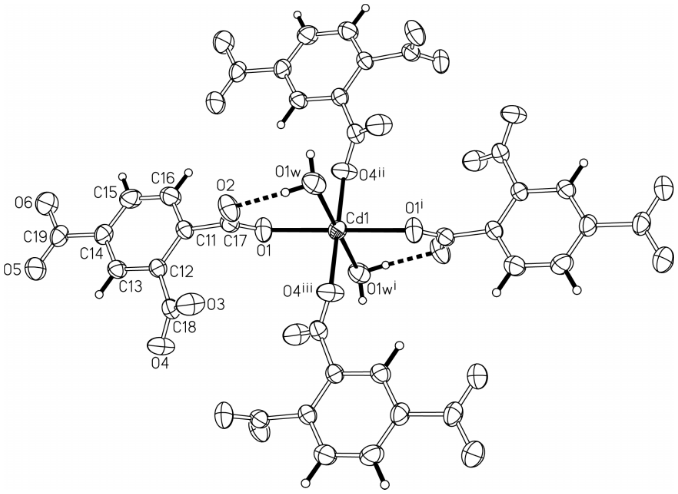


Figure 1
The coordination of the Cd1 atom in (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 70% probability level and H atoms are shown as small spheres of arbitrary radii. The Cd1 atom lies at ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$). [Symmetry/translational codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $x - 1, y, z$; (iii) $2 - x, 1 - y, 1 - z$.]

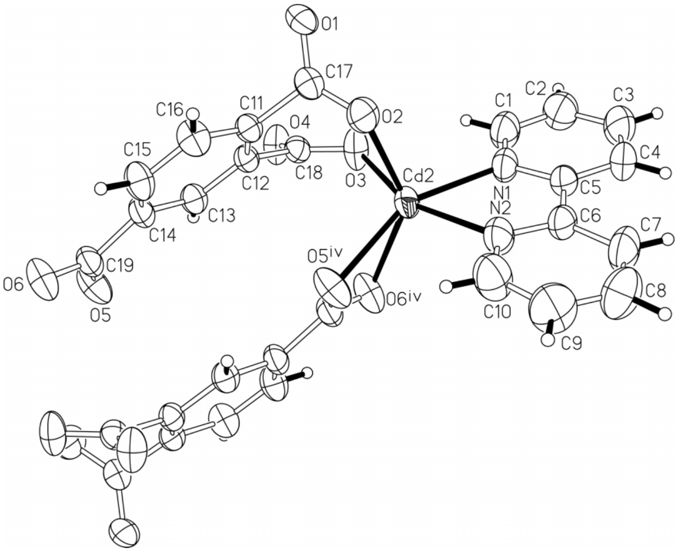


Figure 2
The coordination of the Cd2 atom in (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 70% probability level and H atoms are shown as small spheres of arbitrary radii. The Cd2 atom lies on a general position. [Symmetry code: (iv) $2 - x, 1 - y, 2 - z$.]

4-CO_2 group of an adjacent trianion. Meanwhile, the O atoms of the 1,2-CO_2 groups that are not involved in chelation to the first Cd atom are each bonded to water-coordinated Cd atoms that lie on centres of inversion (Fig. 1). The geometry of the chelated Cd atom is distorted octahedral (Fig. 2). The trianion links the Cd atoms to form a three-dimensional network structure (Fig. 3), which is further consolidated by hydrogen bonds involving the water molecules (Table 2).

Experimental

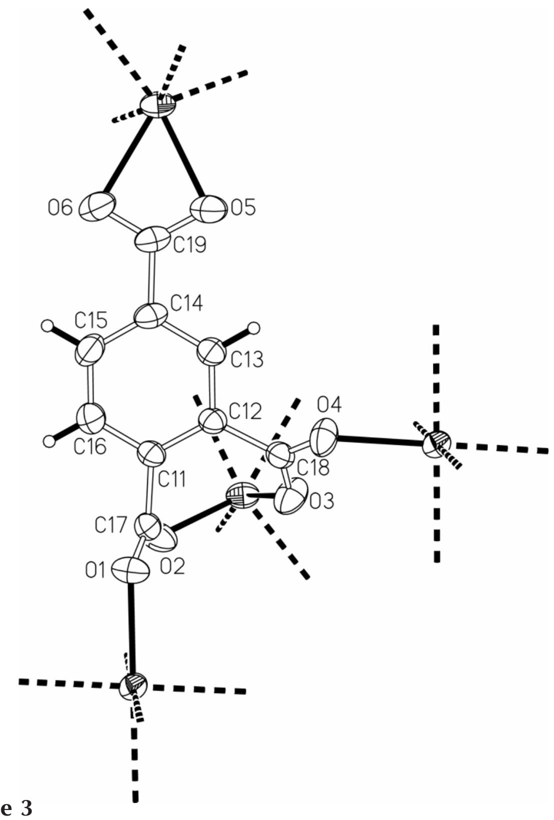


Figure 3
The μ_4 bonding mode of the benzene-1,2,4-tricarboxylate trianaion in (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are shown as small spheres of arbitrary radii.

A mixture of cadmium nitrate hexahydrate (140 mg, 0.4 mmol), benzene-1,2,4-tricarboxylic acid (85 mg, 0.4 mmol) and 2,2′-bipyridine (79 mg, 0.5 mmol) in water (20 ml) was placed in a Teflon-lined stainless-steel Parr bomb, which was then heated to 393 K for 36 h. The bomb was cooled to room temperature over 36 h. Colourless crystals of (I) were isolated in about 30% yield.

Crystal data

$[Cd_3(C_9H_3O_6)_2(C_{10}H_8N_2)_2(H_2O)_2]$
$M_r = 1099.83$
Triclinic, $P\overline{1}$
$a = 7.683$ (4) Å
$b = 11.341$ (8) Å
$c = 11.344$ (5) Å
$\alpha = 82.12$ (2)°
$\beta = 71.01$ (2)°
$\gamma = 79.56$ (3)°
$V = 916.0$ (9) Å^3
$Z = 1$
$D_x = 1.994$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8585 reflections
$\theta = 3.1$–27.5°
$\mu = 1.80$ mm^{-1}
$T = 295$ (2) K
Block, colourless
0.1 × 0.1 × 0.1 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan, (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.594$, $T_{\max} = 0.840$
9039 measured reflections
4131 independent reflections
3756 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\max} = 27.5°$
$h = -7 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.091$
$S = 1.29$
4131 reflections
276 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.4079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.52$ e Å^{-3}
$\Delta\rho_{\min} = -0.62$ e Å^{-3}
Extinction correction: none

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Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.347 (2)	Cd2—O2	2.235 (3)
Cd1—O1$^{\rm i}$	2.347 (2)	Cd2—O3	2.286 (3)
Cd1—O4$^{\rm ii}$	2.244 (2)	Cd2—O5$^{\rm iv}$	2.370 (3)
Cd1—O4$^{\rm iii}$	2.244 (2)	Cd2—O6$^{\rm iv}$	2.349 (3)
Cd1—O1*w*	2.330 (3)	Cd2—N1	2.301 (3)
Cd1—O1*w*$^{\rm i}$	2.330 (3)	Cd2—N2	2.332 (3)
O1—Cd1—O1$^{\rm i}$	180	O2—Cd2—O5$^{\rm iv}$	95.1 (1)
O1—Cd1—O4$^{\rm ii}$	84.6 (1)	O3—Cd2—O5$^{\rm iv}$	109.5 (1)
O1—Cd1—O4$^{\rm iii}$	95.4 (1)	O2—Cd2—O6$^{\rm iv}$	138.4 (1)
O1—Cd1—O1*w*	87.8 (1)	O3—Cd2—O6$^{\rm iv}$	81.4 (1)
O1—Cd1—O1*w*$^{\rm i}$	92.2 (1)	O3—Cd2—N1	87.1 (1)
O4$^{\rm ii}$—Cd1—O4$^{\rm iii}$	180	O3—Cd2—N2	158.0 (1)
O4$^{\rm ii}$—Cd1—O1*w*	91.2 (1)	O5$^{\rm iv}$—Cd2—O6$^{\rm iv}$	55.5 (1)
O4$^{\rm ii}$—Cd1—O1*w*$^{\rm i}$	88.8 (1)	O5$^{\rm iv}$—Cd2—N1	153.9 (1)
O1*w*—Cd1—O1*w*$^{\rm i}$	180	O5$^{\rm iv}$—Cd2—N2	92.3 (1)
O2—Cd2—O3	82.7 (1)	O6$^{\rm iv}$—Cd2—N1	110.2 (1)
O2—Cd2—N1	107.1 (1)	O6$^{\rm iv}$—Cd2—N2	109.8 (1)
O2—Cd2—N2	99.0 (1)		

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $x-1, y, z$; (iii) $2-x, 1-y, 1-z$; (iv) $2-x, 1-y, 2-z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O2	0.85 (1)	1.79 (2)	2.624 (3)	164 (8)
O1*w*—H1*w*2···O6$^{\rm v}$	0.85 (1)	2.00 (2)	2.836 (4)	170 (6)

Symmetry code: (v) $1-x, 1-y, 2-z$.

The C-bound H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$C] and were included in the refinement in the riding-model approximation. The water H atoms were located in a difference map and refined with a distance restraint of 0.85 (1) Å.

Data collection: *RAPID AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Acta Cryst. (2005). E**61**, m123–m125 Wang *et al.* • $[\mathrm{Cd_3(C_9H_3O_6)_2(C_{10}H_8N_2)_2(H_2O)_2}]$ **m125**