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Poly[cadmium(II)-μ_4-benzene-1,3-dioxyacetato]: a two-dimensional layer cadmium(II) coordination polymer

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.064
Data-to-parameter ratio = 14.2

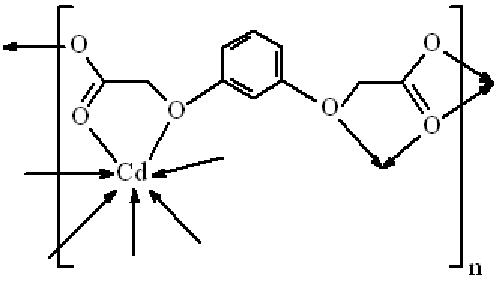
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, poly[cadmium(II)-μ_4-*m*-phenylenebis(oxyacetato)], [Cd($C_{10}H_8O_6$)]$_n$, the Cd^{II} atom exists in a distorted monocapped octahedral coordination environment with seven O atoms from four carboxylate groups. The Cd atoms are bridged by benzene-1,3-dioxyacetate dianions with tridentate and tetradentate modes of the oxyacetate groups, leading to a two-dimensional layer structure parallel to (001).

Comment

Crystal engineering of metal-organic supramolecular architectures by employing covalent linkages is a rapidly expanding field that offers potential for new classes of functional solids, in which the choice of suitable ligand is an important factor that greatly influences the structure and stabilization of the coordination architecture formed (Tao *et al.*, 2000; Choi & Jeon, 2003). Phenylenedioxydiacetic acids (bdoaH$_2$), which have versatile binding modes, are good candidates for the construction of supramolecular complexes. Previously, we have reported some Cu^{II}, Zn^{II}, Co^{II} and Cd^{II} coordination polymers constructed by 1,4-bdoaH$_2$ and coligands (or solvent), in which the 1,4-bdoa^{2-} group shows the good capability of the bridging ligand in various coordination fashions, including bidentate (Gao, Liu, Huo, Zhao & Zhao, 2004*b,c*; Gao, Liu, Huo, Zhao & Ng, 2004*a*), tridentate (Gao, Liu, Huo, Zhao & Zhao, 2004*a*) or tetradentate (Gao, Liu, Huo, Zhao & Ng, 2004*b*; Gao *et al.*, 2004). For example, in the Cd^{II} coordination polymer, [Cd(1,4-bdoa)($C_3H_4N_2$)$_3$]$_n$, the 1,4-bdoa^{2-} ligand is in a tridentate coordination mode (Gao, Liu, Huo, Zhao & Zhao, 2004*d*). However, compared with the extensively studied complexes with the 1,4-bdoa^{2-} ligand and rigid terephthalate groups (Xu *et al.*, 2004; Banerjee *et al.*, 2003), complexes with the 1,3-bdoaH$_2$ ligand have been documented very little to date. Recently, we have reported the structures of three one-dimensional chain Zn^{II}, Cd^{II} and Cu^{II} polymers (Gao, Li *et al.*, 2004; Gao, Liu, Huo, Zhao & Ng, 2004*c*; Liu *et al.*, 2004), within which the 1,3-bdoa^{2-} dianions function as bidentate bridging ligands. In the case of the Cd^{II} coordination polymer, [Cd(1,3-bdoa)(C_5H_5N)$_3$(H_2O]$_n$ (Gao, Liu, Huo, Zhao & Ng, 2004*c*), the Cd^{II} ion has an octahedral geometry. In this paper, we report the crystal structure of the title compound, (I), [Cd(1,3-bdoa)]$_n$, which is the first example of a coordination polymer based on just the 1,3-bdoa^{2-} ligand and Cd^{II} ions.

As shown in Fig. 1, the asymmetric unit of (I) comprises one Cd^{II} ion and one 1,3-bdoa^{2-} dianion. The oxyacetate groups combined with the Cd^{II} atom give two different five-membered chelate rings and one four-membered ring. The Cd^{II} ion is seven-coordinated by four 1,3-bdoa^{2-} groups, and the local coordination around the Cd^{II} ion can best be described as a distorted monocapped octahedron with a CdO_7 chromophore. Its equatorial plane is defined by atoms O1, O2^{i}, O4^{ii} and O5^{ii} [symmetry codes: (i) $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $x, y + 1, z$], with an r.m.s. deviation of 0.08 (4) Å, the deviation of atom Cd1 from this plane being 0.46 (4) Å. The axial positions are occupied by atoms O3 and O6^{iii} [symmetry code: (iii) $1 - x, y + \frac{3}{2}, \frac{1}{2} - z$], with an angle of 160.54 (6)°. The capping atom O5^{iii} deviates by 1.858 (3) Å from the plane defined by atoms O4^{ii}, O5^{ii} and O6^{iii}. The Cd1—O4^{ii} and Cd1—O5^{iii} distances are 2.709 (2) and 2.614 (2) Å, respectively, which are considerably longer than those other Cd—O distances but lie within the range of Cd—O$_{\text{carboxylate}}$ bond distances [2.209 (2)–2.879 (2) Å] reported for Cd^{II}–carboxylate coordination polymers (Clegg *et al.*, 1995). The C10—O5 and O2—C1 distances are longer than the C10—O6 and O1—C1 distances (Table 1), suggesting greater double-bond character of the latter bonds.



(I)

In the two-dimensional coordination polymer, the 1,3-bdoa^{2-} ligand displays interesting coordination modes. One of the oxyacetate groups adopts a tridentate mode, the other a tetradentate mode. In the former case, the oxyacetate group (O1—C1—O2) in the bidentate chelating mode is coordinated to atom Cd1 through ether atom O3 and carboxyl atom O1, and connects to the adjacent atom Cd1*A* through the bridging O2 atom, the Cd1···Cd1*A* separation being 5.601 (3) Å [symmetry code: (*A*) $2 - x, y + \frac{1}{2}, \frac{1}{2} - z$]. In the latter case, the oxyacetate carboxyl group (O5^{ii}—C10^{ii}—O6^{ii}) chelates atom Cd1 through ether atom O4^{ii} and carboxyl atom O5^{ii}, and bridges to a neighboring atom Cd1*D* through atoms O5^{ii} and O6^{ii}, with a Cd1···Cd1*D* separation of 4.606 (3) Å [symmetry code: (*D*) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$]. Thus, the 1,3-bdoa^{2-} ligand with a heptadentate bridging mode is linked to four Cd atoms, with Cd1···Cd1*B* and Cd1···Cd1*C* separations of 5.988 (3) and 9.640 (3) Å, respectively [symmetry codes: (*B*) $x, y - 1, z$; (*C*) $1 - x, y - \frac{3}{2}, \frac{1}{2} - z$], and further gives rise to a two-dimensional layer structure (Fig. 2). To the best our knowledge, such a heptadentate bridging mode of the 1,3-bdoa^{2-} ligand is rare and is a novel structural feature for aromatic carboxylate coordination architectures.

Experimental

Benzene-1,3-dioxyacetic acid was prepared following the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). Cadmium dinitrate tetrahydrate (6.16 g, 20 mmol), imidazole (1.90 g, 20 mmol) and 1,3-bdoaH$_2$ (4.52 g, 20 mmol) were dissolved in an ethanol/water (1:1) solution, and then the pH was adjusted to 7 with 0.1 *M* NaOH. The mixture was sealed in a 25 ml Teflon-lined stainless steel bomb and held at 393 K for 5 d. The bomb was cooled naturally to room temperature, and colorless prismatic crystals of (I) were obtained after several days. Analysis calculated: C 35.69, H 2.40%; found: C 35.82, H 2.35%.

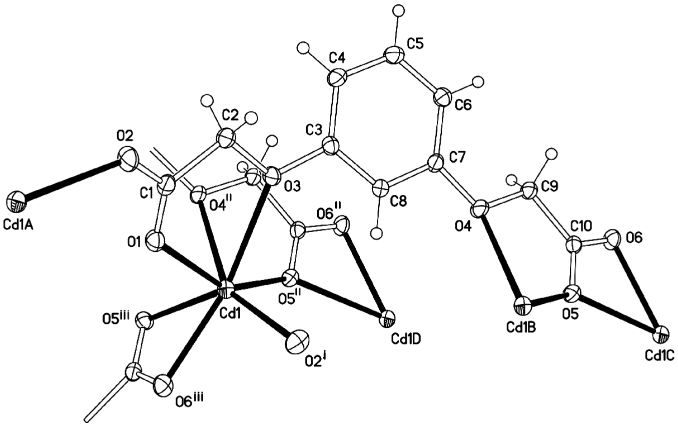


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), showing 30% probability displacement ellipsoids. [Symmetry codes: (i) $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $x, y + 1, z$; (iii) $1 - x, y + \frac{3}{2}, \frac{1}{2} - z$; (*A*) $2 - x, y + \frac{1}{2}, \frac{1}{2} - z$; (*B*) $x, y - 1, z$; (*C*) $1 - x, y - \frac{3}{2}, \frac{1}{2} - z$; (*D*) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.]

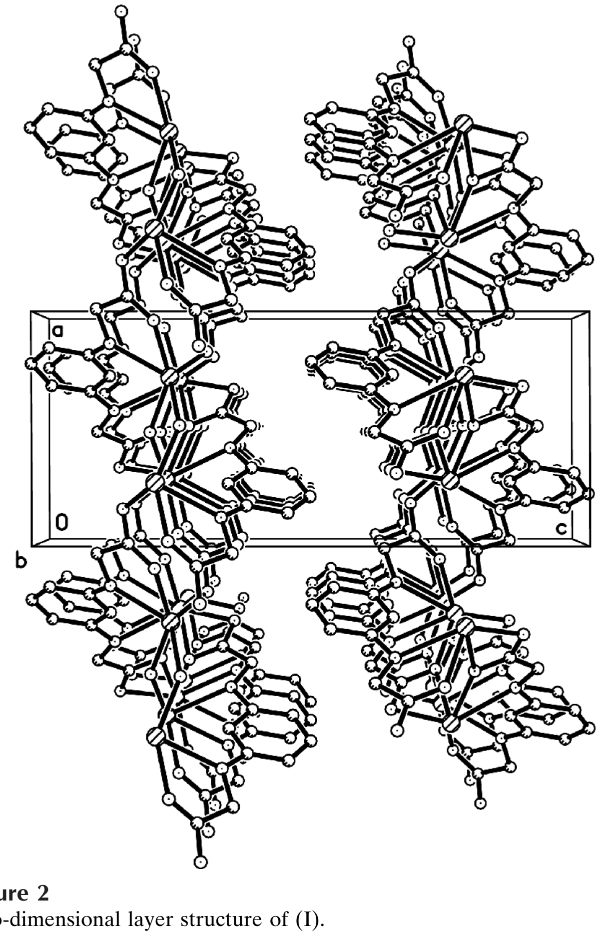


Figure 2
Two-dimensional layer structure of (I).

m1876 Shan Gao *et al.* • [Cd(C$_{10}$H$_8$O$_6$)] *Acta Cryst.* (2004). E**60**, m1875–m1877

Crystal data

[Cd($C_{10}H_8O_6$)]
M_r = 336.57
Monoclinic, $P2_1/c$
a = 8.2104 (16) Å
b = 5.9881 (12) Å
c = 19.473 (4) Å
β = 90.21 (3)°
V = 957.4 (3) Å^3
Z = 4
D_x = 2.335 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6536 reflections
θ = 3.6–27.5°
μ = 2.30 mm^{-1}
T = 293 (2) K
Prism, colorless
0.37 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min}$ = 0.469, $T_{\max}$ = 0.663
8736 measured reflections
2188 independent reflections
2135 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.021
$\theta_{\max}$ = 27.5°
$h = -10 \rightarrow 10$
$k = -7 \rightarrow 7$
$l = -25 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.064
S = 1.02
2188 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.9652P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.002
$\Delta\rho_{\max}$ = 0.70 e Å^{-3}
$\Delta\rho_{\min}$ = −0.60 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.209 (2)	Cd1—O6$^{\rm iii}$	2.322 (2)
Cd1—O2$^{\rm i}$	2.232 (2)	O1—C1	1.247 (3)
Cd1—O3	2.554 (2)	O2—C1	1.263 (3)
Cd1—O4$^{\rm ii}$	2.709 (2)	O5—C10	1.264 (3)
Cd1—O5$^{\rm ii}$	2.230 (2)	O6—C10	1.248 (3)
Cd1—O5$^{\rm iii}$	2.614 (2)		
O1—Cd1—O2$^{\rm i}$	98.95 (7)	O3—Cd1—O5$^{\rm iii}$	133.48 (6)
O1—Cd1—O3	68.31 (6)	O5$^{\rm ii}$—Cd1—O2$^{\rm i}$	99.85 (7)
O1—Cd1—O4$^{\rm ii}$	88.19 (6)	O5$^{\rm ii}$—Cd1—O3	87.03 (6)
O1—Cd1—O5$^{\rm ii}$	148.48 (7)	O5$^{\rm ii}$—Cd1—O4$^{\rm ii}$	63.85 (6)
O1—Cd1—O5$^{\rm iii}$	99.68 (6)	O5$^{\rm iii}$—Cd1—O4$^{\rm ii}$	66.37 (6)
O1—Cd1—O6$^{\rm iii}$	92.99 (7)	O5$^{\rm ii}$—Cd1—O5$^{\rm iii}$	82.88 (3)
O2$^{\rm i}$—Cd1—O3	88.78 (7)	O5$^{\rm ii}$—Cd1—O6$^{\rm iii}$	112.40 (7)
O2$^{\rm i}$—Cd1—O4$^{\rm ii}$	151.76 (6)	O6$^{\rm iii}$—Cd1—O3	160.54 (6)
O2$^{\rm i}$—Cd1—O5$^{\rm iii}$	137.66 (6)	O6$^{\rm iii}$—Cd1—O4$^{\rm ii}$	118.11 (6)
O2$^{\rm i}$—Cd1—O6$^{\rm iii}$	88.95 (7)	O6$^{\rm iii}$—Cd1—O5$^{\rm iii}$	52.46 (6)
O3—Cd1—O4$^{\rm ii}$	68.42 (6)	Cd1$^{\rm iv}$—O5—Cd1$^{\rm v}$	143.9 (8)
O1—C1—C2—O3	−18.2 (3)	C3—O3—C2—C1	−170.4 (2)
O4—C9—C10—O5	−11.3 (3)	C7—O4—C9—C10	172.0 (2)

Symmetry codes: (i) $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $x, 1 + y, z$; (iii) $1 - x, \frac{3}{2} + y, \frac{1}{2} - z$; (iv) $x, y - 1, z$; (v) $1 - x, y - \frac{3}{2}, \frac{1}{2} - z$.

H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C), and were refined in the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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Acta Cryst. (2004). E**60**, m1875–m1877 Shan Gao *et al.* • [Cd($C_{10}H_8O_6$)] **m1877**