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A one-dimensional chain Cd^{II} polymer: *catena*-poly[[tris(1*H*-imidazole-κN^3)cadmium(II)]-μ-benzene-1,4-dioxyacetato-$\kappa^3 O,O':O''$]

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In the title coordination polymer, [Cd(1,4-BDOA)($C_3H_4N_2$)$_3$]$_n$ (1,4-BDOA^{2-} is benzene-1,4-dioxyacetate, $C_{10}H_8O_6$), each Cd^{II} atom exists in a distorted octahedral coordination sphere, involving three carboxyl O atoms from different 1,4-BDOA^{2-} groups and three N atoms from the imidazole co-ligands. The Cd^{II} ions are linked by carboxylate groups into a one-dimensional infinite chain. The Cd$\cdots$Cd separation within the polymer is 15.009 (2) Å. N—H$\cdots$O hydrogen bonds help to establish the crystal packing.

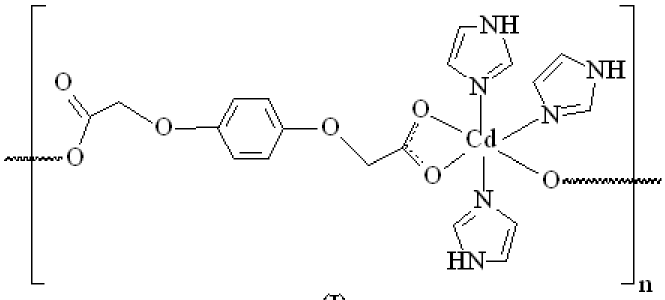
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.027
wR factor = 0.064
Data-to-parameter ratio = 16.4

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

Comment

The self-assembly of metal ions with aromatic carboxylate groups is a rapidly developing research area of modern coordination chemistry within which ligand design is an important aspect in adjusting the coordination framework and functionalities of the compounds formed. Compared with the extensively studied Cd^{II} complexes with the rigid terephthalate group (Xu *et al.*, 2004; Banerjee *et al.*, 2003; Tao *et al.*, 2000), the coordination chemistry and structural property of flexible multidentate ligand with versatile binding modes, such as benzene-1,4-dioxyacetic acid, has received little attention to date. As a contribution to this work, we have reported the structures of a number of complexes in which the benzene-1,4-dioxyacetate dianion acts as counter-ion in the Mn^{II} and Zn^{II} complexes (Gao *et al.*, 2004*a*,*b*), or only one of two oxyacetate groups is involved in coordination in the Co^{II} complex (Gao, Liu, Huo & Zhao 2004), as well as when it functions as a bridging ligand in the one-dimensional chain Zn^{II} and Cu^{II} polymers (Gao *et al.*, 2004*c*; Gao, Liu, Huo, Zhao & Ng, 2004). In the present work, a new Cd^{II} polymer, *viz* [Cd(1,4-BDOA)($C_3H_4N_2$)$_3$]$_n$ (1,4-BDOA^{2-} is benzene-1,4-dioxyacetate), (I), has been prepared by the reaction of Cd(NO_3)$_2$·4H_2O, imidazole and 1,4-BDOAH$_2$. The crystal structure of (I) is reported here.



(I)

As shown in Fig. 1, each Cd^{II} atom exists in a distorted octahedral environment, defined by three carboxyl O atoms

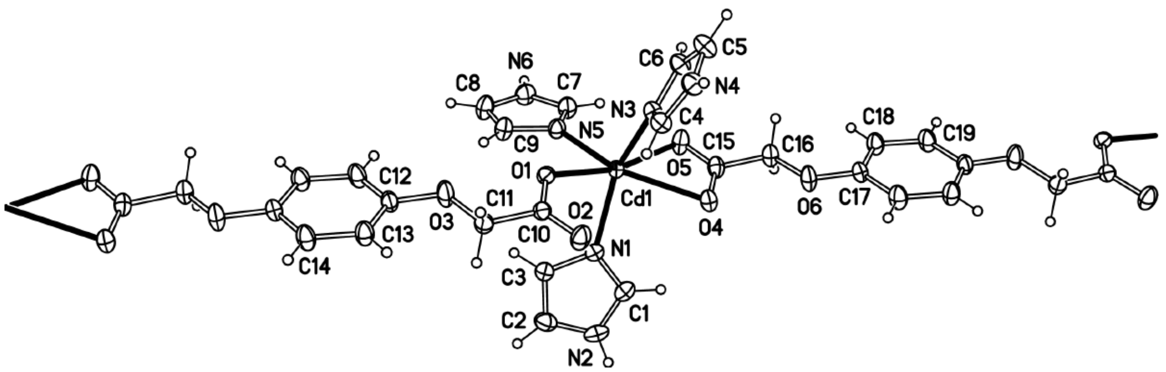


Figure 1
View of the title complex, with displacement ellipsoids drawn at the 30% probability level. H atoms are represented by small spheres of arbitrary radius.

from two different 1,4-BDOA^{2-} groups and three N atoms from the three imidazole co-ligands. Its equatorial plane is defined by atoms O1, O4, O5 and N5, with a mean deviation from this plane of 0.17 (2) Å and the deviation of the Cd atom from the mean plane being 0.043 (2) Å. The imidazole molecules act as typical monodentate ligands terminally coordinated to the metal center. The Cd—O$_{\text{carboxyl}}$ distances [2.347 (2)–2.481 (2) Å] are in the range of the corresponding bond distances of Cd–terephthalate complexes [2.251 (2)–2.879 (2) Å] (Yuan *et al.*, 2001; Fun *et al.*, 1999).

It should be noted that the O1—C10 distance [1.254 (3) Å] is longer than the O2—C10 distance [1.231 (3) Å], agreeing with the greater double-bond character of the latter bond. In contrast, the O4—C15 [1.251 (3) Å] and O5—C15 [1.253 (3) Å] distances are nearly identical, suggesting delocalization of electrons throughout. This can be explained by the influence of the different coordination modes of the carboxyl groups. In the former (O1—C10—O2), the carboxyl group is in a monodentate bridging mode through the O1 atom, and the other carboxyl group (O4—C15—O5) is in a bidentate chelating mode through atoms O4 and O5. The oxyacetate groups and phenyl ring are almost coplanar, with torsion angles of −174.2 (3) (C11—O3—C12—C19) and 178.7 (2)° (C17—O6—C16—C15). The dihedral angles between imidazole co-ligands 1–3, 3–5 and 5–1 are 88.9 (2), 57.8 (3) and 78.4 (3)°, respectively.

Each 1,4-BDOA^{2-} group adopts a tridentate coordinated mode to link two Cd$^{\text{II}}$ atoms into a one-dimensional infinite chain, running along the diagonal line of the *ac* plane. In the chain, the adjacent Cd···Cd distance is 15.009 (2) Å, longer than that found in the Cd–terephthalate complex (11.304 Å; Xu *et al.*, 2004). The chains are crosslinked by N—H···O hydrogen bonds involving the uncoordinated imidazole N atoms and 1,4–BDOA^{2-} carboxyl O atoms (Table 2 and Fig. 2).

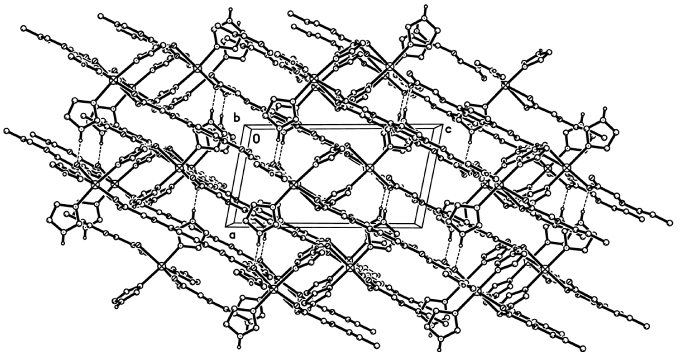


Figure 2
Packing diagram of the title complex.

Experimental

Benzene-1,4-dioxyacetic acid was prepared following the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). The title complex was synthesized by the addition of cadmium dinitrate tetrahydrate (6.16 g, 20 mmol) and imidazole (0.95 g, 10 mmol) to a hot aqueous solution of 1,4-BDOAH$_2$ (0.68 g, 20 mmol). The solution was allowed to evaporate at room temperature and colorless prismatic crystals were obtained after several days. Analysis calculated for $C_{19}H_{20}CdN_6O_6$: C 42.20, H 3.73, N 15.54%; found: C 42.09, H 3.68, N 15.37%.

Crystal data

$[Cd(C_{10}H_8O_6)(C_3H_4N_2)_3]$
$M_r = 540.82$
Triclinic, $P\bar{1}$
$a = 7.7036$ (15) Å
$b = 9.962$ (2) Å
$c = 14.548$ (3) Å
$\alpha = 82.60$ (3)°
$\beta = 78.23$ (3)°
$\gamma = 82.77$ (3)°
$V = 1078.2$ (4) Å^3
$Z = 2$
$D_x = 1.666$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10113 reflections
$\theta = 3.2$–27.5°
$\mu = 1.06$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.38 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.688$, $T_{\max} = 0.824$
10115 measured reflections
4743 independent reflections
4356 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.017$
$\theta_{\max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.064$
$S = 1.06$
4743 reflections
289 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.5293P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.66$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}

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Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.254 (2)	Cd1—O5	2.435 (2)
Cd1—N3	2.252 (2)	O1—C10	1.254 (3)
Cd1—N5	2.276 (2)	O2—C10	1.231 (3)
Cd1—O1	2.347 (2)	O4—C15	1.251 (3)
Cd1—O4	2.481 (2)	O5—C15	1.253 (3)
N1—Cd1—N5	97.91 (8)	N3—Cd1—O5	89.19 (7)
N1—Cd1—O1	85.10 (7)	N5—Cd1—O1	85.53 (7)
N1—Cd1—O4	85.13 (7)	N5—Cd1—O4	138.38 (7)
N1—Cd1—O5	106.68 (7)	N5—Cd1—O5	86.62 (7)
N3—Cd1—N1	147.74 (7)	O1—Cd1—O4	135.96 (6)
N3—Cd1—N5	111.19 (8)	O1—Cd1—O5	166.66 (6)
N3—Cd1—O1	83.63 (7)	O5—Cd1—O4	53.35 (6)
N3—Cd1—O4	82.26 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H20···O1^{i}	0.86	1.93	2.781 (3)	173
N4—H21···O4^{ii}	0.86	1.94	2.752 (3)	157
N6—H22···O2^{iii}	0.86	1.90	2.753 (3)	174

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

The H atoms attached to the C atoms and imidazole N atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (aliphatic) and N—H = 0.86 Å (imidazole), and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C, N), and were refined in the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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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