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## Key indicators

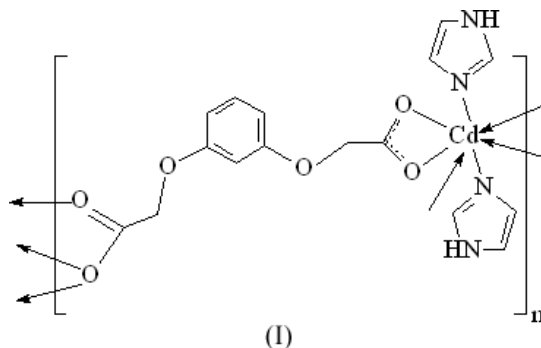
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.029  
 $wR$  factor = 0.071  
Data-to-parameter ratio = 16.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Poly[[bis(1*H*-imidazole- $\kappa N^3$ )cadmium(II)]-  
 $\mu_3$ -benzene-1,3-dioxyacetato]

Each seven-coordinate  $\text{Cd}^{\text{II}}$  atom in the title coordination polymer, poly[[bis(1*H*-imidazole- $\kappa N^3$ )cadmium(II)]- $\mu_3$ -*m*-phenylenebis(oxyacetato)],  $[\text{Cd}(1,3\text{-BDOA})(\text{C}_3\text{H}_4\text{N}_2)_2]_n$  (1,3-BDOA $^{2-}$  is the benzene-1,3-dioxyacetate dianion,  $\text{C}_{10}\text{H}_8\text{O}_6$ ), displays a distorted monocapped octahedral coordination geometry, defined by two N atoms from the imidazole ligands and five O atoms from three 1,3-BDOA $^{2-}$  anions. Adjacent  $\text{Cd}^{\text{II}}$  atoms are bridged by two 1,3-BDOA $^{2-}$  ligands, forming a one-dimensional double-chain structure, with  $\text{Cd}\cdots\text{Cd}$  separations of 4.014 (3) Å across the double chain and 13.105 (2) Å along the chain. A network of  $\text{N}-\text{H}\cdots\text{O}$  interchain hydrogen bonds is also present.

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## Comment

Recently, there has been growing interest in cadmium(II) carboxylate polymers, due to the recognition of their role in biological organisms (Strasdeit *et al.*, 1988), as well as in molecular-based materials (Liu *et al.*, 2002), within which the judicious choice of a suitable ligand is an important factor that greatly influences the structure of the coordination architecture and functionality of the complex formed. Phenylene-dioxydiacetic acids (BDOAH $_2$ ) are regarded as excellent candidates with which to construct high-dimensional coordination polymers, because of their interesting structural characteristics. Firstly, they have high symmetry and versatile carboxylate coordination modes. Secondly, they are not only capable of binding to metal centres, but can also form regular hydrogen bonds by functioning as both a hydrogen donor and acceptor, owing to the existence of deprotonated and/or



protonated carboxyl groups. Recently, we have reported some coordination polymers incorporating 1,3- or 1,4-BDOA $^{2-}$  ligands, in which these ligands act in a great variety of coordination modes, such as bidentate (Gao, Li *et al.*, 2004; Gao, Liu, Huo, Zhao & Zhao, 2004*b*; Gao, Liu, Huo, Zhao & Ng, 2004*a*; Liu *et al.*, 2004), tridentate (Gao, Liu, Huo, Zhao & Zhao, 2004*a,c,d*) or tetradentate (Gao, Liu, Huo, Zhao & Ng,

2004*b*) modes. Here, we report the structural characterization of the title novel double-chain cadmium(II) coordination polymer,  $[\text{Cd}(\text{1,3-BDOA})(\text{C}_3\text{H}_4\text{N}_2)_2]_n$ , (I) (Fig. 1), obtained by the self-assembly reaction of cadmium dinitrate tetrahydrate, imidazole and 1,3-BDOAH<sub>2</sub>. This compound represents the first example of a coordination polymer with a pentadentate 1,3-BDOA<sup>2-</sup> ligand coordinating in bridging mode.

The asymmetric unit of (I) consists of a Cd<sup>II</sup> ion, two imidazole molecules and one 1,3-BDOA<sup>2-</sup> dianion. The seven-coordinate Cd<sup>II</sup> ion is coordinated by two N atoms from the imidazole ligands and five O atoms from three different carboxylate groups (Table 1). The local coordination around the Cd<sup>II</sup> ion can best be described as distorted monocapped octahedral with a CdN<sub>2</sub>O<sub>5</sub> chromophore. Its equatorial plane is defined by atoms O1, O2, N1 and O6<sup>i</sup> [symmetry code: (i)  $x + 1, y + 1, z$ ] [r.m.s. deviation 0.12 Å; deviation of Cd1 from the mean plane 0.47 (4) Å]. Atoms N3 and O6<sup>ii</sup> occupy the axial sites, with an N3–Cd1–O6<sup>ii</sup> angle of 162.59 (7)° [symmetry code: (ii)  $-x, -y, 1 - z$ ]. The capping atom O5<sup>i</sup> lies 2.342 (3) Å out of the plane of atoms N1, N3 and O6<sup>i</sup>. The Cd–O5<sup>i</sup> and Cd–O6<sup>ii</sup> distances (Table 1) are considerably longer than the other Cd–O bonds but lie within the range of the corresponding bond distances reported for related Cd<sup>II</sup> carboxylate coordination polymers [2.639 (2) and 2.879 (2) Å; Clegg *et al.*, 1995]. The imidazole molecules serve as typical monodentate ligands coordinated to the metal centre. The dihedral angle between the two imidazole molecules is 72.04 (8)°.

The Cd–O<sub>carboxyl</sub> distances in (I) range from 2.251 (2) to 2.771 (2) Å, whereas in the related polymer,  $[\text{Cd}(\text{1,4-BDOA})(\text{C}_3\text{H}_4\text{N}_2)_3]_n$ , (II) (Gao, Liu, Huo, Zhao & Zhao, 2004*c*), the Cd–O<sub>carboxyl</sub> distances range from 2.347 (2) to 2.481 (2) Å. In (II), the Cd<sup>II</sup> atom is coordinated by three carboxyl O atoms from two different 1,4-BDOA<sup>2-</sup> groups and three N atoms from three imidazole molecules, displaying an octahedral configuration, and the 1,4-BDOA<sup>2-</sup> dianion behaves as a bridging ligand with both a monodentate and a bidentate chelating mode, to form a one-dimensional chain polymer.

In (I), the two C–O bond distances of one of the carboxyl groups (C10/O5/O6) are significantly different, while those of the other carboxyl group (C1/O1/O2) are essentially the same. This may be attributed to the influence of the different coordination modes of the carboxyl groups. In the former, the carboxyl group is in a tridentate bridging mode through atoms O5 and O6<sub>bridge</sub> between two metal ions. In the latter, the carboxyl group is in a bidentate chelating mode through atoms O1 and O2. One of the oxyacetate groups and the aromatic ring are nearly coplanar, with a C7–O4–C9–C10 torsion angle of –176.3 (2)°, while the other oxyacetate group is twisted out the aromatic ring plane, with a C3–O3–C2–C1 torsion angle of 72.9 (4)°. The dihedral angles between the aromatic ring and imidazole molecules are 52.55 (8) and 57.99 (7)°. In contrast, in (II), both oxyacetate groups and the aromatic ring are almost coplanar, with torsion angles of

–174.2 (3)° (C11–O3–C12–C19) and 178.7 (2)° (C17–O6–C16–C15).

Each 1,3-BDOA<sup>2-</sup> dianion links two Cd<sup>II</sup> atoms in a bis-bidentate mode, giving rise to a one-dimensional chain running along a diagonal of the *ab* plane. The intrachain Cd···Cd separation is 13.105 (2) Å, which is somewhat shorter than that in (II) of 15.009 (2) Å. Neighbouring chains share carboxyl atoms O6 and O6<sup>ii</sup> to generate a four-membered ring with a centrosymmetric Cd<sub>2</sub>O<sub>2</sub> core, in which the Cd···Cd separation is 4.014 (3) Å. The three four-membered rings with Cd–O bonds as shared edges have an overall chair shape (Fig. 2).

Imidazole atoms N2 and N4 do not participate in coordination to the metal atom, owing to their weak coordination ability, but engage in intermolecular hydrogen bonds with carboxyl O atoms (Table 2), consolidating the crystal structure and leading to a three-dimensional supramolecular architecture.

## Experimental

Benzene-1,3-dioxyacetic acid was prepared following by the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). Compound (I) was synthesized by the addition of cadmium dinitrate tetrahydrate (6.16 g, 20 mmol) and imidazole (1.90 g, 20 mmol) to a hot aqueous solution of 1,3-BDOAH<sub>2</sub> (4.52 g, 20 mmol), and the pH was adjusted to 6 with 0.2 M NaOH. The solution was allowed to evaporate at room temperature, and colourless prismatic crystals of (I) were obtained after several days. CHN analysis, calculated for C<sub>16</sub>H<sub>16</sub>N<sub>4</sub>O<sub>6</sub>Cd: C 40.65, H 3.41, N 11.85%; found: C 40.71, H 3.36, N 11.80%.

### Crystal data

$[\text{Cd}(\text{C}_{10}\text{H}_8\text{O}_6)(\text{C}_3\text{H}_4\text{N}_2)_2]$   
 $M_r = 472.74$   
 Triclinic,  $P\bar{1}$   
 $a = 9.4084$  (19) Å  
 $b = 10.062$  (2) Å  
 $c = 11.130$  (2) Å  
 $\alpha = 108.46$  (3)°  
 $\beta = 111.04$  (3)°  
 $\gamma = 95.46$  (3)°  
 $V = 906.5$  (5) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.732$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 6222 reflections  
 $\theta = 3.6$ – $27.4$ °  
 $\mu = 1.25$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, colourless  
 $0.38 \times 0.24 \times 0.17$  mm

### Data collection

Rigaku R-AXIS RAPID diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.649$ ,  $T_{\max} = 0.816$   
 8787 measured reflections

4122 independent reflections  
 3923 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$   
 $\theta_{\max} = 27.5$ °  
 $h = -10 \rightarrow 12$   
 $k = -12 \rightarrow 13$   
 $l = -14 \rightarrow 14$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.071$   
 $S = 1.08$   
 4122 reflections  
 244 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.4978P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.79$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.59$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cd1—N1	2.239 (2)	Cd1—O6 <sup>ii</sup>	2.636 (2)
Cd1—N3	2.299 (2)	C1—O1	1.248 (3)
Cd1—O1	2.476 (2)	C1—O2	1.249 (3)
Cd1—O2	2.367 (2)	C10—O5	1.232 (3)
Cd1—O5 <sup>i</sup>	2.771 (2)	C10—O6	1.261 (3)
Cd1—O6 <sup>i</sup>	2.251 (2)		
N1—Cd1—N3	94.28 (8)	O1—Cd1—O6 <sup>ii</sup>	79.79 (6)
N1—Cd1—O1	100.19 (8)	O2—Cd1—O1	53.89 (6)
N1—Cd1—O2	151.85 (8)	O2—Cd1—O5 <sup>i</sup>	108.80 (7)
N1—Cd1—O5 <sup>i</sup>	99.27 (8)	O2—Cd1—O6 <sup>ii</sup>	81.51 (7)
N1—Cd1—O6 <sup>i</sup>	104.64 (8)	O5 <sup>i</sup> —Cd1—O6 <sup>ii</sup>	119.04 (7)
N1—Cd1—O6 <sup>ii</sup>	83.11 (7)	O6 <sup>i</sup> —Cd1—N3	127.24 (7)
N3—Cd1—O1	83.76 (7)	O6 <sup>i</sup> —Cd1—O1	137.56 (6)
N3—Cd1—O2	93.42 (8)	O6 <sup>i</sup> —Cd1—O2	91.95 (7)
N3—Cd1—O5 <sup>i</sup>	78.37 (7)	O6 <sup>i</sup> —Cd1—O5 <sup>i</sup>	50.48 (6)
N3—Cd1—O6 <sup>ii</sup>	162.59 (7)	O6 <sup>i</sup> —Cd1—O6 <sup>ii</sup>	69.81 (7)
O1—Cd1—O5 <sup>i</sup>	154.42 (6)		

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

**Table 2**

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H17...O1 <sup>iv</sup>	0.86	1.96	2.786 (3)	160
N4—H18...O4 <sup>v</sup>	0.86	2.57	3.148 (3)	125
N4—H18...O5 <sup>v</sup>	0.86	2.02	2.792 (3)	149

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

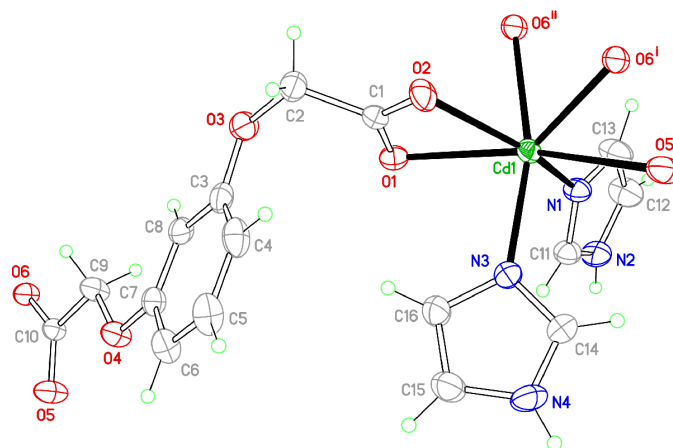
All H atoms were placed in calculated positions, with C—H = 0.93 Å (aromatic) or 0.97 Å (aliphatic) and N—H = 0.86 Å (imidazole), and were refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ .

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); *SHELXL97*.

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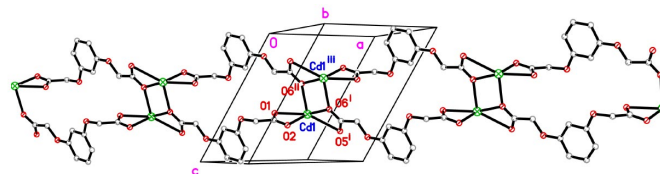
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**Figure 1**

A view of the asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes as in Table 1.]



**Figure 2**

The double-chain structure of (I), with the imidazole ligands and H atoms omitted for clarity. [Symmetry codes as in Table 1; (iii)  $1-x, 1-y, 1-z$ .]

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