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## Key indicators

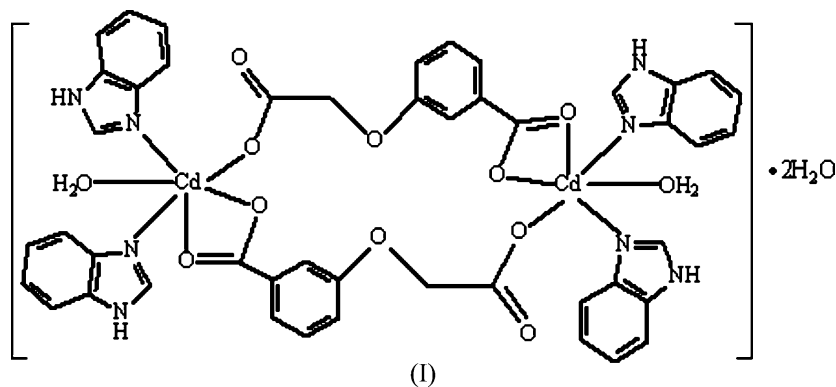
Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
H-atom completeness 91%  
 $R$  factor = 0.046  
 $wR$  factor = 0.105  
Data-to-parameter ratio = 16.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis( $\mu$ -3-carboxylatophenoxyacetato)bis-  
[aquabis(1*H*-benzimidazole)cadmium(II)]  
dihydrate

In the title complex,  $[\text{Cd}_2(\text{C}_9\text{H}_6\text{O}_5)_2(\text{C}_7\text{H}_6\text{N}_2)_4(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ , the  $\text{Cd}^{\text{II}}$  atoms are linked by two 3-carboxyphenoxyacetate groups into a centrosymmetric dimer. Each  $\text{Cd}^{\text{II}}$  atom displays a distorted octahedral coordination geometry, with three carboxylate O atoms from different 3-carboxyphenoxyacetate groups, two N atoms from two benzimidazole co-ligands and one water molecule. Intermolecular hydrogen bonding leads to a two-dimensional supramolecular network.

Received 10 October 2005  
Accepted 9 November 2005  
Online 26 November 2005

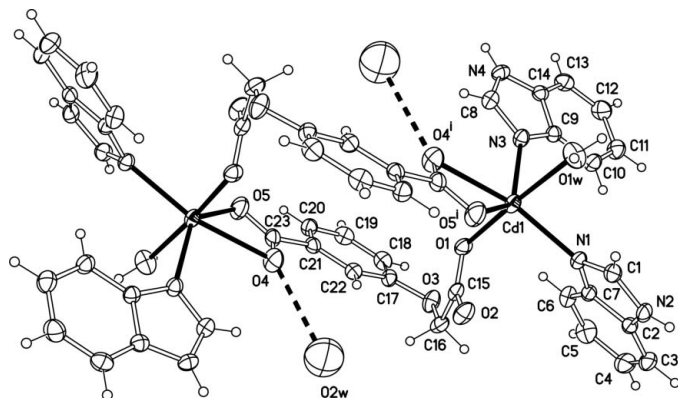
## Comment

3-Carboxyphenoxyacetic acid (3-CPOAH<sub>2</sub>), which is an excellent bridging ligand with both rigid and flexible parts, is used to form coordination polymers. Recently, we have reported the structure of a one-dimensional  $\text{Cd}^{\text{II}}$  coordination polymer  $[\text{Cd}(3\text{-CPOA})(\text{imidazole})(\text{H}_2\text{O})_2] \cdot 3\text{H}_2\text{O}$  (Gao *et al.*, 2005), in which the  $\text{Cd}^{\text{II}}$  atom has a pentagonal bipyramidal geometry and the 3-CPOA<sup>2-</sup> ligand is in the tetradentate coordination mode. Here, we have extended our research to ternary mixed-ligand metal complexes with 3-CPOA<sup>2-</sup> as bridging ligands and heteroaromatic *N*-donor benzimidazole as co-ligands, and generated a new dinuclear  $\text{Cd}^{\text{II}}$  complex,  $[\text{Cd}_2(3\text{-CPOA})_2(1H\text{-benzimidazole})_4(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ , (I).



As illustrated in Fig. 1, the structure of (I) consists of a centrosymmetric neutral dinuclear  $\text{Cd}^{\text{II}}$  complex and two uncoordinated water molecules. Each  $\text{Cd}^{\text{II}}$  atom displays a distorted octahedral coordination defined by three carboxylate O atoms from different 3-CPOA<sup>2-</sup> groups, two N atoms from two benzimidazole co-ligands and one water molecule.

As a consequence of two 3-CPOA<sup>2-</sup> bridges, two  $\text{Cd}^{\text{II}}$  atoms are linked into a dinuclear unit, with a  $\text{Cd} \cdots \text{Cd}$  separation of 8.506 (3) Å. These dinuclear units are further connected through hydrogen bonding involving uncoordinated benzimidazole N atoms, water molecules and carbox-



**Figure 1**  
ORTEP plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines. The symmetry code is as in Table 1.

ylate O atoms, resulting in the formation a two-dimensional supramolecular network (Table 2 and Fig. 2).

## Experimental

The title complex was prepared by the addition of a stoichiometric amount of cadmium dinitrate tetrahydrate (3.08 g, 10 mmol) and benzimidazole (2.34 g, 20 mmol) to an aqueous solution of 3-CPOAH<sub>2</sub> (1.96 g, 10 mmol); the pH was adjusted to 7 with 0.1 M NaOH. The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb and held at 423 K for 4 d. The bomb was cooled naturally to room temperature and colorless prismatic crystals were obtained over several days. Analysis calculated for C<sub>46</sub>H<sub>44</sub>Cd<sub>2</sub>N<sub>8</sub>O<sub>14</sub>: C 47.72, H 3.83, N 9.68%; found: C 47.78, H 3.79, N 9.71%.

### Crystal data

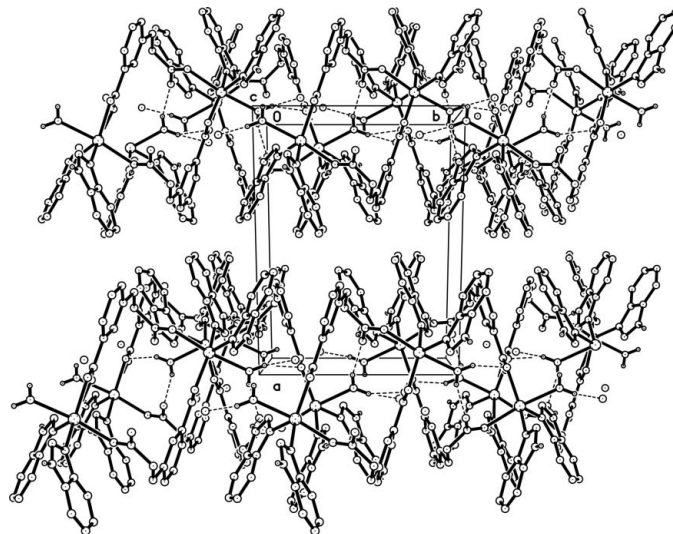
[Cd <sub>2</sub> (C <sub>9</sub> H <sub>6</sub> O <sub>5</sub> ) <sub>2</sub> (C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ) <sub>4</sub> ·(H <sub>2</sub> O) <sub>2</sub> ·2H <sub>2</sub> O]	$D_x = 1.626 \text{ Mg m}^{-3}$
$M_r = 1157.69$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 18370 reflections
$a = 15.744 (3) \text{ \AA}$	$\theta = 3.0\text{--}27.4^\circ$
$b = 10.956 (2) \text{ \AA}$	$\mu = 0.98 \text{ mm}^{-1}$
$c = 15.094 (3) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 114.74 (3)^\circ$	Prism, colorless
$V = 2364.6 (10) \text{ \AA}^3$	$0.32 \times 0.27 \times 0.18 \text{ mm}$
$Z = 2$	

### Data collection

Rigaku R-Axis RAPID diffractometer	5290 independent reflections
$\omega$ scans	4113 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.056$
$T_{\text{min}} = 0.745$ , $T_{\text{max}} = 0.844$	$\theta_{\text{max}} = 27.5^\circ$
22000 measured reflections	$h = -20 \rightarrow 20$
	$k = -14 \rightarrow 14$
	$l = -19 \rightarrow 18$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 1.9238P]$
$R[F^2 > 2\sigma(F^2)] = 0.046$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.75 \text{ e \AA}^{-3}$
5290 reflections	$\Delta\rho_{\text{min}} = -0.70 \text{ e \AA}^{-3}$
322 parameters	
H atoms treated by a mixture of independent and constrained refinement	



**Figure 2**  
A packing diagram of the title complex. Hydrogen bonds are shown as dashed lines and C-bound H atoms have been omitted for clarity.

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cd1—N1	2.304 (3)	Cd1—O1W	2.418 (3)
Cd1—N3	2.260 (3)	O1—C15	1.260 (5)
Cd1—O1	2.362 (3)	O2—C15	1.241 (4)
Cd1—O4 <sup>i</sup>	2.498 (3)	O4—C23	1.230 (6)
Cd1—O5 <sup>i</sup>	2.318 (3)	O5—C23	1.274 (5)
N1—Cd1—O1	90.87 (10)	N3—Cd1—O1W	83.68 (13)
N1—Cd1—O4 <sup>i</sup>	163.36 (11)	O1—Cd1—O4 <sup>i</sup>	88.91 (11)
N1—Cd1—O5 <sup>i</sup>	110.49 (12)	O1—Cd1—O1W	173.23 (11)
N1—Cd1—O1W	85.49 (13)	O5 <sup>i</sup> —Cd1—O1	108.20 (11)
N3—Cd1—N1	110.53 (11)	O5 <sup>i</sup> —Cd1—O4 <sup>i</sup>	54.11 (12)
N3—Cd1—O1	92.30 (11)	O5 <sup>i</sup> —Cd1—O1W	78.45 (13)
N3—Cd1—O4 <sup>i</sup>	86.10 (11)	O1W—Cd1—O4 <sup>i</sup>	96.21 (13)
N3—Cd1—O5 <sup>i</sup>	133.41 (12)		

Symmetry code: (i)  $-x, -y + 1, -z + 1$ .

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
N2—H24 $\cdots$ O1 <sup>ii</sup>	0.86	1.97	2.831 (4)	176
N4—H25 $\cdots$ O2 <sup>iii</sup>	0.86	2.04	2.861 (4)	160
O1W—H1W2 $\cdots$ O2 <sup>iv</sup>	0.85 (4)	1.96 (3)	2.748 (5)	155 (6)
O1W—H1W1 $\cdots$ O5 <sup>ii</sup>	0.85 (3)	2.29 (4)	2.999 (5)	141 (4)
O1W—H1W1 $\cdots$ O2W <sup>v</sup>	0.85 (3)	2.18 (4)	2.869 (10)	138 (6)

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

H atoms on C and N atoms were placed in calculated positions, with C—H = 0.93 or 0.97  $\text{\AA}$ , N—H = 0.86  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ , and were refined in the riding-model approximation. The H atoms of the O1W water molecule were located in a difference Fourier map and refined with O—H distance restraints of 0.85 (1)  $\text{\AA}$  and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ ; the H atoms of the O2W water molecule were not located. Hydrogen-bond interactions are expected to exist between water O2W and carboxylate O4 atoms, with an  $\text{O}\cdots\text{O}$

distance of 2.98 Å, and between water O2W and carboxylate O5 at  $(x, -y + \frac{3}{2}, z + \frac{1}{2})$ , with an O...O distance of 2.68 Å.

Data collection: *RAPID-AUTO* (Rigaku, 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*.

The authors thank the National Natural Science Foundation of China (No. 20101003), the Scientific Fund of Remarkable

Teachers of Heilongjiang Province (No. 1054 G036), and Heilongjiang University for supporting this study.

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