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Key indicators

Single-crystal X-ray study
T = 295 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
Disorder in solvent or counterion
R factor = 0.024
wR factor = 0.063
Data-to-parameter ratio = 16.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[[diaqua(imidazole)cadmium(II)]-
 μ -3-carboxylatophenoxyacetato] trihydrate]**

In the title compound, $[\text{Cd}(\text{C}_9\text{H}_6\text{O}_5)(\text{C}_3\text{H}_4\text{N}_2)(\text{H}_2\text{O})_2] \cdot 3\text{H}_2\text{O}$, the carboxylatophenoxyacetate dianion links the water- and imidazole-coordinated Cd atoms into a zigzag chain that runs along the *c* axis of the monoclinic unit cell; the chelation by the carboxylate arms leads to a seven-coordinate pentagonal-bipyramidal geometry for the Cd atom. The chains are linked into a three-dimensional network by hydrogen bonds.

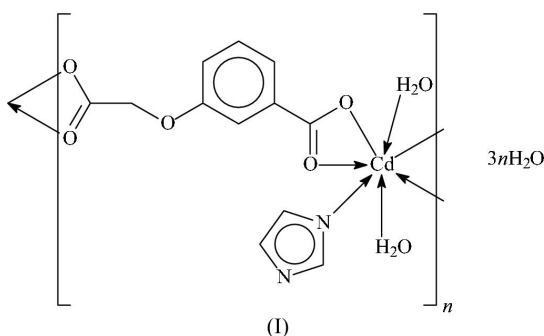
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Comment

Structural reports on metal derivatives of 3-carboxyphenoxyacetic acid (Gao, Li *et al.*, 2004; Li *et al.*, 2004) comprise one part of the studies on metal complexes of the 2-, 3- and 4-carboxyphenoxyacetic acids. An earlier attempt to synthesize the benzimidazole adduct of cadmium 3-carboxyphenoxyacetate by reacting the cadmium carboxylate, prepared *in situ*, yielded only benzimidazolium hydrogen bis(3-carboxyphenoxyacetate) (Gao, Huo *et al.*, 2004). In other attempts to synthesize adducts with nitrogen-containing heterocycles, the metal complexes that are isolated have the 3-carboxyphenoxyacetate dianion uncoordinated to the metal atom (Zhao, Gu, Gao *et al.*, 2005; Zhao, Gu, Huo *et al.*, 2005). Possibly, the isolation of the present cadmium–imidazole adduct, (I), should be attributed to the particularly small size of the nitrogen-containing heterocycle, as well as the participation of the heterocycle in hydrogen-bonding interactions. The dianion chelates to two adjacent Cd atoms through its carboxylate arms; the four O atoms along with a water molecule constitute a pentagonal plane. The heterocycle and another water molecule occupy the apical sites (Fig. 1). The manner of bridging by the dianion leads to a helical chain that runs along the *c* axis (Fig. 2); the chains are linked into a three-dimensional network by hydrogen bonds (Table 2).



Experimental

Cadmium dinitrate tetrahydrate (0.31 g, 1 mmol) was added to an aqueous solution of 3-carboxyphenoxyacetic acid (0.19 g, 1 mmol). The pH was adjusted to 7 with 0.1 M sodium hydroxide. Imidazole

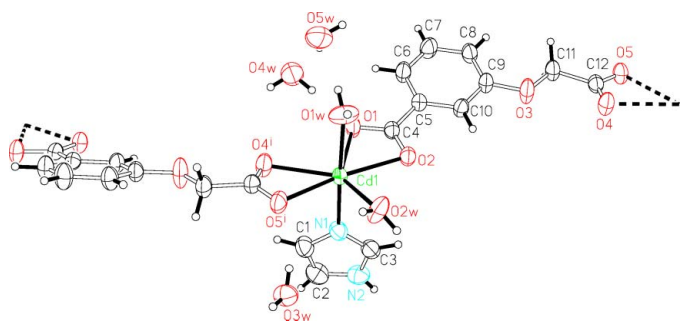


Figure 1
ORTEP (Johnson, 1976) plot of a portion of the chain of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. The minor component of the disordered water molecule O5w is not shown. [Symmetry code: (i) $x - \frac{1}{2}, \frac{3}{2} - y, \frac{1}{2} + z$.]

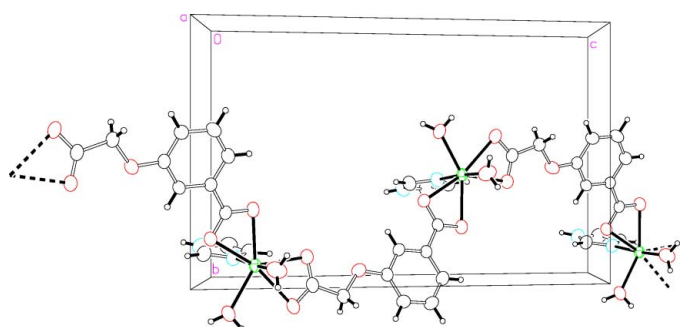


Figure 2
ORTEP (Johnson, 1976) plot of the polymeric chain structure. The uncoordinated water molecules are not shown.

(0.14 g, 2 mmol) was then added. Colorless crystals separated from the clear solution after several days. Analysis calculated for $C_{12}H_{20}CdN_2O_{10}$: C 31.02, H 4.34, N 6.03%; found: C 31.19, H 4.30, N 6.06%.

Crystal data

$[Cd(C_9H_6O_5)(C_3H_4N_2)(H_2O)_2] \cdot 3H_2O$
 $M_r = 464.70$
 Monoclinic, $P2_1/n$
 $a = 8.574(2) \text{ \AA}$
 $b = 11.467(2) \text{ \AA}$
 $c = 18.374(3) \text{ \AA}$
 $\beta = 101.88(3)^\circ$
 $V = 1767.9(6) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.746 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 15434 reflections
 $\theta = 3.0\text{--}27.5^\circ$
 $\mu = 1.29 \text{ mm}^{-1}$
 $T = 295(2) \text{ K}$
 Block, colorless
 $0.36 \times 0.25 \times 0.18 \text{ mm}$

Data collection

Rigaku R-Axis RAPID IP diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{min} = 0.478, T_{max} = 0.801$
 16669 measured reflections
 3995 independent reflections
 3607 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.018$
 $\theta_{max} = 27.5^\circ$
 $h = -11 \rightarrow 9$
 $k = -14 \rightarrow 14$
 $l = -23 \rightarrow 23$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.063$
 $S = 1.06$
 3995 reflections
 237 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 0.5011P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.67 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.31 \text{ e \AA}^{-3}$

Table 1
Selected geometric parameters ($\text{\AA}, ^\circ$).

Cd1—O1	2.418 (2)	Cd1—O1w	2.270 (2)
Cd1—O2	2.398 (1)	Cd1—O2w	2.350 (2)
Cd1—O4 ⁱ	2.424 (2)	Cd1—N1	2.244 (2)
Cd1—O5 ⁱ	2.484 (2)		
O1—Cd1—O2	53.98 (5)	O4 ⁱ —Cd1—O5 ⁱ	53.00 (5)
O1—Cd1—O4 ⁱ	89.16 (5)	O4 ⁱ —Cd1—O1w	90.63 (8)
O1—Cd1—O5 ⁱ	140.81 (5)	O4 ⁱ —Cd1—O2w	130.29 (6)
O1—Cd1—O1w	81.97 (6)	O4 ⁱ —Cd1—N1	90.60 (7)
O1—Cd1—O2w	138.24 (6)	O5 ⁱ —Cd1—O1w	88.01 (7)
O1—Cd1—N1	93.80 (6)	O5 ⁱ —Cd1—O2w	77.38 (6)
O2—Cd1—O4 ⁱ	143.11 (5)	O5 ⁱ —Cd1—N1	96.11 (6)
O2—Cd1—O5 ⁱ	162.83 (5)	O1w—Cd1—O2w	84.25 (7)
O2—Cd1—O1w	86.15 (7)	O1w—Cd1—N1	175.58 (7)
O2—Cd1—O2w	85.97 (6)	O2w—Cd1—N1	98.17 (7)
O2—Cd1—N1	90.32 (6)		

Symmetry code: (i) $x - \frac{1}{2}, \frac{3}{2} - y, \frac{1}{2} + z$.

Table 2
Hydrogen-bonding geometry ($\text{\AA}, ^\circ$).

D—H...A	D—H	H...A	D...A	D—H...A
O1w—H1w1...O5w	0.82	1.94	2.760 (3)	171
O1w—H1w2...O4w ⁱⁱ	0.81	1.85	2.662 (3)	176
O2w—H2w1...O5w ⁱⁱ	0.82	2.03	2.828 (3)	163
O2w—H2w2...O2w ⁱⁱⁱ	0.83	1.88	2.703 (2)	171
O3w—H3w1...O4 ⁱⁱⁱ	0.82	2.02	2.809 (2)	161
O3w—H3w2...O5 ⁱ	0.83	2.03	2.839 (2)	163
O4w—H4w2...O3w ^{iv}	0.83	1.96	2.775 (3)	172
O4w—H4w1...O1	0.83	1.84	2.663 (3)	172
O5w—H5w1...O4w	0.83	1.97	2.729 (5)	152
O5w—H5w2...O5 ^v	0.82	2.16	2.784 (3)	133
O5w ^v —H5w3...O5 ^v	0.83	2.30	2.799 (8)	119
N2—H2n...O3w ^{vi}	0.86	1.97	2.823 (3)	170

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

The carbon-bound H atoms were positioned geometrically (C—H = 0.93 \AA for the aromatic H atoms and 0.97 \AA for the others) and were included in the refinement with $U_{iso}(H)$ values set at $1.2U_{eq}(C)$ in the riding-model approximation. The amino H atom of the nitrogen-containing heterocycle was similarly treated [$N-H = 0.86 \text{ \AA}$ and $U_{iso}(H) = 1.2U_{eq}(N)$]. One of the uncoordinated water molecules, O5w, is disordered over two positions; the occupancies refined to 0.747 (7):0.253 (7). The H atoms of the water molecules, including the disorder components, were placed at chemically sensible positions on the basis of O—H distances of approximately 0.82 \AA and hydrogen bonds of approximately 2 \AA . These were not refined; their displacement parameters were also set to 1.2 times U_{eq} of the O atoms. Positioning the H atoms in this way leads to a satisfactory scheme of hydrogen bonds and all H...H contacts exceed 2 \AA . For example, atom H5w1 is 2.01 \AA from H4w1 and the minor O5w^v component forms only one hydrogen bond whereas the major O5w component forms two.

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

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