

A two-dimensional cadmium(II) coordination polymer: poly[*diaquabis*(μ_2 -2,4-dichlorophenoxyacetato)cadmium(II)]Wen-Dong Song,^{a*} Chang-Sheng Gu,^a Ji-Wei Liu^b and Xiao-Min Hao^a^aDepartment of Applied Chemistry, Guangdong University of Ocean, Zhanjiang 524006, People's Republic of China, and ^bCollege of Chemistry and Chemical Technology, Daqing Petroleum Institute, Daqing 163318, People's Republic of ChinaCorrespondence e-mail:
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Key indicators

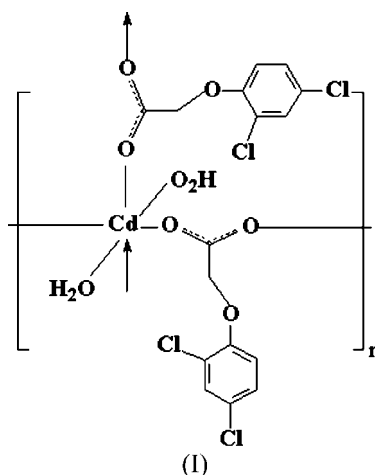
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(C-C) = 0.004$ Å
 R factor = 0.026
 wR factor = 0.067
Data-to-parameter ratio = 17.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title coordination polymer, $[Cd(C_8H_5Cl_2O_3)_2(H_2O)_2]_n$, each Cd^{II} atom lies on an inversion center. The Cd^{II} atom exists in a slightly distorted octahedral coordination polyhedron, involving four carboxyl O atoms from different 2,4-dichlorophenoxyacetate ligands and two water molecules. The Cd^{II} ions are bridged by carboxylate groups in a bis(monodentate) mode, leading to a two-dimensional layer structure. This supramolecular network is consolidated by intermolecular hydrogen-bonding interactions.

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Comment

2,4-Dichlorophenoxyacetic acid is one of the important biologically active compounds that have been commonly used in herbicides and plant growth substances (Lv *et al.*, 1998). The mono-phenoxyacetate group can be used as a terminal ligand or a bridging ligand with different coordination numbers and with various metal ions (Liang *et al.*, 2002). In addition to its versatile coordination modes, 2,4-dichlorophenoxyacetic acid may take part in hydrogen-bonding interactions by functioning as either hydrogen-bond donor or acceptor. The work described here is an investigation into the synthesis and structural characterization of a two-dimensional layer Cd^{II} coordination polymer, (I). A completely isomorphous and isostructural compound has been reported by Kruszynski & Turek (2004). The only difference is that one of the Cl atoms of the phenoxy ligand is exchanged for a CH_3 group.



As illustrated in Fig. 1, the Cd^{II} atom is located on an inversion center and displays a slightly distorted octahedral coordination polyhedron. Each Cd^{II} atom is six-coordinated by four carboxyl O atoms from four different symmetry-related 2,4-dichlorophenoxyacetate ligands [$Cd-O$ mean =

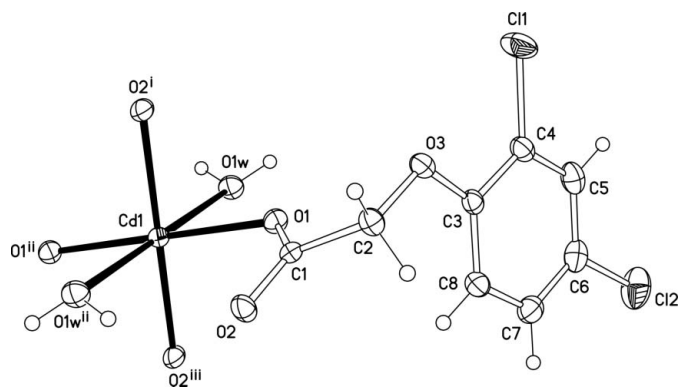


Figure 1
Part of the structure of (I), with displacement ellipsoids shown at the 30% probability level.

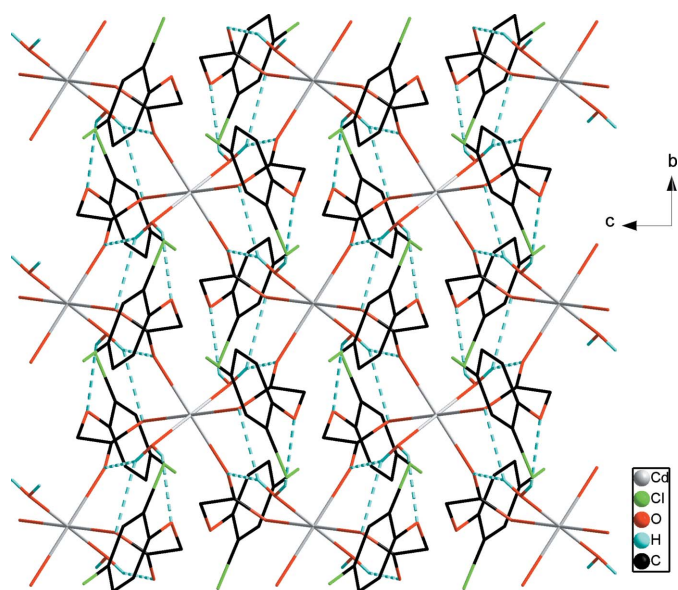


Figure 2
The two-dimensional layer structure of (I), viewed down *a*. H atoms not involved in hydrogen bonding have been omitted. Hydrogen bonds are indicated by dashed lines.

2.274 (2) Å] and two water molecules. The oxyacetate group is twisted out of the benzene ring plane in (I), the C3–O3–C2–C1 torsion angle being $-82.0(2)^\circ$. The C–O bond lengths of the carboxyl group confirm the deprotonated nature of this group and the delocalization of the double bond (Table 1).

Each 2,4-dichlorophenoxyacetate group adopts a bis(monodentate) bridging mode, linking two adjacent Cd^{II} atoms into a one-dimensional infinite chain. In the chain, the adjacent Cd···Cd distance is 5.431 (2) Å. Adjacent chains are parallel to each other, and are further connected by other 2,4-dichlorophenoxyacetate groups, resulting in the formation of a two-dimensional layer structure (Fig. 2).

In the packing arrangement of (I), the two-dimensional supramolecular framework is further stabilized by intermolecular hydrogen bonds involving the uncoordinated ether O3 atom, the coordinated carboxylate O atoms and the water molecule (Table 2).

Experimental

2,4-Dichlorophenoxyacetic acid was synthesized according to the literature (Wu *et al.*, 1996). Cadmium dinitrate tetrahydrate (6.16 g, 20 mmol) and 2,4-dichlorophenoxyacetic acid (4.42 g, 20 mmol) were dissolved in a 1:2 ethanol/water mixture. The pH of the solution was adjusted to 7 with 0.1 M sodium hydroxide. The reaction mixture was stirred for 30 min at room temperature and then filtered. The solution was left to stand at room temperature and colorless crystals formed after a few days. Analysis. Calculated for C₁₆H₁₄CdCl₄O₈: C 32.65, H 2.40%; found: C 32.69, H 2.39%.

Crystal data

[Cd(C₈H₅Cl₂O₃)₂(H₂O)₂]
M_r = 588.47
 Monoclinic, *P*2₁/*c*
a = 17.732 (4) Å
b = 7.2796 (15) Å
c = 8.0624 (16) Å
 β = 95.20 (3)°
V = 1036.4 (4) Å³

Z = 2
D_x = 1.886 Mg m⁻³
 Mo *K*α radiation
 μ = 1.61 mm⁻¹
T = 295 (2) K
 Prism, colorless
 0.36 × 0.25 × 0.18 mm

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
T_{min} = 0.620, *T_{max}* = 0.750

9832 measured reflections
 2373 independent reflections
 2069 reflections with *I* > 2σ(*I*)
R_{int} = 0.024
 θ_{\max} = 27.5°

Refinement

Refinement on *F*²
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.067$
S = 1.07
 2373 reflections
 139 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 0.6209P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.64 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.48 \text{ e } \text{Å}^{-3}$

H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected geometric parameters (Å, °).

Cd1–O1	2.2703 (17)	O1–C1	1.249 (2)
Cd1–O2 ⁱ	2.2784 (16)	O2–C1	1.253 (3)
Cd1–O1W	2.3325 (18)		
O1–Cd1–O2 ⁱⁱ	102.57 (6)	O1–Cd1–O1W	84.05 (6)
O1–Cd1–O2 ⁱ	77.43 (6)	O1W–Cd1–O2 ⁱ	90.10 (7)
O1–Cd1–O1W ⁱⁱⁱ	95.95 (6)	O1W–Cd1–O2 ⁱⁱ	89.90 (7)

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

Table 2

Hydrogen-bond 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>
O1W–H1W1···O1 ^{iv}	0.839 (10)	2.41 (2)	3.105 (2)	141 (2)
O1W–H1W1···O2 ⁱⁱⁱ	0.839 (10)	2.165 (18)	2.845 (3)	138 (2)
O1W–H1W2···O3 ^{iv}	0.837 (10)	2.37 (2)	3.035 (2)	137 (2)

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

H atoms attached to C atoms were placed in calculated positions, with C–H = 0.93 (aromatic) or 0.97 Å (methylene) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of the water molecule were located in a difference Fourier map and refined with an O–H distance restraint of 0.85 (1) Å, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

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*.

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