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Key indicators

Single-crystal X-ray study T = 273 K Mean σ (C–C) = 0.005 Å R factor = 0.052 wR factor = 0.159 Data-to-parameter ratio = 15.8

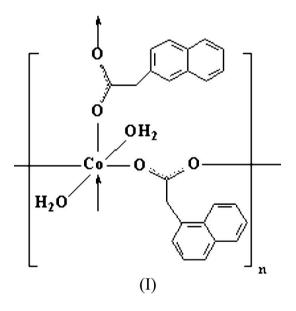
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

A two-dimensional grid-like cobalt^{II} coordination polymer: poly[[diaquacobalt(II)]-di- μ_2 -naphthalene-1-acetato]

In the title compound, $[Co(C_{12}H_9O_2)_2(H_2O)_2]_n$, the Co^{II} atom lies on an inversion centre and has a slightly distorted octahedral coordination environment involving four carboxylate and two water O atoms. In the crystal structure, each naphthaleneacetate ligand coordinates two metal centres through its carboxylate O atoms, adopting a bis-monodentate mode to give rise to a two-dimensional network. A threedimensional supramolecular network is consolidated by intermolecular O-H···O hydrogen bonds.

Comment

As an interesting field of crystal engineering and materials chemistry, coordination polymers have been rapidly developed in recent years (Żurowska *et al.*, 2006; Ye *et al.*, 2006). In an effort to establish strategies aimed at designing novel metal–organic frameworks, we have chosen some carboxylate ligands, such as 2,4-dichlorophenoxyacetate (Gu *et al.*, 2006), phenylenedioxydiacetate (Gao *et al.*, 2005) and carboxylphenoxyacetate (Huo *et al.*, 2005), to bind metal centres into novel metal–organic networks. We report here the synthesis and crystal structure of the title coordination polymer, (I).



As illustrated in Fig. 1, the Co^{II} atom of (I) occupies a special position on an inversion centre, and has a slightly distorted octahedral coordination environment. The Co^{II} atom is coordinated by six O atoms, four from three different naphthaleneacetate ligands [average Co–O distance = 2.096 (2) Å] and two from two water molecules [Co–OW = 2.126 (2) Å]. The carboxylate groups of the anionic ligands are

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metal-organic papers

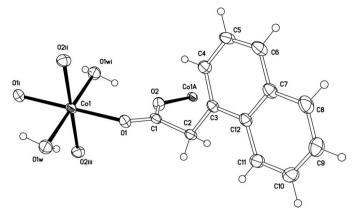


Figure 1

The asymmetric unit of (I), together with additional atoms to complete the coordination of Co1 and the carboxylate bridge, with the atomnumbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $-x + \frac{1}{2}$, $-y + \frac{3}{2}$, -z; (ii) x, -y + 1, $z = \frac{1}{2}$; (iii) $-x + \frac{1}{2}$, $y + \frac{1}{2}$, $-z + \frac{1}{2}$; (A) $-x + \frac{1}{2}$, $y = \frac{1}{2}$, $-z + \frac{1}{2}$].

all electron-delocalized, as evidenced by the characteristic C-O bond lengths (Table 1).

Each naphthaleneacetate group displays a bis-monodentate bridging mode, connecting two adjacent Co^{II} atoms. As a result, a polynuclear one-dimensional cobalt chain is formed. running along the diagonal of the bc plane, in which the adjacent Co \cdots Co distance is 5.358 (2) Å. Adjacent chains are parallel to each other and are further connected by other naphthaleneacetate groups, resulting in the formation of a two-dimensional grid-like lamellar framework (Fig. 2).

Intermolecular $O-H \cdots O$ hydrogen bonds (Table 2) link the sheets of (I) into a three-dimensional supramolecular framework, and may be effective in the stabilization of the crystal structure.

Experimental

Cobalt(II) diacetate trihydrate (4.76 g, 20 mmol) and naphthaleneacetic acid (3.72 g, 20 mmol) were dissolved in a 1:1 ethanol-water mixture (100 ml), and the pH was adjusted to 7 with 0.1 M sodium hydroxide. The resulting solution was stirred for 20 min at room temperature and then filtered. Pink single crystals of (I) were isolated from the solution at room temperature over several days.

Crystal data [Co(C12H9O2)2(H2O)2] Z = 4 $D_r = 1.566 \text{ Mg m}^{-3}$ $M_{r} = 465.35$ Mo $K\alpha$ radiation Monoclinic, C2/c a = 36.954 (5) Å $\mu = 0.91 \text{ mm}^{-1}$ b = 6.1913 (10) Å T = 273 (2) K c = 8.7464 (13) ÅBlock, pink $0.31 \times 0.26 \times 0.18 \text{ mm}$ $\beta = 99.524 \ (9)^{\circ}$ V = 1973.5 (5) Å³ Data collection

6297 measured reflections

 $R_{\rm int} = 0.043$

 $\theta_{\rm max} = 27.5^{\circ}$

2238 independent reflections

1628 reflections with $I > 2\sigma(I)$

Bruker SMART diffractometer ω scans Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{\rm min}=0.765,\ T_{\rm max}=0.853$

Table 2 Hydrogen-bond geometry (Å, °). $D - H \cdot \cdot \cdot A$ $O1W - H1W1 \cdots O2^{ii}$ $O1W-H1W2\cdots O2^{i}$

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

D-H

0.85

H atoms were positioned geometrically, with O-H = 0.85 Å (for water H) and C-H = 0.93 and 0.97 Å, for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$, where x = 1.5 for water H and x = 1.2 for all other H atoms.

 $H \cdot \cdot \cdot A$

1.85

2.16

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

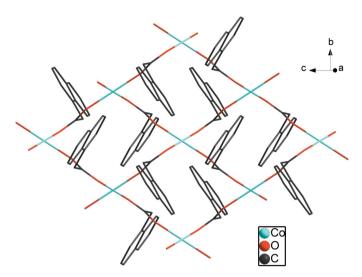


Figure 2

A view of the two-dimensional layer structure of (I). H atoms and aqua ligands have been omitted.

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0977P)^2]$
$wR(F^2) = 0.159$	where $P = (F_0^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{\rm max} < 0.001$
2238 reflections	$\Delta \rho_{\rm max} = 0.61 \ {\rm e} \ {\rm \AA}^{-3}$
142 parameters	$\Delta \rho_{\rm min} = -0.83 \ {\rm e} \ {\rm \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Co1-O1	2.062 (2)	O1-C1	1.256 (4)
Co1-O2 ⁱ	2.130 (2)	O2-C1	1.265 (4)
Co1-O1W	2.126 (2)		
O1 ⁱⁱ -Co1-O1	180	O2 ⁱⁱⁱ -Co1-O2 ⁱ	180
O1 ⁱⁱ -Co1-O2 ⁱ	94.17 (9)	$O1W^{ii}$ -Co1-O2 ⁱ	90.23 (10)
$O1-Co1-O2^i$	85.83 (9)	$O1W-Co1-O2^{i}$	89.77 (10)
O1 ⁱⁱ -Co1-O1W	89.31 (10)	$O1W^{ii}$ -Co1-O1W	180
O1-Co1-O1W	90.69 (10)		
Symmetry codes:	(i) $-x + \frac{1}{2}, y + \frac{1}{2}, -$	$-z + \frac{1}{2};$ (ii) $-x + \frac{1}{2}, -y$	$z + \frac{3}{2}, -z;$ (iii)
$x, -y + 1, z - \frac{1}{2}$	2 - 2	2 2 -	2

 $D \cdots A$

2.701 (3)

3.004(3)

 $D - H \cdot \cdot \cdot A$

176

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SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXL97.

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