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## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=273 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.005 \AA$
$R$ factor $=0.052$
$w R$ 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.

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## A two-dimensional grid-like cobalt ${ }^{\prime \prime}$ coordination polymer: poly[[diaquacobalt(II)]-di- $\mu_{2}$-naphthalene1 -acetato]

In the title compound, $\left[\mathrm{Co}\left(\mathrm{C}_{12} \mathrm{H}_{9} \mathrm{O}_{2}\right)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{2}\right]_{n}$, the $\mathrm{Co}^{\mathrm{II}}$ 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 $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ 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 $\mathrm{Co}^{\mathrm{II}}$ atom of (I) occupies a special position on an inversion centre, and has a slightly distorted octahedral coordination environment. The $\mathrm{Co}^{\mathrm{II}}$ atom is coordinated by six O atoms, four from three different naphthaleneacetate ligands [average $\mathrm{Co}-\mathrm{O}$ distance $=$ 2.096 (2) A] and two from two water molecules [ $\mathrm{Co}-\mathrm{OW}=$ 2.126 (2) A]. The carboxylate groups of the anionic ligands are

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Figure 1
The asymmetric unit of (I), together with additional atoms to complete the coordination of Co 1 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) $\left.-x+\frac{1}{2}, y-\frac{1}{2},-z+\frac{1}{2}\right]$.
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 $\mathrm{Co}^{\mathrm{II}}$ atoms. As a result, a polynuclear one-dimensional cobalt chain is formed, running along the diagonal of the $b c$ plane, in which the adjacent Co $\cdots$ Co distance is 5.358 (2) $\AA$. 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 $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ 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 $(4.76 \mathrm{~g}, 20 \mathrm{mmol})$ and naphthaleneacetic acid ( $3.72 \mathrm{~g}, 20 \mathrm{mmol}$ ) 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

| $\left[\mathrm{Co}\left(\mathrm{C}_{12} \mathrm{H}_{9} \mathrm{O}_{2}\right)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{2}\right]$ | $Z=4$ |
| :--- | :--- |
| $M_{r}=465.35$ | $D_{x}=1.566 \mathrm{Mg} \mathrm{m}^{-3}$ |
| Monoclinic, $C 2 / c$ | Mo $K \alpha$ radiation |
| $a=36.954(5) \AA \AA$$\circ$ <br> $b=6.1913(10) \AA$ <br> $c=8.7464(13) \AA$ | $\mu=0.91 \mathrm{~mm}^{-1}$ |
| $\beta=99.524(9)^{\circ}$ | $T=273(2) \mathrm{K}$ |
| $V=1973.5(5) \AA^{3}$ | Block, pink |
|  | $0.31 \times 0.26 \times 0.18 \mathrm{~mm}$ |
|  |  |

## Data collection

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

## $Z=4$

.566 Mg m
Mo $K \alpha$ radiation
$T=273$
Block, pink
$0.31 \times 0.26 \times 0.18 \mathrm{~mm}$

6297 measured reflections
2238 independent reflections
1628 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.043$
$\theta_{\text {max }}=27.5^{\circ}$

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2},-z+\frac{1}{2}$; (ii) $-x+\frac{1}{2},-y+\frac{3}{2},-z$.
H atoms were positioned geometrically, with $\mathrm{O}-\mathrm{H}=0.85 \AA$ (for water H ) and $\mathrm{C}-\mathrm{H}=0.93$ and $0.97 \AA$, for aromatic and methylene H , respectively, and constrained to ride on their parent atoms, with $U_{\text {iso }}(\mathrm{H})=x U_{\text {eq }}(\mathrm{C}, O)$, where $x=1.5$ for water H and $x=1.2$ for all other H atoms.

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 $F^{2}$
H -atom parameters constrained
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.052$
$w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}{ }^{2}\right)+(0.0977 P)^{2}\right]$
where $P=\left(F_{\mathrm{o}}{ }^{2}+2 F_{\mathrm{c}}{ }^{2}\right) / 3$
$(\Delta / \sigma)_{\max }<0.001$
$S=1.06$
$\Delta \rho_{\text {max }}=0.61 \mathrm{e} \mathrm{A}^{-3}$
$\Delta \rho_{\min }=-0.83 \mathrm{e}^{\AA^{-3}}$

Table 1
Selected geometric parameters ( $\left({ }^{\circ},{ }^{\circ}\right)$.

| Co1-O1 | 2.062 (2) | O1-C1 | 1.256 (4) |
| :---: | :---: | :---: | :---: |
| $\mathrm{Co} 1-\mathrm{O} 2^{\text {i }}$ | 2.130 (2) | $\mathrm{O} 2-\mathrm{C} 1$ | 1.265 (4) |
| Co1-O1W | 2.126 (2) |  |  |
| $\mathrm{O} 1^{\text {ii }}-\mathrm{Co} 1-\mathrm{O} 1$ | 180 | $\mathrm{O} 2{ }^{\text {iii }}-\mathrm{Co} 1-\mathrm{O} 2{ }^{\text {i }}$ | 180 |
| $\mathrm{O} 1^{\mathrm{ii}}-\mathrm{Co} 1-\mathrm{O} 2^{\text {i }}$ | 94.17 (9) | $\mathrm{O} 1 W^{\mathrm{ii}}-\mathrm{Co} 1-\mathrm{O} 2^{\mathrm{i}}$ | 90.23 (10) |
| $\mathrm{O} 1-\mathrm{Co} 1-\mathrm{O} 2^{\mathrm{i}}$ | 85.83 (9) | $\mathrm{O} 1 W-\mathrm{Co} 1-\mathrm{O} 2^{\mathrm{i}}$ | 89.77 (10) |
| $\mathrm{O} 1{ }^{\text {ii }}-\mathrm{Co} 1-\mathrm{O} 1 \mathrm{~W}$ | 89.31 (10) | $\mathrm{O} 1 W^{\text {ii }}-\mathrm{Co} 1-\mathrm{O} 1 W$ | 180 |
| $\mathrm{O} 1-\mathrm{Co} 1-\mathrm{O} 1 W$ | 90.69 (10) |  |  |
| Symmetry codes: $x,-y+1, z-\frac{1}{2} .$ | $-x+\frac{1}{2}, y+\frac{1}{2},-z+\frac{1}{2} ; \quad$ (ii) |  | -z; (iii) |

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

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| O1 $W-\mathrm{H} 1 W 1 \cdots \mathrm{O}^{\text {ii }}$ | 0.85 | 1.85 | $2.701(3)$ | 176 |
| O1 $^{\mathrm{ii}}-\mathrm{H} 1 W 2 \cdots$ O2 $^{\mathrm{i}}$ | 0.85 | 2.16 | $3.004(3)$ | 176 |

## metal-organic papers

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

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