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catena-Poly[[tetraaquacobalt(II)]-μ-benzene-1,4-dioxyacetato-κ^2O:O']

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The Co^{II} atom in the title coordination polymer, $[Co(1,4\text{-BDOA})(H_2O)_4]_n$ (where $1,4\text{-BDOA}^{2-}$ is benzene-1,4-dioxyacetate, $C_{10}H_8O_6$), lies on an inversion center. The Co^{II} atom has an octahedral coordination configuration, involving two carboxyl O atoms of different benzene-1,4-dioxyacetate ligands and four water molecules. Adjacent Co^{II} atoms are bridged by anions with two monodentate carboxylate groups, forming a one-dimensional chain along the *c* axis; the Co$\cdots$Co separation within the polymer is 14.699 (2) Å. A supramolecular network structure is formed by O—H$\cdots$O hydrogen bonds.

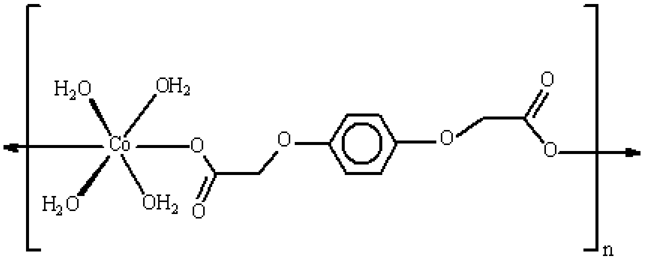
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.072
Data-to-parameter ratio = 14.0

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

Comment

Many promising supramolecular architectures sustained by coordination covalent bonds and hydrogen bonds have been designed and constructed in recent years. The selection of appropriate ligands is crucial to determining the structure of the coordination framework and its properties. Fortunately, multicarboxylate ligands are good candidates because of their versatile binding modes, and numerous polymeric complexes have been reported (Lee *et al.*, 2003; Gomez-Lor *et al.*, 2002; Bian *et al.*, 2003). However, the structural characterization of polymers with the multidentate benzene-1,4-dioxyacetic acid ligand is less well developed. Recently, we have reported the structures of the mononuclear cobalt complexes $[Co(H_2O)_6](1,4\text{-BDOA})$ (Liu *et al.*, 2004) and $[Co(1,4\text{-BDOA})(C_{10}H_8N_2)_2(H_2O)]\cdot 4H_2O$, (II) (Gao *et al.*, 2004); the $1,4\text{-BDOA}^{2-}$ ($1,4\text{-BDOA}^{2-}$ is benzene-1,4-dioxyacetate) ligand functions as a counter-ion in the former, and only one of the two oxyacetate groups is coordinated to Co^{II} ion in the latter. We present here the crystal structure of a one-dimensional chain Co^{II} polymer, $[Co(1,4\text{-BDOA})(H_2O)_4]_n$, (I).



(I)

In (I), the Co^{II} atom exists in an octahedral coordination environment (Fig. 1), defined by two carboxyl O atoms of different $1,4\text{-BDOA}^{2-}$ ligands [Co—O = 2.090 (1) Å] and four water molecules [$\text{Co—O}_{\text{mean}}$ = 2.095 (2) Å]. The Co^{II} atom and the $1,4\text{–BDOA}^{2-}$ ligand lie on inversion centers.

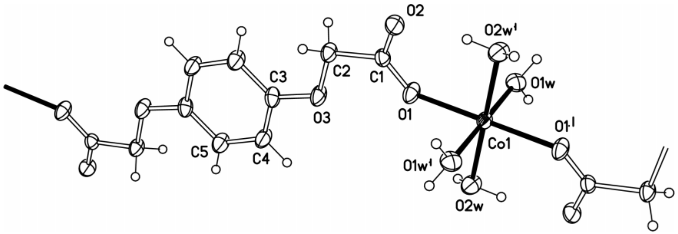


Figure 1
A view of the title complex, with 30% probability displacement ellipsoids. Symmetry code (i) as in Table 1.

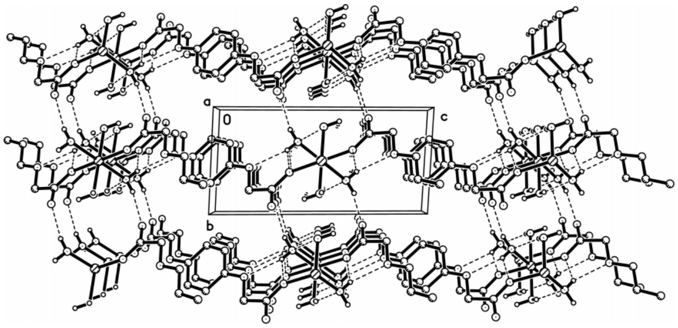


Figure 2
A packing diagram of the title complex. Hydrogen bonds are shown as dashed lines.

The C1—O1 bond distance [1.263 (2) Å; Table 1] is slightly longer than C1—O2 [1.252 (2) Å], appropriate for the monodentate coordination mode of carboxyl groups. The oxyacetate group and benzene ring are almost coplanar, with a C3—O3—C2—C1 torsion angle of 176.9 (2)°, whereas the torsion angles of the two oxyacetate groups and the benzene ring in (II) are 80.7 (3) and −90.2 (3) °.

In (II), the Co atom has the same coordination geometry as in (I). However, only one of the two oxyacetate groups in the monodentate mode is coordinated to the Co^{II} center, and the other oxyacetate group is not involved in coordination. The Co—O$_{\rm carboxylate}$ bond distance [2.106 (2) Å] is slightly longer than the corresponding bond distance in (I).

In (I), each 1,4-BDOA^{2-} group acts in a bis-monodentate mode to bridge two Co^{II} atoms, forming a one-dimensional chain along the *c* axis. In the chain, the Co···Co distance is 14.699 (2) Å. Furthermore, chains are connected through intermolecular hydrogen bonds involving the water molecules and O atoms of 1,4-BDOA^{2-} groups, with O···O distances ranging from 2.692 (2) to 2.979 (2) Å and O—H···O angles ranging from 135 (2) to 158 (2)° (Table 2), yielding a hydrogen-bonding supramolecular network (Fig. 2).

Experimental

Benzene-1,4-dioxyacetic acid was prepared according to the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). The title complex was synthesized by the addition of cobalt diacetate trihydrate (4.76 g, 20 mmol) and 3-hydroxypyridine (0.95 g, 10 mmol) to a hot aqueous solution of 1,4-BDOAH$_2$ (4.52 g, 20 mmol). The solution was allowed to evaporate at room temperature, and pink prismatic crystals were obtained after about six days. Analysis calculated for $C_{10}H_{16}CoO_{10}$: C 33.82, H 4.54%; found: C 33.91, H 4.46%.

Crystal data

$[Co(C_{10}H_8O_6)(H_2O)_4]$
M_r = 355.16
Triclinic, $P\overline{1}$
a = 4.9218 (10) Å
b = 5.7966 (12) Å
c = 11.804 (2) Å
α = 92.41 (3)°
β = 94.98 (3)°
γ = 96.91 (3)°
V = 332.59 (12) Å^3
Z = 1
D_x = 1.773 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2096 reflections
θ = 3.5–27.5°
μ = 1.34 mm^{-1}
T = 293 (2) K
Prism, pink
0.37 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\rm min}$ = 0.637, $T_{\rm max}$ = 0.794
3183 measured reflections
1526 independent reflections
1351 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.024
$\theta_{\rm max}$ = 27.5°
$h = -6 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.072
S = 1.05
1526 reflections
109 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.0781P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.37 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.090 (1)	O1—C1	1.263 (2)
Co1—O1*W*	2.118 (2)	O2—C1	1.252 (2)
Co1—O2*W*	2.072 (2)		
O1—Co1—O1^{i}	180	O2*W*—Co1—O1	88.56 (6)
O1—Co1—O1*W*^{i}	91.79 (6)	O2*W*—Co1—O1*W*	90.47 (6)
O1—Co1—O1*W*	88.21 (6)	O2*W*—Co1—O1*W*^{i}	89.53 (6)
O1*W*—Co1—O1*W*^{i}	180	O2*W*—Co1—O2*W*^{i}	180
O2*W*—Co1—O1^{i}	91.44 (6)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{ii}	0.85 (2)	1.93 (1)	2.733 (2)	158 (2)
O1*W*—H1*W*2···O1^{iii}	0.84 (2)	2.22 (2)	2.876 (2)	135 (2)
O1*W*—H1*W*2···O3^{iii}	0.84 (2)	2.21 (2)	2.979 (2)	153 (2)
O2*W*—H2*W*2···O2^{i}	0.85 (2)	1.89 (1)	2.692 (2)	158 (2)
O2*W*—H2*W*1···O1*W*^{iii}	0.85 (2)	2.12 (1)	2.869 (2)	148 (2)

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $-x, -y, 1-z$; (iii) $1-x, 1-y, 1-z$.

C-bound H atoms were placed in calculated positions, with C—H = 0.93 and 0.97 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$, and were refined in the riding-model approximation. The H atoms of water molecules were located in a difference map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97

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(Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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