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Hexaaquacobalt(II) bis[2-(4-carboxyphenoxy)-propionate] trihydrate

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Key indicators

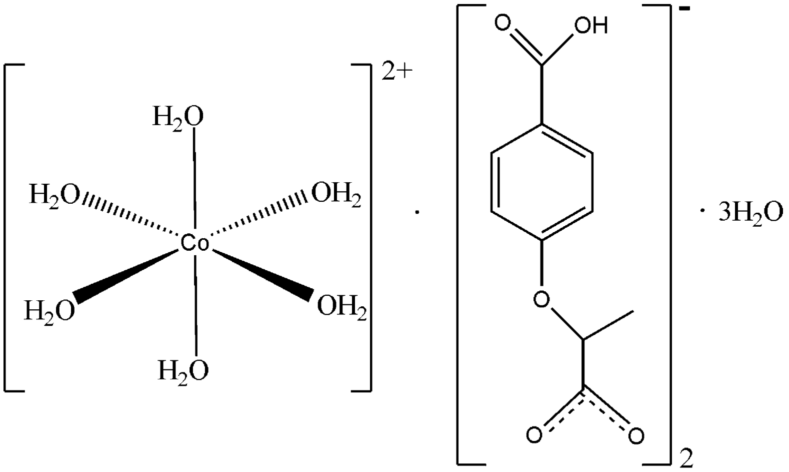
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
Disorder in solvent or counterion
R factor = 0.033
wR factor = 0.100
Data-to-parameter ratio = 15.6

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

The title complex, $[Co(H_2O)_6](C_{10}H_9O_5)_2 \cdot 3H_2O$, consists of $[Co(H_2O)_6]^{2+}$ cations and 2-(4-carboxylatophenoxy)propionate anions along with uncoordinated water molecules. The Co atoms, which each lie on a center of symmetry, have octahedral coordination. The cations and anions are linked by O—H···O hydrogen bonds into a three-dimensional supramolecular framework.

Comment

The structure of 3-(4-carboxylatophenoxy)propionic acid [3-(p-CPOPH$_2$)] has been reported recently (Gao & Ng, 2006); the present study used isomeric 2-(4-carboxylatophenoxy)propionic acid [2-(p-CPOPH$_2$)] in an attempted synthesis of the cobalt derivative. Our previous work detailed the structure of the cobalt(II) derivative of 3-(p-CPOPH$_2$) (Xiao *et al.*, 2006); the present synthesis afforded hexaaquacobalt(II) 2-(4-carboxyphenoxy)propionate hexahydrate, (I) (Fig. 1).



(I)

Both the two independent Co^{II} atoms, which lie on inversion centers, are six-coordinate in octahedral environments. In the anion, the oxyacetate group and aromatic ring are twisted by 67.93 (17) (C5—O3—C8—C10) and 110.84 (17)° (C15—O8—C18—C20). The cations and anions are linked by extensive hydrogen bonds into a three-dimensional supramolecular network (Table 2).

Experimental

Cobalt(II) acetate trihydrate (2.28 g, 10 mmol) was added to a hot aqueous solution of 2-(4-carboxylatophenoxy)propionic acid (2.10 g,

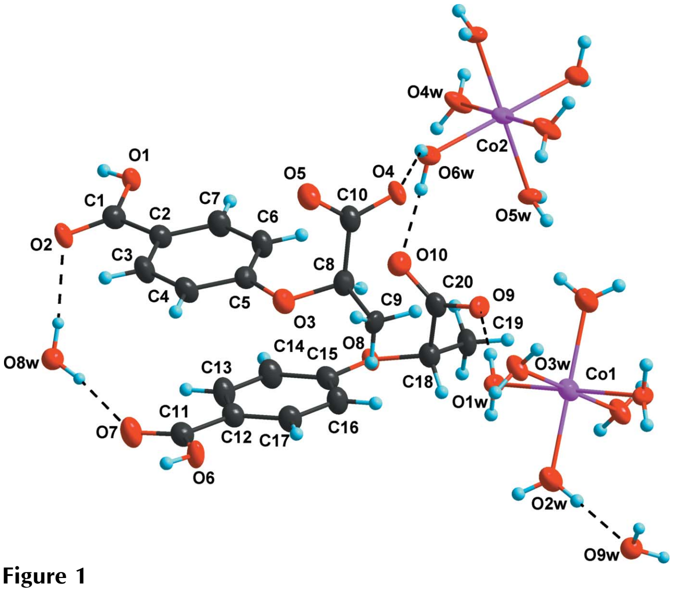


Figure 1
The asymmetric unit of (I), together with symmetry-equivalent aqua ligands to complete the coordination. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Hydrogen bonds are denoted by dashed lines. The disordered water molecule is not shown. [Symmetry codes for unlabeled ligands bonded to Co1 and Co2: $1 - x$, $1 - y$, $1 - z$ and $-x$, $-y$, $1 - z$, respectively.]

10 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the solution registered a pH of 6. The filtered solution was allowed to evaporate at room temperature, and pink prismatic crystals of (I) were separated from the filtered solution after several days. Analysis calculated for $C_{40}H_{72}Co_2O_{38}$: C 37.57, H 5.67%; found: C 37.62, H 5.64%.

Crystal data

$[Co(H_2O)_6](C_{10}H_9O_5)_2\cdot 3H_2O$
$M_r = 637.40$
Monoclinic, $P2_1/n$
$a = 8.0171$ (16) Å
$b = 13.288$ (3) Å
$c = 27.352$ (6) Å
$\beta = 95.99$ (3)°
$V = 2898.0$ (10) Å^3
$Z = 4$
$D_x = 1.461$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.67$ mm^{-1}
$T = 295$ (2) K
Prism, pink
0.36 × 0.28 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.794$, $T_{\max} = 0.883$
45283 measured reflections
6615 independent reflections
5127 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.031$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.100$
$S = 1.04$
6615 reflections
424 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2 + 0.6509P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.44$ e Å^{-3}
$\Delta\rho_{\min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2*W*	2.0825 (13)	Co2—O4*W*	2.0661 (15)
Co1—O3*W*	2.0888 (13)	Co2—O5*W*	2.0710 (14)
Co1—O1*W*	2.0897 (12)	Co2—O6*W*	2.1042 (14)
O2*W*—Co1—O2*W*$^{\text{i}}$	180	O4*W*$^{\text{ii}}$—Co2—O4*W*	180
O2*W*—Co1—O3*W*	93.97 (6)	O4*W*—Co2—O5*W*$^{\text{ii}}$	91.37 (8)
O2*W*$^{\text{i}}$—Co1—O3*W*	86.03 (6)	O4*W*—Co2—O5*W*	88.63 (8)
O3*W*—Co1—O3*W*$^{\text{i}}$	180	O5*W*$^{\text{ii}}$—Co2—O5*W*	180
O2*W*—Co1—O1*W*$^{\text{i}}$	93.01 (5)	O4*W*$^{\text{ii}}$—Co2—O6*W*	88.21 (7)
O3*W*—Co1—O1*W*$^{\text{i}}$	90.21 (6)	O4*W*—Co2—O6*W*	91.79 (7)
O2*W*—Co1—O1*W*	86.99 (5)	O5*W*$^{\text{ii}}$—Co2—O6*W*	89.92 (6)
O3*W*—Co1—O1*W*	89.79 (6)	O5*W*—Co2—O6*W*	90.08 (6)
O1*W*$^{\text{i}}$—Co1—O1*W*	180	O6*W*—Co2—O6*W*$^{\text{ii}}$	180

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*W*1···O5$^{\text{iii}}$	0.844 (9)	1.802 (10)	2.6404 (18)	172 (2)
O1*W*—H1*W*2···O9	0.834 (9)	2.064 (12)	2.8566 (18)	158.5 (18)
O2*W*—H2*W*1···O9*W*	0.809 (9)	1.935 (11)	2.7277 (18)	166 (2)
O2*W*—H2*W*2···O2$^{\text{iv}}$	0.817 (9)	1.946 (11)	2.7405 (17)	164 (2)
O3*W*—H3*W*1···O4$^{\text{v}}$	0.823 (9)	1.972 (10)	2.7921 (18)	174 (2)
O3*W*—H3*W*2···O8*W*$^{\text{iv}}$	0.826 (9)	1.969 (9)	2.790 (2)	172 (2)
O4*W*—H4*W*1···O7$^{\text{vi}}$	0.826 (10)	1.958 (10)	2.782 (2)	176 (3)
O4*W*—H4*W*2···O9*W*$^{\text{vii}}$	0.820 (10)	2.003 (12)	2.778 (2)	157 (3)
O6*W*—H6*W*1···O10	0.835 (9)	1.841 (10)	2.6740 (19)	175 (2)
O6*W*—H6*W*2···O4	0.821 (9)	2.378 (15)	3.1094 (19)	148.7 (19)
O8*W*—H8*W*1···O2	0.824 (19)	2.00 (2)	2.821 (2)	171 (2)
O8*W*—H8*W*2···O7	0.83 (2)	1.963 (10)	2.7860 (19)	170 (3)
O9*W*—H9*W*1···O9$^{\text{i}}$	0.848 (9)	1.911 (10)	2.7497 (19)	169 (2)
O9*W*—H9*W*2···O4$^{\text{i}}$	0.841 (9)	1.924 (10)	2.7531 (18)	168 (2)
O1—H100···O5$^{\text{viii}}$	0.822 (10)	1.829 (10)	2.6452 (16)	172 (3)
O6—H200···O10$^{\text{iv}}$	0.807 (10)	1.851 (11)	2.6485 (16)	170 (3)

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

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93–0.97Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the other H atoms, and were refined in the riding-model approximation. The uncoordinated water molecule O7*W* is disordered over two positions; the occupancies of O7*W* and O7*W*′ refined to 0.783 (4) and 0.217 (4). H atoms could not be placed in any chemical sensible positions owing to the disorder. Other H atoms of the water molecules and hydroxyl groups were located in a difference Fourier map and refined with O—H and H···H distance restraints of 0.82 (1) and 1.39 (1) Å, respectively, 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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