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mer-Triaqua(2-carboxylatophenoxyacetato)cobalt(II)

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Key indicators

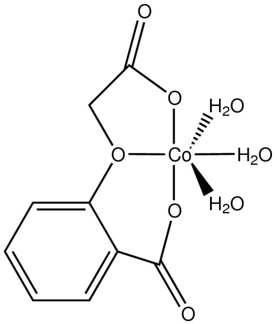
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.078
Data-to-parameter ratio = 13.6

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

In the title compound, [Co($C_9H_6O_5$)(H_2O)$_3$], the Co^{II} atom is coordinated by three O atoms from the 2-carboxylatophenoxyacetate ligand in meridional sites, forming chelate rings. The other three coordination sites of the octahedron are occupied by the water molecules.

Comment

The preceding report describes a polymeric zinc(II) complex with 2-carboxylatophenoxyacetic acid (2-cbphacH_2) as a ligand, [Zn(2-cbphac)(H_2O)]$_n$; this was synthesized hydrothermally. The compound adopts a carboxylate-bridged chain motif (Zhu *et al.*, 2005). Under non-hydrothermal conditions, the cobalt(II) compound crystallizes as the title monomeric complex, [Co(2-cbphac)(H_2O)$_3$], (I).



(I)

In (I), the Co^{II} atom is coordinated by three O atoms from the 2-cbphac^{2-} ligand which occupy *mer* sites; adjacent complexes are linked by O—H···O hydrogen bonds (Table 2) into a three-dimensional network. The cobalt(II) complex of 3-carboxyphenoxyacetic acid (3-cbphacH_2) exists as [Co(3-cbphacH)$_2$(H_2O)$_4$], in which the 3-carboxyl group retains the acid H atom (Li *et al.*, 2004).

Experimental

Cobalt(II) nitrate hexahydrate (0.149 g, 0.5 mmol) and 2-carboxyphenoxyacetic acid (0.196 g, 1 mmol) were dissolved in ethanol (3 ml) and water (15 ml) to give a purple solution. Crystals of (I) separated from the solution after a week (yield *ca* 70%).

Crystal data

[Co($C_9H_6O_5$)(H_2O)$_3$]
M_r = 307.12
Monoclinic, $P2_1/c$
a = 8.762 (1) Å
b = 6.7707 (8) Å
c = 19.841 (2) Å
β = 96.515 (2)°
V = 1169.5 (2) Å^3
Z = 4

D_x = 1.744 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 934 reflections
θ = 3.2–27.0°
μ = 1.50 mm^{-1}
T = 295 (2) K
Block, dark purple
0.36 × 0.25 × 0.21 mm

Data collection

Bruker SMART 1K area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.615$, $T_{\max} = 0.744$
6758 measured reflections

2549 independent reflections
2132 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 27.0^\circ$
$h = -9 \rightarrow 11$
$k = -8 \rightarrow 7$
$l = -25 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.078$
$S = 1.06$
2549 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.1445P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.34$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.031 (1)	Co1—O1*w*	2.097 (2)
Co1—O3	2.203 (1)	Co1—O2*w*	2.044 (1)
Co1—O4	1.989 (1)	Co1—O3*w*	2.108 (2)
O2—Co1—O3	76.77 (5)	O3—Co1—O3*w*	90.14 (6)
O2—Co1—O4	160.59 (6)	O4—Co1—O1*w*	90.28 (7)
O2—Co1—O1*w*	90.82 (7)	O4—Co1—O2*w*	102.11 (6)
O2—Co1—O2*w*	97.28 (6)	O4—Co1—O3*w*	89.96 (7)
O2—Co1—O3*w*	89.57 (7)	O1*w*—Co1—O2*w*	88.81 (6)
O3—Co1—O4	83.83 (5)	O1*w*—Co1—O3*w*	178.16 (6)
O3—Co1—O1*w*	91.69 (6)	O2*w*—Co1—O3*w*	89.35 (6)
O3—Co1—O2*w*	174.04 (6)		
O2—C1—C2—O3	0.0 (3)	O3—C3—C8—C9	−1.7 (3)
C2—O3—C3—C4	1.5 (3)	C3—C8—C9—O4	−3.2 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O5$^{\rm i}$	0.85 (1)	1.93 (1)	2.760 (2)	166 (3)
O1*w*—H1*w*2···O4$^{\rm ii}$	0.85 (1)	1.97 (1)	2.804 (2)	169 (2)
O2*w*—H2*w*2···O1$^{\rm iii}$	0.84 (1)	1.93 (1)	2.766 (2)	173 (2)
O2*w*—H2*w*1···O5$^{\rm ii}$	0.84 (1)	1.87 (1)	2.703 (2)	171 (2)
O3*w*—H3*w*1···O2$^{\rm iii}$	0.85 (1)	1.92 (1)	2.757 (2)	167 (3)
O3*w*—H3*w*2···O1$^{\rm iv}$	0.84 (1)	2.03 (1)	2.861 (2)	172 (2)

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

The carbon-bound H atoms were positioned geometrically (C—H = 0.93 Å for the aromatic H atoms and 0.97 Å for the methylene H atoms) and were included in the refinement in the riding-model approximation, with $U_{\rm iso}$(H) values set at 1.2 times $U_{\rm eq}$(C). The water H atoms were located in difference Fourier maps and refined isotropically, with restraints of O—H and H···H distances to 0.85 (1) and 1.39 (1) Å, respectively.

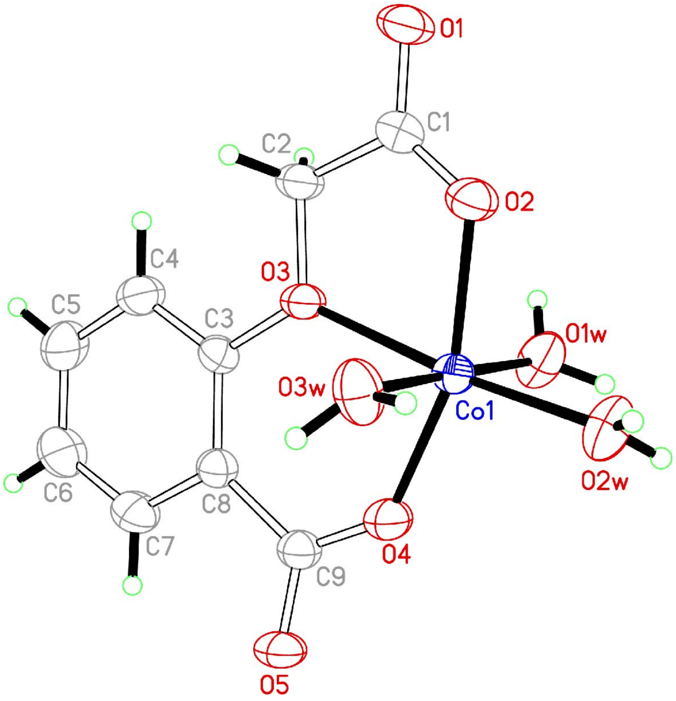


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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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