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Hexaaquacobalt(II) bis(4-formylbenzoate) dihydrate

Zhao-Peng Deng,[a] Shan Gao[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

The crystal structure of the title compound, $[Co(H_2O)_6](C_8H_5O_3)_2{\cdot}2H_2O$, consists of octahedral Co^{II} complex cations that interact with the anions and uncoordinated water molecules, forming a tightly held, hydrogen-bonded layer. The Co^{II} complex cation lies on a special position of site symmetry $\overline{1}$.

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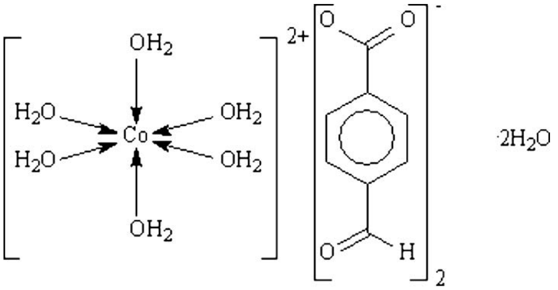
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.029
wR factor = 0.080
Data-to-parameter ratio = 13.1

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

Comment

The known transition metal derivatives of 4-formylbenzoic acid are water-coordinated compounds showing covalent metal–carboxylate bonds, for example the nickel(II) (Deng *et al.*, 2006*a*) and copper(II) (Deng *et al.*, 2006*b*) derivatives. However, the cobalt(II) derivative does not have this feature; the title compound (I) has a hexaaquacobalt cation (Table 1), and its charge is balanced by two uncoordinated 4-formylbenzoate ions. There are one cation and two anions in the asymmetric unit along with two uncoordinated water molecules (Fig. 1). These are linked by hydrogen bonds (Table 2) into a layer structure. The Co^{II} complex cation lies on a special position of site symmetry $\overline{1}$.



(I)

Experimental

Cobalt diacetate trihydrate (0.116 g, 0.5 mmol) was added to an aqueous solution (20 ml) of 4-formylbenzoic acid (0.15 g, 1 mmol). Sodium hydroxide solution was added to obtain a pH 5. The filtered solution was allowed to stand for a few days for the pink prismatic crystals to separate. Elemental analysis calculated for $C_{16}H_{26}CoO_{14}$: C 38.33, H 5.23%; found: C 38.31, H 5.24%.

Crystal data

$[Co(H_2O)_6](C_8H_5O_3)_2{\cdot}2H_2O$
M_r = 501.30
Triclinic, $P\overline{1}$
a = 6.3470 (3) Å
b = 7.4194 (4) Å
c = 12.5041 (7) Å
α = 92.353 (2)°
β = 90.029 (3)°
γ = 113.801 (6)°
V = 538.20 (5) Å^3
Z = 1
D_x = 1.547 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 295 (2) K
Prism, pink
0.36 × 0.28 × 0.18 mm

Data collection

Rigaku RAXIS-RAPID IP diffractometer
ω scans
Absorption correction: multi-scan *ABSCOR* (Higashi, 1995)
$T_{\min} = 0.614$, $T_{\max} = 0.860$
5333 measured reflections
2451 independent reflections
2325 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.017$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.080$
$S = 1.00$
2451 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.2223P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.55$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1*w*	2.127 (1)	Co1—O3*w*	2.065 (1)
Co1—O2*w*	2.071 (1)		
O1*w*—Co1—O2*w*	89.57 (5)	O2*w*—Co1—O3*w*	88.04 (6)
O1*w*—Co1—O3*w*	92.73 (6)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O1	0.84 (1)	1.95 (1)	2.778 (2)	166 (2)
O1*w*—H1*w*2···O2$^{\rm i}$	0.85 (1)	1.78 (1)	2.629 (2)	178 (3)
O2*w*—H2*w*1···O1$^{\rm i}$	0.85 (1)	1.90 (1)	2.746 (2)	171 (2)
O2*w*—H2*w*2···O4*w*$^{\rm ii}$	0.84 (1)	1.93 (1)	2.760 (2)	172 (2)
O3*w*—H3*w*1···O3$^{\rm iii}$	0.84 (1)	1.89 (1)	2.715 (2)	165 (3)
O3*w*—H3*w*2···O4*w*$^{\rm iv}$	0.84 (1)	1.92 (1)	2.743 (2)	169 (2)
O4*w*—H4*w*1···O1$^{\rm v}$	0.84 (1)	2.03 (2)	2.812 (2)	155 (3)
O4*w*—H4*w*2···O1*w*	0.84 (1)	2.05 (1)	2.872 (2)	168 (2)

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1, y-1, z$; (iii) $-x+1, -y+1, -z$; (iv) $x, y-1, z$; (v) $-x+2, -y+2, -z+1$.

The –C_6H_4– ring is disordered over two positions about the C2···C5 vector; the atoms C2 and C5 are ordered. The C–C distances in the ring were restrained to 1.39 (1) Å, and both components were restrained to be approximately planar. The displacement parameters of the primed atoms were set equal to those of the unprimed atoms. The occupancy factors refined to 0.52 (1):0.48 (1).

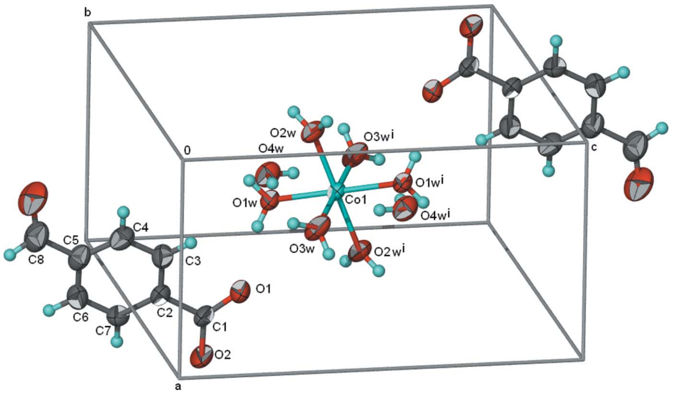


Figure 1
Displacement ellipsoid plot of the unit-cell contents. Displacement ellipsoids are drawn at the 70% probability level, and H atoms are shown as spheres of arbitrary radii. Only one disorder component is shown. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

Carbon-bound H atoms were positioned geometrically (C—H 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The water H atoms were located in a difference Fourier map, and were refined with a distance restraint of O—H 0.85 (1) Å; their displacement parameters were freely refined.

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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