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Hexaaquacobalt(II) bis(4-hydroxyisophthalate) tetrahydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.095
Data-to-parameter ratio = 10.2

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

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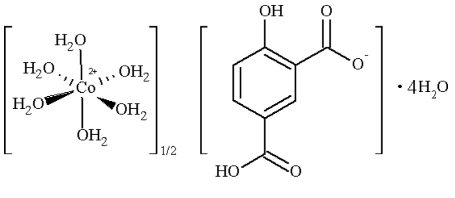
Hydrothermal reaction of 4-hydroxyisophthalic acid and $Co(NO_3)_2 \cdot 6H_2O$ in water resulted in a new mononuclear cobalt compound, $[Co(H_2O)_6](C_8H_5O_5)_2 \cdot 4H_2O$. The occurrence of an intricate hydrogen-bond network leads to the formation of a three-dimensional structure. The cation lies on a crystallographic inversion center, while the anion and water molecules are in general positions.

Comment

The design and synthesis of new compounds with structures defined through non-covalent connections is currently of great interest because of their potential application in certain areas, such as gas storage (Atwood *et al.*, 2002), catalysis (Thomas, 1998), molecular transport (Gardner *et al.*, 1995) and biosynthesis (Lippert, 1997). In the fields of supramolecular chemistry and crystal engineering, hydrogen bonding plays an important role. Many examples of compounds that assemble by hydrogen-bonding interactions have been reported in previous publications (Yuan *et al.*, 2002). The great structural diversity of crystal packing results not only from the variability of the organic ligands and the ligand-to-metal connections, but also from the types and fashions of hydrogen bonding and other weak intermolecular interactions (Naumann *et al.*, 2002). Although 4-hydroxyisophthalic acid, which possesses four carboxylic O atoms and one hydroxyl O atom, is a good candidate for the generation of many linking modes, including hydrogen bonding, it has rarely been reported in recent years. Here we report the preparation and characterization of the first 4-hydroxyisophthalate–cobalt(II) complex, $[Co(H_2O)_6]$-$(C_8H_5O_5)_2 \cdot 4H_2O$, (I).



(I)

An X-ray analysis reveals that (I) possesses a mononuclear structure, with the cation on a crystallographic inversion center. A view of the cobalt ion coordination is shown in Fig. 1; the metal center is coordinated in an octahedral geometry by six water molecules with Co—O distances ranging from 2.0386 (18) to 2.1371 (18) Å. The 4-hydroxyisophthalate ligand, in which only one carboxylic acid group is deprotonated, is not directly coordinated to the cobalt ion but is involved in a hydrogen-bond interaction with a coordinated water molecule. Different types of hydrogen-bonding interactions are observed (Table 2) in which O atoms may act as

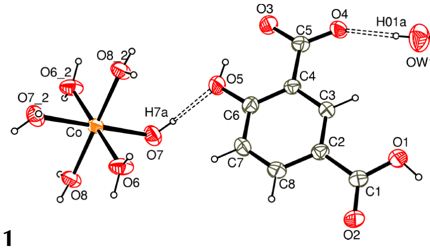


Figure 1
The cation, anion and water molecules, with their hydrogen-bond interactions. Displacement ellipsoids are drawn at the 50% probability level. The suffix 2 corresponds to symmetry code (i) in Table 1 .

donors or acceptors: (*a*) hydrogen bonds between coordinated water and isolated water molecules, with O···O distances ranging from 2.627 (3) to 2.982 (3) Å; (*b*) hydrogen bonds between coordinated water molecules and carboxylic acid O atoms, with O···O distances ranging from 2.744 (2) to 3.031 (3) Å; (*c*) hydrogen bond between coordinated water and hydroxyl atom O5, with an O···O distance of 2.886 (3) Å; (*d*) hydrogen bonds between isolated water molecules and carboxylic acid oxygen atoms, with O···O distances of 2.754 (3) and 2.865 (3) Å; (*e*) hydrogen bond between the hydroxyl and carboxylic acid groups, with an O···O distance of 2.675 (2) Å. These hydrogen-bonding interactions result in a three-dimensional network (Fig. 2).

Experimental

A mixture of 4-hydroxyisophthalic acid (0.25 mmol, 0.045 g), $Co(NO_3)_2 \cdot 6H_2O$ (0.2 mmol, 0.05 g) and H_2O (20 ml) was sealed in a 25 ml Teflon-lined stainless-steel reactor and heated at 433 K for 72 h, and yielding a red solution. After cooling and evaporation of the red solution over two weeks, red crystals were isolated by filtration (yield, 50%).

Crystal data

$[Co(H_2O)_6](C_8H_5O_5)_2 \cdot 4H_2O$
$M_r = 601.33$
Triclinic, $P\overline{1}$
$a = 7.1863$ (6) Å
$b = 8.5173$ (7) Å
$c = 9.8959$ (7) Å
$\alpha = 92.088$ (1)°
$\beta = 91.424$ (1)°
$\gamma = 90.548$ (1)°
$V = 605.08$ (8) $Å^3$

$Z = 1$
$D_x = 1.650$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 34 reflections
$\theta = 2.1$–25.0°
$\mu = 0.80$ mm^{-1}
$T = 293$ (2) K
Block, red
0.28 × 0.16 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.857$, $T_{max} = 0.923$
3102 measured reflections

2076 independent reflections
1847 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.0°$
$h = -7 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.095$
$S = 1.07$
2076 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.2322P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.54$ e $Å^{-3}$
$\Delta\rho_{min} = -0.43$ e $Å^{-3}$

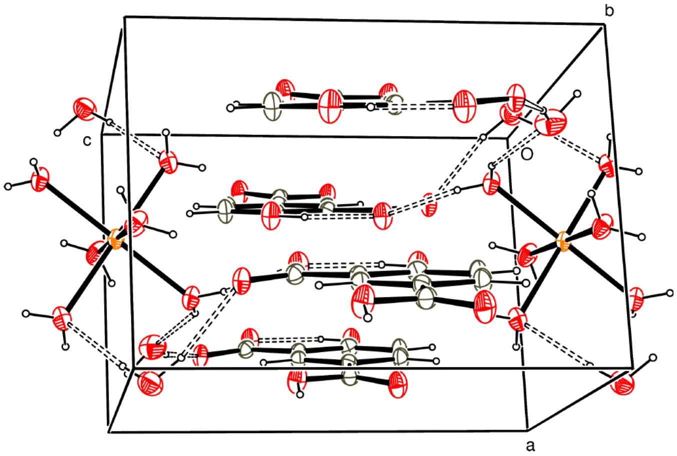


Figure 2
Packing of the title complex, showing the three-dimensional hydrogen-bonding network.

Table 1
Selected geometric parameters (Å, °).

Co—O6	2.0386 (18)	O2—C1	1.230 (3)
Co—O8	2.0873 (17)	O3—C5	1.270 (3)
Co—O7	2.1371 (18)	O4—C5	1.263 (3)
O1—C1	1.310 (3)	O5—C6	1.344 (3)
O6—Co—O8^{i}	90.38 (7)	O2—C1—O1	122.6 (2)
O6—Co—O8	89.62 (7)	O2—C1—C2	122.5 (2)
O6—Co—O7	88.04 (8)	O1—C1—C2	114.8 (2)
O6^{i}—Co—O7	91.96 (8)	O4—C5—O3	123.1 (2)
O8^{i}—Co—O7	93.09 (8)	O4—C5—C4	119.2 (2)
O8—Co—O7	86.91 (8)	O3—C5—C4	117.7 (2)

Symmetry code: (i) $1 - x, 1 - y, 2 - z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.86	2.675 (2)	173
O5—H5···O3	0.82	1.80	2.527 (2)	148
O6—H6*A*···O*W*1^{ii}	0.84 (3)	1.82 (3)	2.627 (3)	161 (3)
O6—H6*B*···O4^{iii}	0.84 (1)	1.86 (1)	2.674 (2)	164 (3)
O7—H7*A*···O5	0.84 (1)	2.10 (2)	2.886 (3)	156 (3)
O7—H7*A*···O2^{iv}	0.84 (1)	2.59 (3)	3.031 (3)	115 (3)
O7—H7*B*···O*W*2^{v}	0.81 (3)	2.05 (3)	2.847 (3)	167 (3)
O8—H8*A*···O*W*1^{v}	0.84 (1)	2.25 (2)	2.982 (3)	147 (2)
O8—H8*B*···O3^{iii}	0.84 (1)	1.92 (1)	2.744 (2)	169 (3)
O*W*2—H*W*2*A*···O7^{vi}	0.84 (3)	2.12 (3)	2.952 (3)	175 (3)
O*W*2—H*W*2*B*···O4^{vii}	0.84 (1)	2.04 (3)	2.865 (3)	167 (4)
O*W*1—H*W*1*A*···O4	0.85 (2)	1.90 (2)	2.754 (3)	174 (4)
O*W*1—H*W*1*B*···O*W*2	0.85 (3)	2.07 (3)	2.759 (3)	138 (3)

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

The H atoms were located in an electron-density difference map. The H atoms of C—H and hydroxyl O—H groups were placed in calculated positions (C—H = 0.96 Å and O—H = 0.82 Å), and were allowed to refine as riding, with displacement parameters fixed at 120% of those of their parent atoms. The H atoms of the water molecules (free and coordinated) were refined with O—H distances restrained to 0.84 (1) Å and H···H distances restrained to 1.37 (1) Å with displacement parameters fixed at 150% of the parent O atoms.

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These restraints ensure a reasonable geometry for the water molecules.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXTL*.

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