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Hexaaquacobalt(II) bis(6-hydroxypyridine-3-carboxylate)

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In the title compound, $[Co(H_2O)_6](C_6H_4NO_3)_2$, the Co^{II} atom lies on a special position of $2/m$ site symmetry in an octahedron made up of water molecules. The anions show orientational disorder over mirror planes and are linked together by a pair of N—H···O hydrogen bonds into a dianion. The complex cations and dianions are connected through O—H···O hydrogen bonds to form a three-dimensional network.

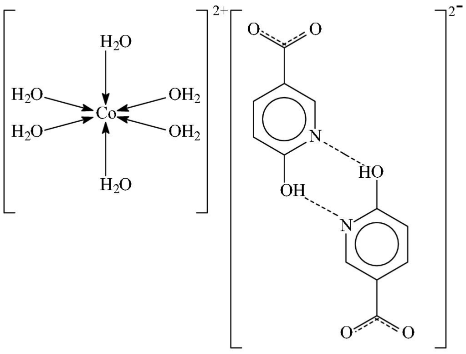
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(o–O) = 0.004 Å
Disorder in main residue
R factor = 0.054
wR factor = 0.159
Data-to-parameter ratio = 8.6

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

Comment

The title compound, (I), is isostructural with the Zn^{II} (Zhang *et al.*, 2005) and Ni^{II} analogues (Zhang & Ng, 2005).



(I)

The crystal structure of (I) consists of octahedral cations and hydrogen-bonded dianions (Fig. 1). Atom Co1 lies on a position of $2/m$ site symmetry and atom O2w also lies on the mirror plane, which bisects the O1w—Co1—O1w^{iii} bond angle

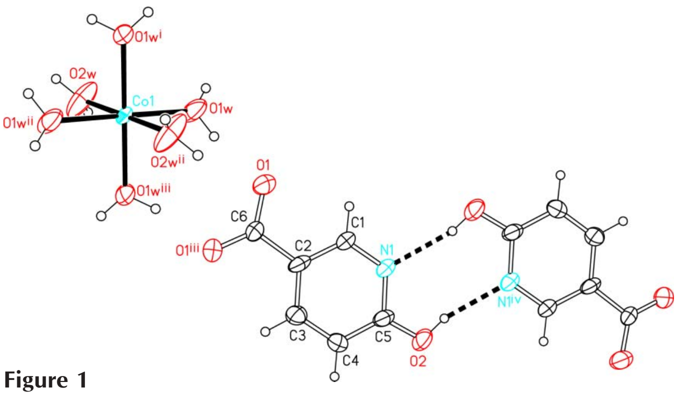


Figure 1
A plot of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Dashed lines indicate hydrogen bonds. [Symmetry codes: (i) $1-x, y, 1-z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, 1-y, z$; (iv) $\frac{5}{2}-x, \frac{3}{2}-y, 2-z$.]

[Fig. 1; symmetry code: (iii) x, $1 - y$, z]. In the anion, a crystallographic mirror plane passes through atom C6 perpendicular to the carboxylate group. As a result, the hydroxypyridyl group of the anion shows orientational disorder.

The cations and dianions of (I) are linked by hydrogen bonds (Table 2) to form a three-dimensional network.

Experimental

A mixture of cobalt(II) chloride hexahydrate (0.238 g, 1 mmol), 6-hydroxypyridyl-3-carboxylic acid (0.139 g, 1 mmol), sodium hydroxide (0.040 g, 1 mmol) and water (10 ml) were sealed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was heated to 433 K for 2 d. It was then cooled to room temperature at 10 K h^{-1} to yield red crystals of (I).

Crystal data

$[Co(H_2O)_6](C_6H_4NO_3)_2$
$M_r = 443.23$
Monoclinic, $C2/m$
$a = 11.609$ (1) Å
$b = 9.754$ (1) Å
$c = 7.6157$ (8) Å
$\beta = 91.448$ (2)°
$V = 862.1$ (2) Å^3
$Z = 2$
$D_x = 1.707$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1422 reflections
$\theta = 2.7$–27.4°
$\mu = 1.07$ mm^{-1}
$T = 295$ (2) K
Plate, red
0.34 × 0.20 × 0.08 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.499$, $T_{max} = 0.920$
2296 measured reflections
968 independent reflections
956 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.4°$
$h = -14 \rightarrow 15$
$k = -12 \rightarrow 12$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.159$
$S = 1.19$
968 reflections
113 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 7.1943P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1*w*	2.042 (3)	Co1—O2*w*	2.113 (5)
O1*w*—Co1—O2*w*	91.9 (2)		
C1—C2—C6—O1	12.0 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O1	0.85 (1)	1.83 (2)	2.659 (4)	168 (4)
O1*w*—H1*w*2···O1^{i}	0.84 (1)	1.87 (1)	2.710 (5)	171 (5)
O2*w*—H2*w*1···O2^{ii}	0.85 (1)	2.02 (3)	2.791 (8)	151 (4)
O2*w*—H2*w*1···O2^{ii}	0.85 (1)	2.02 (3)	2.791 (8)	151 (4)
O2*w*—H2*w*2···O2^{iii}	0.85 (1)	1.97 (1)	2.769 (9)	157 (2)
O2*w*—H2*w*2···O2^{iv}	0.85 (1)	1.97 (1)	2.769 (9)	157 (2)
O2—H2o···N1^{v}	0.85	2.04	2.86 (1)	159

Symmetry codes: (i) $\frac{3}{2} - x, \frac{3}{2} - y, 1 - z$; (ii) $x - 1, y, z - 1$; (iii) $2 - x, 1 - y, 1 - z$; (iv) $2 - x, y, 1 - z$; (v) $\frac{5}{2} - x, \frac{3}{2} - y, 2 - z$.

Atoms C1–C5/N1/O2 in the anion are disordered over two possible positions related by mirror symmetry; the C—C distances were restrained to 1.39 (1) Å, and the two N—C distances were restrained to within 0.01 Å of each other. Additionally, the ring was restrained to near planarity. Water H atoms were located in difference Fourier maps and were refined with a distance restraint of O—H = 0.85 (1) Å. OH groups were allowed to rotate about the C—O bond to fit the electron density, with O—H constrained to 0.85 Å and C—O—H = 109.5°. Carbon-bound H atoms were placed in calculated positions (C—H = 0.93 Å) and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: atomic coordinates taken from the isostructural Zn analogue (Zhang *et al.*, 2005); 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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