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Hexaaquacobalt(II) bis[(4-oxo-4*H*-pyridin-1-yl)acetate] dihydrate

Zhu-Yan Zhang,[a] Shan Gao,[a]* Li-Hua Huo,[a] Hui Zhao,[a] Jing-Gui Zhao[a] and Seik Weng Ng[b]

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

Correspondence e-mail:
shangao67@yahoo.com

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The title complex, $[Co(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$, was synthesized by the reaction of $Co(CH_3COO)_2\cdot 4H_2O$ and 4-oxo-4*H*-pyridine-1-acetic acid in an aqueous solution. The cobalt(II) ion, which lies on a center of symmetry, is coordinated by six water molecules to form an octahedron [Co—O = 2.077 (1)–2.084 (1) Å]. A three-dimensional supramolecular framework is formed *via* O—H···O hydrogen bonds between the anions and cations.

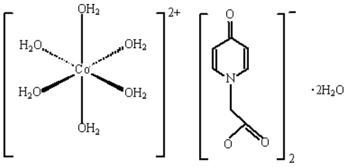
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.080
Data-to-parameter ratio = 14.7

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

Comment

(4-Oxo-4*H*-pyridin-1-yl)acetic acid is known as an important medical intermediate (Edwards *et al.*, 1977), but there is little information on the structure of its metal complexes. We have recently reported the structure of hexaaquazinc(II) bis[(4-oxo-4*H*-pyridin-1-yl)acetate] dihydrate (Gao *et al.*, 2004) and hexaaquanickel(II) bis[(4-oxo-4*H*-pyridin-1-yl)acetate] dihydrate (Zhang *et al.*, 2004). Recently, we found that (4-oxo-4*H*-pyridin-1-yl)acetic acid crystallizes as a hexaaquacobalt(II) complex, (I), under similar reaction conditions, and that it is isomorphous with the Zn^{II} and Ni^{II} analogs. Similar structural descriptions of the Zn^{II} and Ni^{II} complexes apply to the present isomorphous complex (Fig. 1).



(I)

As shown in Fig. 1, the Co^{II} atom occupies an inversion site and is coordinated by six water molecules in an octahedral geometry. The Co—O bond lengths are in the range 2.077 (1)–2.084 (1) Å (Table 1). The C3—C4, C6—C7 and C5—O3 bond lengths are 1.352 (2), 1.357 (2) and 1.274 (2) Å, respectively. The carboxylate group and the pyridone ring in the acetate anion form a dihedral angle of 77.7 (2)°. A three-dimensional supramolecular network is formed by intermolecular O—H···O hydrogen bonds between water molecules and O atoms of (4-oxo-4*H*-pyridin-1-yl)acetate (Table 2 and Fig. 2).

Experimental

The title complex was prepared by the addition of $Co(CH_3COO)_2\cdot 4H_2O$ (4.98 g, 20 mmol) to an aqueous solution of (4-oxo-4*H*-pyridin-1-yl)acetic acid (5.84 g, 40 mmol). The pH was adjusted to 7 with 0.2 *M* NaOH solution. Pink single crystals were obtained from the filtered solution over a period of several days. Analysis calculated for

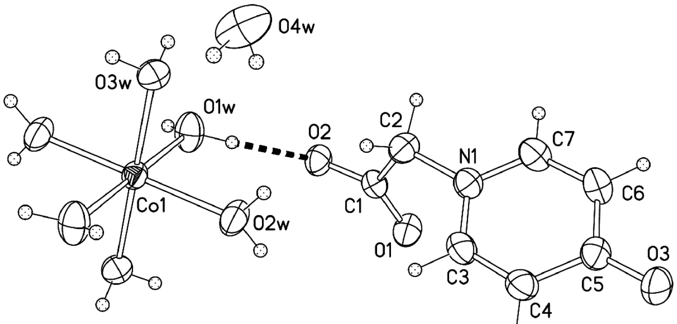


Figure 1
The components of the title compound, showing 50% probability displacement ellipsoids for the non-H atoms. The dashed line indicates a hydrogen bond.

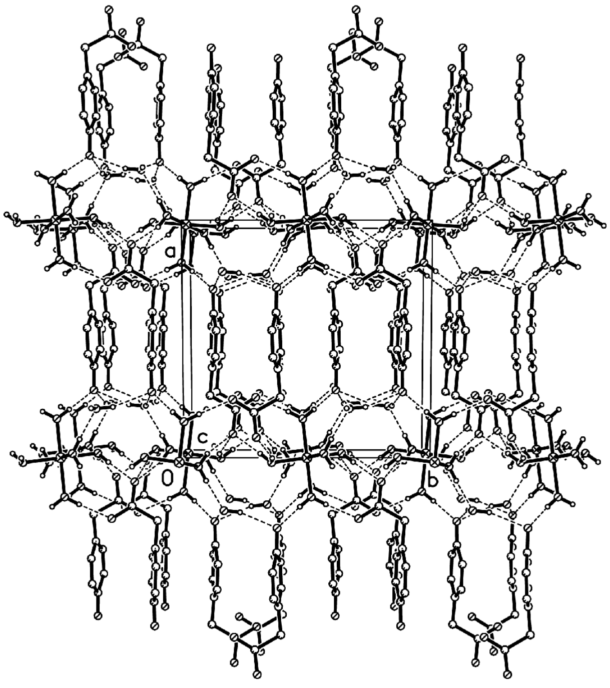


Figure 2
Packing diagram of the complex, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

$C_{14}H_{28}CoN_2O_{14}$: C 33.15, H 5.56, N 5.52%; found: C 33.00, H 5.72, N 5.37%.

Crystal data

$[Co(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$
$M_r = 507.31$
Monoclinic, $P2_1/c$
$a = 12.387$ (3) Å
$b = 12.816$ (3) Å
$c = 6.766$ (1) Å
$\beta = 98.42$ (3)°
$V = 1062.6$ (4) Å^3
$Z = 2$

$D_x = 1.586$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8329 reflections
$\theta = 3.7$–27.5°
$\mu = 0.88$ mm^{-1}
$T = 293$ (2) K
Prism, pink
0.37 × 0.26 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.736$, $T_{max} = 0.865$
10160 measured reflections

2452 independent reflections
2312 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.6°$
$h = -16 \rightarrow 15$
$k = -16 \rightarrow 16$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.080$
$S = 1.04$
2452 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.2260P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.049 (3)

Table 1
Selected geometric parameters (Å, °).

Co1—O1*W*	2.084 (1)	O2—C1	1.261 (2)
Co1—O2*W*	2.077 (1)	O3—C5	1.274 (2)
Co1—O3*W*	2.081 (1)	C3—C4	1.352 (2)
O1—C1	1.236 (2)	C6—C7	1.357 (2)
O2*W*—Co1—O1*W*	91.84 (5)	O3*W*—Co1—O1*W*	89.45 (4)
O2*W*—Co1—O1*W*^{i}	88.16 (5)	O3*W*—Co1—O1*W*^{i}	90.55 (4)
O2*W*—Co1—O3*W*	88.27 (4)	N1—C2—C1	113.9 (1)
O2*W*—Co1—O3*W*^{i}	91.74 (4)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*2···O2	0.852 (19)	1.99 (1)	2.821 (2)	164 (2)
O1*W*—H1*W*1···O4*W*^{ii}	0.845 (9)	1.87 (1)	2.709 (2)	176 (2)
O2*W*—H2*W*1···O1^{iii}	0.850 (9)	1.839 (9)	2.684 (2)	173 (2)
O2*W*—H2*W*2···O3^{iv}	0.849 (19)	1.88 (1)	2.725 (2)	170 (2)
O3*W*—H3*W*1···O2^{v}	0.859 (9)	2.06 (1)	2.832 (2)	150 (2)
O3*W*—H3*W*2···O2^{vi}	0.852 (9)	1.84 (1)	2.684 (1)	173 (2)
O4*W*—H4*W*1···O3^{vii}	0.865 (9)	1.95 (1)	2.790 (2)	162 (2)
O4*W*—H4*W*2···O3^{iv}	0.855 (9)	2.17 (1)	2.969 (2)	155 (2)

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

H atoms of the water molecules were located in difference Fourier maps and were refined subject to the restraints O—H = 0.85 (1) Å and H···H = 1.39 (1) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$. All other H atoms were placed in calculated positions [C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$] and were included in the refinement in the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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