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Tetraaquabis[(2-oxo-1,2-dihydropyridin-1-yl)-acetato-κO^2]cobalt(II)

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Key indicators

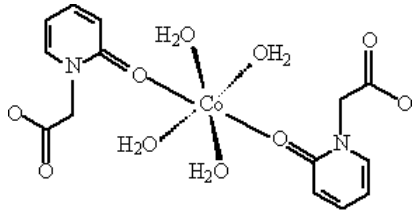
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.100
Data-to-parameter ratio = 14.9

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

The title complex, $[Co(2\text{-}OPA)_2(H_2O)_4]$ [2-OPA$^-$ = (2-oxo-1,2-dihydropyridin-1-yl)acetate, C_7H_6NO], is a neutral mononuclear compound. The Co^{II} atom, located on an inversion center, has an octahedral coordination geometry involving two carbonyl O atoms of different 2-OPA$^-$ ligands and four water molecules. A layer structure is formed *via* O—H···O intermolecular hydrogen bonds.

Comment

(2-Oxo-4*H*-pyridin-1-yl)acetic acid, 2-OPAH, known as an important medical intermediate (Klopman & Buyukbingol, 1988), is a potential multidentate ligand with versatile binding ability. However, there is little information on the structure of metal complexes formed by the 2-OPAH$^-$ ligand. Recently, we have reported the structure of $[Mg(2\text{-}OPA)_2(H_2O)_4]$ (Gao *et al.*, 2004). The cobalt(II) analog was synthesized under similar reaction conditions in this study. The structure of the Mg(II) complex has been presented in detail; a similar description applies to the present isomorphous complex.



(I)

As shown in Fig. 1, the Co(II) atom is located on an inversion center and is coordinated by two carbonyl O atoms of the 2-OPA$^-$ ligands, in a *trans* configuration, and four water molecules, resulting in octahedral coordination geometry. The

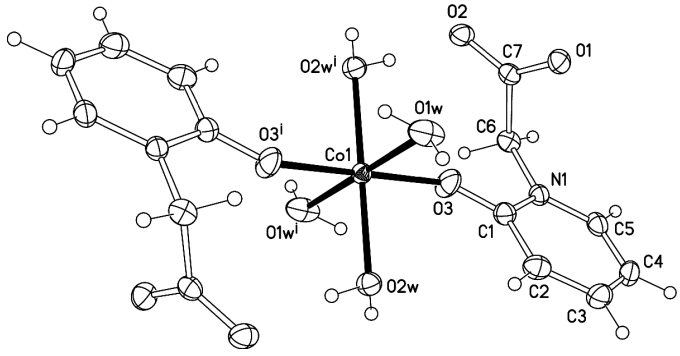


Figure 1
View of the title compound, with 30% probability ellipsoids for the non-H atoms. [Symmetry code: (i) $-x, -y, 1-z$.]

Co—$O_{carbonyl}$ and mean Co—O_{water} bond distances are 2.0364 (17) and 2.1071 (19) Å, respectively. The C1—O3 bond length is 1.250 (3) Å, which indicates unambiguously that the 2-OPA^- anion possesses a doubly bonded O1 atom connected to the ring. The carboxyl group and pyridine ring in the 2-OPA^- anion are not coplanar; the dihedral angle is 79.68 (3)°. O—H···O intermolecular hydrogen bonds are formed between the coordinated water molecules and the uncoordinated carboxylic acid groups of adjacent molecules, with hydrogen-bond lengths of 2.709 (2)–2.971 (3) Å and bond angles of 121 (3)–175 (3)°, resulting in a layer structure (Table 2, Fig. 2).

Experimental

The title complex was prepared by the addition of $Co(CH_3COO)_2{\cdot}2H_2O$ (6.28 g, 20 mmol) to an aqueous solution of (2-oxo-4*H*-pyridin-1-yl)acetic acid (5.84 g, 40 mmol). The resulting solution was stirred and the pH was adjusted to 7 with 0.2 *M* NaOH solution. After evaporation at room temperature for a week, pink single crystals were obtained from the filtered solution. CH&N analysis. Calc. for $C_{14}H_{20}CoN_2O_{10}$: C 38.63, H 4.63, N 6.44%. Found: C 38.96, H 4.89, N 5.99%.

Crystal data

$[Co(C_7H_6NO)_2(H_2O)_4]$
M_r = 435.25
Monoclinic, $P2_1/c$
a = 10.527 (2) Å
b = 7.0943 (14) Å
c = 13.007 (3) Å
β = 113.83 (3)°
V = 888.6 (4) Å^3
Z = 2
D_x = 1.627 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6681 reflections
θ = 3.3–27.5°
μ = 1.02 mm^{-1}
T = 293 (2) K
Prism, pink
0.36 × 0.25 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.709, T_{max} = 0.837
7469 measured reflections
2031 independent reflections
1776 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -9 \rightarrow 9$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.100
S = 1.06
2031 reflections
136 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.7445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °) for (I).

Co1—O1*W*	2.0694 (19)	C2—C3	1.356 (4)
Co1—O2*W*	2.1447 (17)	C4—C5	1.353 (4)
Co1—O3	2.0364 (17)	O1—C7	1.238 (3)
O3—C1	1.250 (3)	O2—C7	1.263 (3)
O3—Co1—O1*W*	90.63 (10)	O1*W*—Co1—O2*W*	90.57 (7)
O3—Co1—O1*W*^{i}	89.37 (10)	O1*W*—Co1—O2*W*^{i}	89.43 (7)
O3—Co1—O2*W*	93.73 (7)	N1—C6—C7	110.66 (19)
O3—Co1—O2*W*^{i}	86.27 (7)		

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

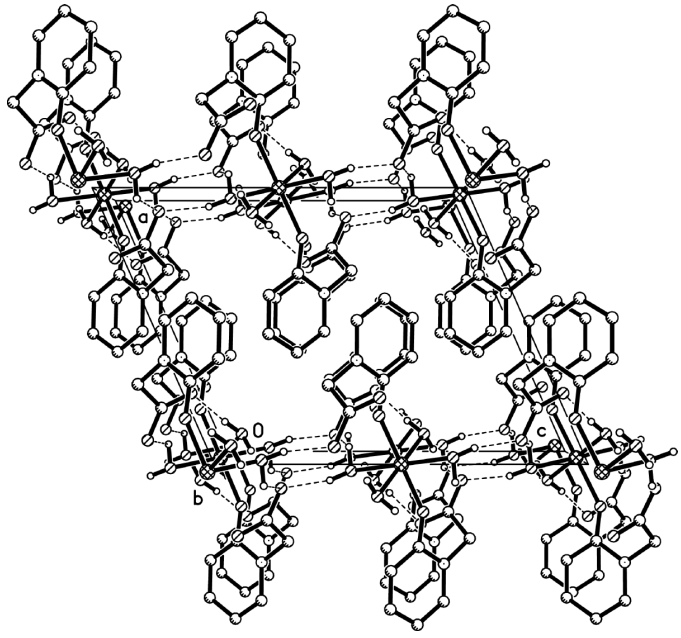


Figure 2
Packing of the complex, viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O3^i	0.86 (3)	2.35 (4)	2.887 (3)	121 (3)
O1*W*—H1*W*2···O2^{ii}	0.86 (3)	1.88 (3)	2.731 (3)	166 (3)
O2*W*—H2*W*1···O1^{iii}	0.86 (3)	1.85 (3)	2.709 (2)	175 (3)
O2*W*—H2*W*2···O2^i	0.85 (3)	2.13 (3)	2.971 (3)	172 (3)

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

The H atoms of water molecules were located in difference Fourier maps and refined isotropically, with O—H distance restrained to 0.85 (1) Å and U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were placed in calculated positions, with 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 Corporation, 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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