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Bis(8-hydroxyquinoline-2-carboxylato-κ^3N,O,O')cobalt(II) trihydrate

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The title compound, $[Co(C_{10}H_7NO_3)_2]\cdot 3H_2O$, contains six-coordinate Co^{II} with a *mer*-octahedral arrangement. The central Co atom is coordinated by the hydroxyl O atom, the quinoline N atom and a carboxylate O atom of each of the two tridentate ligands.

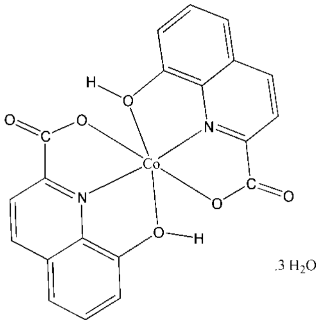
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.007 Å
R factor = 0.043
wR factor = 0.162
Data-to-parameter ratio = 14.2

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

Comment

8-Hydroxyquinoline-2-carboxylic acid (8-hydroxyquinaldic acid) is one of the tryptophan metabolites formed from xanthurenic acid (4,8-dihydroxy-quinoline-2-carboxylic acid), which causes a deficiency of vitamin B_6 (Rodwell, 1983). This metabolite is considered as a tridentate chelating agent through three functional groups, the 8-hydroxyl O, the quinoline N, and a carboxylate O atom (Irving & Pinnington, 1954; Moberg & Weber, 1984). To date, many crystal structures of metal compounds of the analogous tryptophan metabolite, quinoline-2-carboxylic acid (quinaldinic acid), have been determined, such as a vanadium(IV) complex (Okabe & Muranishi, 2002); however, little is known about the structures of the metal compounds of the 8-hydroxy-substituted quinoline-2-carboxylic acid. Investigation of the coordinating behaviour of these compounds is of interest in connection with their physiological role, as well as their use as chelating reagents for the selective recovery of metal ions (Högberg *et al.*, 1985). In this study, the structure of the title cobalt(II) complex, (I), has been determined.



(I)

The molecular structure of (I) is shown in Fig. 1. In the complex, two ligand molecules coordinate to the central Co^{II} ion in a distorted octahedral structure, with the two quinoline rings perpendicular to each other. The carboxylate groups of the ligand molecules are ionized and are essentially coplanar with the quinoline rings, as shown by relevant torsion angles [O1—C10—C1—N1 −8.7 (7)° and O4—C20—C11—N2 −3.5 (5)°]. Three ligand atoms (the hydroxyl O, the quinoline N and a carboxylate O), together with the central Co ion, form

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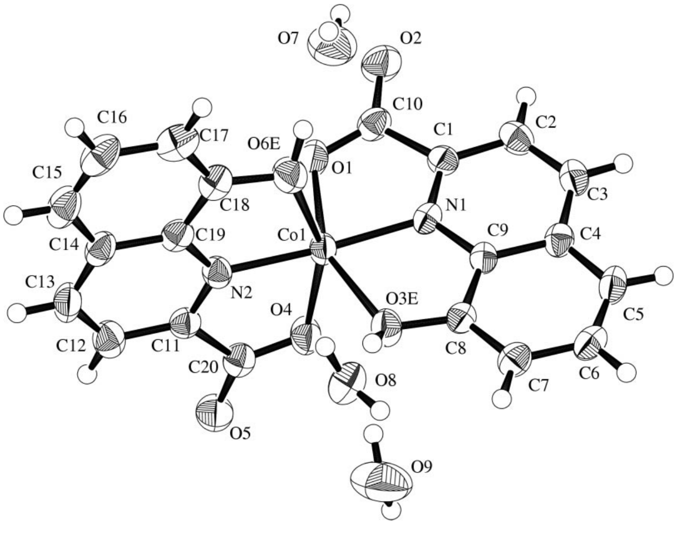

Figure 1

The title compound with the atomic numbering scheme. Ellipsoids for non-H atoms are drawn at the 50% probability level.

the five-membered chelate rings typical of metal complexes of such pyridine or quinoline compounds. The distances between Co and the carboxylate O atoms are shorter than those between Co and the hydroxyl O atoms. The Co—N distances are the shortest for the Co–ligand bonds. There are stacking interactions between neighbouring quinoline rings. The *mer*-octahedral structure with tridentate ligands revealed in this study is the first example of a metal complex of 8-hydroxyquinoline-2-carboxylic acid, although it has been indicated by the NMR study of manganese(II) complexes of 8-substituted quinoline-2-carboxylic acid derivatives (Moberg & Weber, 1984).

Experimental

Yellow prismatic crystals of (I) were obtained by slow evaporation from a 70% ethanol–water solution of a mixture of 8-hydroxyquinoline-2-carboxylic acid and cobalt(II) acetate tetrahydrate (4:1).

Crystal data

$[Co(C_{10}H_7NO_3)_2]\cdot 3H_2O$
$M_r = 489.29$
Triclinic, $P\bar{1}$
$a = 9.255$ (1) Å
$b = 15.852$ (3) Å
$c = 7.192$ (1) Å
$\alpha = 97.46$ (1)°
$\beta = 107.12$ (1)°
$\gamma = 102.03$ (1)°
$V = 965.4$ (3) Å^3

$Z = 2$
$D_x = 1.683$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 12.8$–14.6°
$\mu = 0.95$ mm^{-1}
$T = 296.2$ K
Prism, yellow
0.15 × 0.10 × 0.10 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.892$, $T_{\max} = 0.909$
4707 measured reflections
4438 independent reflections
2256 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.049$
$\theta_{\max} = 27.5°$
$h = 0 \rightarrow 12$
$k = -20 \rightarrow 20$
$l = -9 \rightarrow 8$
3 standard reflections every 150 reflections intensity decay: 0.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.162$
$S = 0.85$
4438 reflections
313 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.43$ e Å^{-3}
$\Delta\rho_{\min} = -0.43$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Co1—O1	2.122 (3)	O1—C10	1.274 (6)
Co1—O3*E*	2.226 (3)	O2—C10	1.250 (6)
Co1—O4	2.082 (4)	O3*E*—C8	1.358 (5)
Co1—O6*E*	2.285 (4)	O4—C20	1.272 (6)
Co1—N1	1.966 (4)	O5—C20	1.244 (7)
Co1—N2	1.979 (4)	O6*E*—C18	1.373 (6)
O1—Co1—O3*E*	153.9 (1)	O4—Co1—N1	105.8 (1)
O1—Co1—O4	98.1 (1)	O4—Co1—N2	79.4 (2)
O1—Co1—O6*E*	91.7 (1)	O6*E*—Co1—N1	100.4 (2)
O1—Co1—N1	77.8 (1)	O6*E*—Co1—N2	74.5 (2)
O1—Co1—N2	101.4 (1)	N1—Co1—N2	174.8 (2)
O3*E*—Co1—O4	88.8 (1)	Co1—O1—C10	113.7 (2)
O3*E*—Co1—O6*E*	93.1 (1)	Co1—O3*E*—C8	111.9 (3)
O3*E*—Co1—N1	76.0 (1)	Co1—O4—C20	113.9 (3)
O3*E*—Co1—N2	104.6 (1)	Co1—O6*E*—C18	111.6 (3)
O4—Co1—O6*E*	153.4 (1)		

All H atoms, located in difference Fourier maps, were idealized. H atoms attached to C atoms were constrained with a riding model, while O—H bonds were refined with bond-length similarity restraints and with similarity restraints for the angles at O atoms in water molecules.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation & Rigaku, 1999); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 1999); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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