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## Key indicators

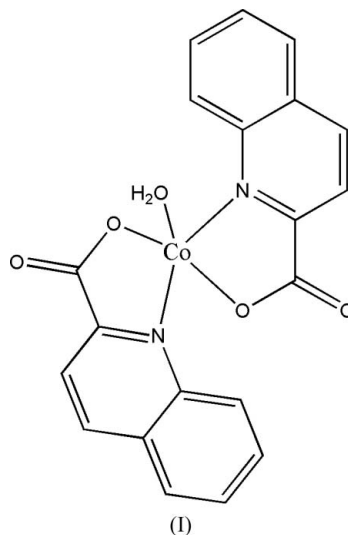
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.038  
 $wR$  factor = 0.082  
Data-to-parameter ratio = 12.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*trans*-Aquabis(quinoline-2-carboxylato- $\kappa^2\text{N,O}$ )-  
cobalt(II)

In the molecule of the title complex,  $[\text{Co}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})]$ , the five-coordinate  $\text{Co}^{\text{II}}$  ion displays a distorted square-pyramidal coordination geometry defined by the two quinoline N atoms and two O atoms of the carboxylate groups located in the basal square plane, and one water O atom in the apical position.  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds involving the water molecule form a layer parallel to the (001) plane.

Received 22 October 2006  
Accepted 1 November 2006

## Comment

Quinoline-2-carboxylate is known to be an effective chelating ligand for many transition metal ions (Martell & Smith, 1974). Some crystal structures of metal complexes of 2-quinoline-carboxylate have been reported, including  $\text{Cu}^{\text{II}}$  (Haendler, 1986),  $\text{Mn}^{\text{II}}$  (Haendler, 1996; Okabe & Koizumi, 1997),  $\text{Fe}^{\text{II}}$  (Okabe & Makino, 1998),  $\text{Co}^{\text{II}}$  (Okabe & Makino, 1999; Okabe & Muranishi, 2003) and  $\text{Ni}^{\text{II}}$  (Odoko *et al.*, 2001; Okabe & Muranishi, 2003).



The  $\text{Co}^{\text{II}}$  atom in the title complex, (I), is five-coordinate in a distorted square-pyramidal environment, with two chelating quinoline-2-carboxylate ligands coordinating through the quinoline N and the carboxylate O atoms, forming a five-membered ring in the basal plane. The apical position is occupied by a water molecule (Fig. 1).

It is interesting to note that the previous  $\text{Co}^{\text{II}}$  complexes (Okabe & Makino, 1999; Okabe & Muranishi, 2003) are hexacoordinate with two water molecules at the apices, whereas in (I) there is only one coordinated water molecule.

An interesting feature is the occurrence of hydrogen-bonding interactions which result in the formation of layers parallel to the (001) plane (Table 1 and Fig. 2). The hydrogen

bonds between the water molecule and the carbonyl O atoms form an  $R_4^2(21)$  ring (Etter *et al.*, 1990) (Fig. 2).

## Experimental

Red crystals of (I) were obtained by slow evaporation of a solution in methanol–water (1:1 *v/v*) of a mixture of quinoline-2-carboxylic acid and  $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$  (molar ratio 2:1).

### Crystal data

$[\text{Co}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})]$	$Z = 4$
$M_r = 421.26$	$D_x = 1.594 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 7.753 (1) \text{ \AA}$	$\mu = 1.01 \text{ mm}^{-1}$
$b = 7.620 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 29.940 (5) \text{ \AA}$	Block, red
$\beta = 97.05 (1)^\circ$	$0.42 \times 0.40 \times 0.20 \text{ mm}$
$V = 1755.4 (6) \text{ \AA}^3$	

### Data collection

Siemens P4 diffractometer	3275 independent reflections
$\omega$ scans	2131 reflections with $I > 2\sigma(I)$
Absorption correction: empirical	$R_{\text{int}} = 0.030$
via $\psi$ scans	$\theta_{\text{max}} = 25.5^\circ$
(North <i>et al.</i> , 1968)	3 standard reflections
$T_{\text{min}} = 0.67$ , $T_{\text{max}} = 0.82$	every 97 reflections
3947 measured reflections	intensity decay: 5.0%

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2]$
$wR(F^2) = 0.082$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.87$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3275 reflections	$\Delta\rho_{\text{max}} = 0.51 \text{ e \AA}^{-3}$
253 parameters	$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O5}-\text{H5A} \cdots \text{O4}^i$	0.83	1.80	2.613 (3)	168
$\text{O5}-\text{H5B} \cdots \text{O2}^{ii}$	0.82	1.82	2.640 (3)	178

Symmetry codes: (i)  $x, y + 1, z$ ; (ii)  $x - 1, y, z$ .

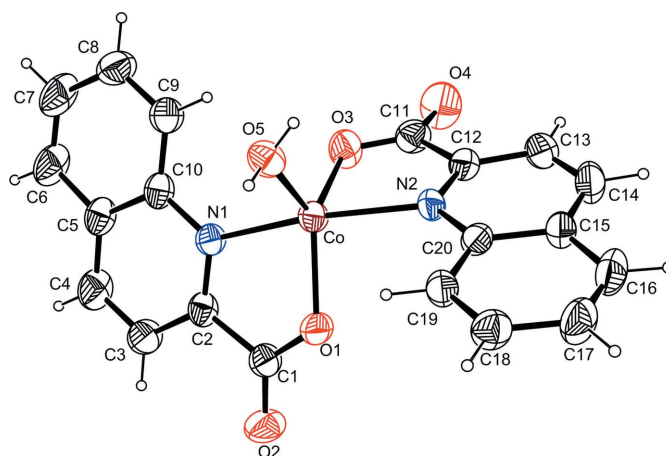
All H atoms attached to C atoms were positioned geometrically and refined as riding, with  $C-H = 0.93 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . Water H atoms were located in difference Fourier maps and then treated as riding on the parent O atom, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

Data collection: XSCANS (Siemens, 1994); cell refinement: XSCANS; data reduction: SHELXTL (Sheldrick, 1997b); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: ORTEPIII (Burnett & Johnson, 1996), ORTEP-3 for Windows (Farrugia, 1997) and MERCURY (Macrae *et al.*, 2006); software used to prepare material for publication: SHELXL97.

We thank the Open Fund (No. hnfc2006005) of Hainan Provincial Key Laboratory of Fine Chemicals for financial support.

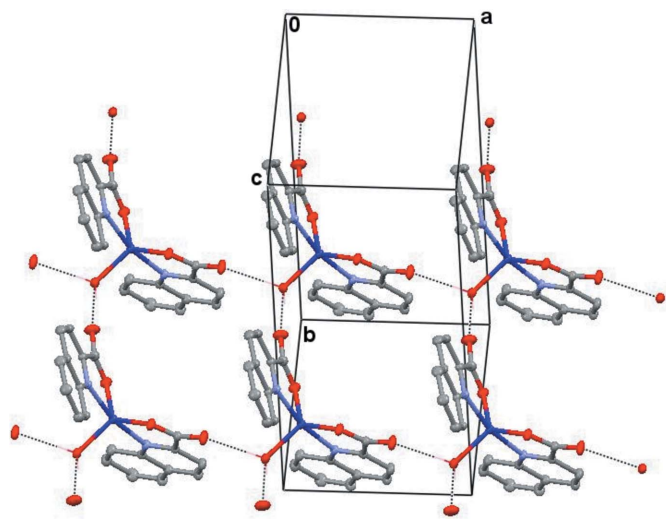
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**Figure 1**

The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.



**Figure 2**

Partial packing view of the title complex, showing the hydrogen-bond interactions and the formation of  $R_4^2(21)$  rings and layers parallel to the (001) plane. H atoms not involved in hydrogen bonding have been omitted for clarity. Hydrogen bonds are represented as dashed lines.

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