

Guang-Bo Che,* Chun-Bo Liu,
Yun-Cheng Cui and Chuan-Bi LiDepartment of Chemistry, Jilin Normal
University, Siping 136000, People's Republic of
ChinaCorrespondence e-mail:
guangbochejl@yahoo.com

Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.036
 wR factor = 0.089
Data-to-parameter ratio = 12.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*trans*-Dimethanolbis(quinoline-8-carboxylato- $\kappa^2\text{N,O}$)-
cobalt(II)

The title complex, $[\text{Co}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{CH}_4\text{O})_2]$, is a neutral mononuclear complex containing a Co^{II} ion in a six-coordinate environment. The Co^{II} center, located on a crystallographic center of symmetry, displays a slightly distorted octahedral geometry, with two quinoline-8-carboxylate and two methanol ligands in *trans* configurations. The complex molecules are linked together by $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds between methanol molecules and carboxylate groups to form a three-dimensional framework.

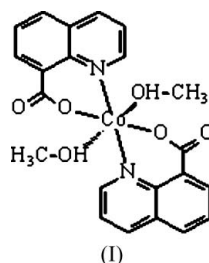
Received 16 September 2005

Accepted 30 September 2005

Online 8 October 2005

Comment

Quinoline-8-carboxylic acid is known to be a potent chelator of transition metal and lanthanide ions. Its metal complexes have been investigated for a long time, with regard to their preparation (Seminara & Musumeci, 1977; Gomez Beltran & Alfaro Lozano, 1974), antitumor activity (Lumme *et al.*, 1984), electrochemical properties (Park *et al.*, 2000), and so on. However, reports on the crystal structures of complexes with quinoline-8-carboxylate are rare (Kuang *et al.*, 2002). Here we report the crystal structure of a quinoline-8-carboxylato-cobalt(II) complex, (I).



As shown in Fig. 1, the molecule of (I) is centrosymmetric. The Co^{II} atom occupies the center of a slightly distorted octahedron. The two quinoline-8-carboxylate ligands chelate the Co^{II} ion through the N and one O atom to form the equatorial plane, and two methanol molecules complete the octahedron at the axial positions. The quinoline-8-carboxylate ligand and the Co^{II} atom form a six-membered chelate ring, which is almost coplanar with the quinoline ring [the dihedral angle is $3.2(1)^\circ$]. The $\text{Co1}-\text{O3}$ distance is slightly longer than the $\text{Co1}-\text{O1}$ distance (Table 1). The carboxyl group of the quinolinecarboxylate ligand is ionized and almost coplanar with the plane defined by the aromatic system [the dihedral angle is $9.8(2)^\circ$].

In the crystal structure, the complex molecules are linked through $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions between the uncoordinated carboxyl O atoms and the hydroxyl H atoms of methanol molecules, and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) to form a three-dimensional framework.

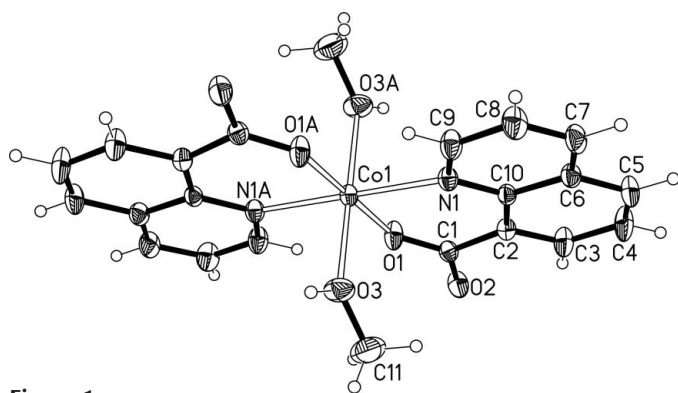


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Atoms labelled with the suffix A are at the symmetry position $(1 - x, -y, -z)$.

Experimental

A solution of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (59.0 mg, 0.2 mmol) in MeOH (10 ml) was added to a solution of quinoline-8-carboxylic acid (69.3 mg, 0.4 mmol) in MeOH (30 ml) in the presence Et_3N . The resulting solution was filtered and left to stand at room temperature. Single crystals suitable for X-ray analysis were obtained after 14 d.

Crystal data

$[\text{Co}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{CH}_4\text{O})_2]$	$D_x = 1.554 \text{ Mg m}^{-3}$
$M_r = 467.33$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 742 reflections
$a = 9.912 (1) \text{ \AA}$	$\theta = 2.3\text{--}28.5^\circ$
$b = 8.740 (2) \text{ \AA}$	$\mu = 0.90 \text{ mm}^{-1}$
$c = 11.689 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 99.51 (3)^\circ$	Block, pink
$V = 998.7 (4) \text{ \AA}^3$	$0.20 \times 0.18 \times 0.18 \text{ mm}$
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	1822 independent reflections
φ and ω scans	1584 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$R_{\text{int}} = 0.032$
$T_{\text{min}} = 0.835$, $T_{\text{max}} = 0.894$	$\theta_{\text{max}} = 25.5^\circ$
6016 measured reflections	$h = -9 \rightarrow 12$
	$k = -10 \rightarrow 10$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.5484P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.089$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
1822 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
142 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Co1—O1	1.9898 (16)	O1—C1	1.255 (3)
Co1—O3	2.1278 (17)	O2—C1	1.242 (3)
Co1—N1	2.1699 (18)	O3—C11	1.381 (3)
O1 ⁱ —Co1—O1	180	O3—Co1—N1	91.52 (7)
O1—Co1—O3 ⁱ	88.59 (8)	O1—Co1—N1 ⁱ	93.58 (7)
O1—Co1—O3	91.41 (8)	O3—Co1—N1 ⁱ	88.48 (7)
O1—Co1—N1	86.42 (7)	N1—Co1—N1 ⁱ	180

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

Table 2

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

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O3—H3B \cdots O2 ⁱⁱ	0.93	1.75	2.645 (3)	160
C5—H5A \cdots O2 ⁱⁱⁱ	0.93	2.57	3.425 (3)	153
C9—H9A \cdots O1 ⁱ	0.93	2.28	2.953 (3)	129

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

H atoms were placed in idealized positions ($\text{O—H} = 0.93 \text{ \AA}$ and $\text{C—H} = 0.93$ or 0.96 \AA) and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{carrier})$ for methyl and hydroxyl H atoms and $1.2U_{\text{eq}}(\text{C})$ for others.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SHELXTL (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97; molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

The authors thank Jilin Normal University for supporting this work.

References

- Bruker (1998). SMART (Version 5.051), SAINT (Version 5.01), SADABS (Version 2.03) and SHELXTL (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
- Gomez Beltran, F. & Alfaro Lozano, T. (1974). *Rev. Acad. Cienc. Exactas Fis. Quim. Nat.* **29**, 229–240.
- Kuang, S.-M., Fanwick, P. E. & Walton, R. A. (2002). *Inorg. Chim. Acta*, **338**, 219–227.
- Lumme, P., Elo, H. & Janne, J. (1984). *Inorg. Chim. Acta*, **92**, 241–251.
- Park, J. Y., Choi, D. S., Kim, Y. K. & Ha, Y. (2000). *J. Korean Chem. Soc.* **44**, 243–248.
- Seminara, A. & Musumeci, A. (1977). *J. Inorg. Nucl. Chem.* **39**, 599–605.
- Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.