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Diaquabis(pyridine-2,5-dicarboxylato)cobalt(II)

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The title mononuclear complex, $[Co(C_7H_4NO_4)_2(H_2O)_2]$, is a stereoisomer of a structure reported earlier [Liang *et al.* (2001). *Acta Cryst*. E**57**, m382–m383]. The centrosymmetric molecule crystallizes in the triclinic space group $P\overline{1}$.

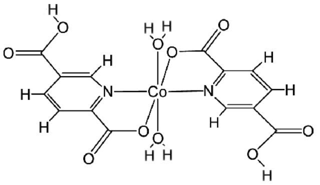
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.124
Data-to-parameter ratio = 10.0

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

Comment

The study of cobalt coordination complexes is especially interesting as these compounds exhibit special magnetic properties, due to strong orbital contributions to the magnetic moments (Liu *et al.*, 2003; Tong *et al.*, 2004; Palii *et al.*, 2003). In our work on the preparation of cobalt complexes, a mononuclear compound, (I), was obtained, and its synthesis and structure are reported here.



(I)

The crystallographic analysis of (I) reveals that the compound is centrosymmetric, and that each cobalt ion is hexacoordinated in an N_2O_4 environment. The complex exhibits regular octahedral geometry in which the two chelating rings of the ligand are coplanar, and the N—Co—N angle of 180°. However, the stereoisomer (Liang *et al.*, 2001) has a slightly distorted octahedral geometry with an N—Co—N angle of 160.3°, and the two chelating rings are nearly perpendicular to each other. Selected bond lengths and angles of (I) are listed in Table 1.

The crystal structure involves O—H···O hydrogen bonds, leading to the formation of a three-dimensional network structure, as shown in Fig. 2.

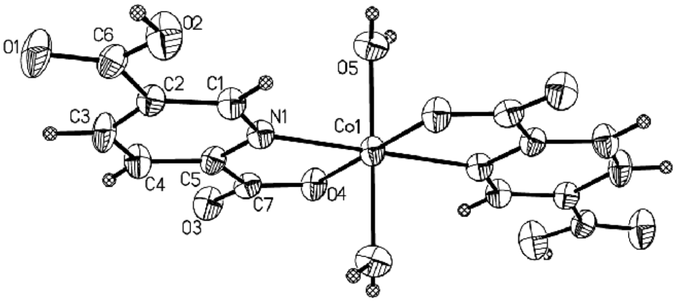


Figure 1
The structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level.

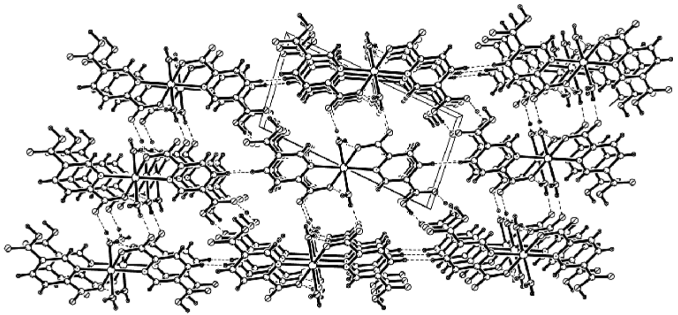


Figure 2
The three-dimensional packing of the complex. Dashed lines indicate the hydrogen bonds.

Experimental

The complex was prepared by the hydrothermal reaction of cobalt powder (0.012 g, 0.2 mmol) and H_2pydc (0.033 g, 0,2 mmol; pydc is pyridine-2,5-dicarboxylate) in water (14 ml) at pH 1. After heating at 433 K for 3 d and cooling to room temperature at 13 K h^{-1}, two types of crystals were obtained. Pale-yellow crystals correspond to the structure reported here, whereas the golden-red crystals are the stereoisomer already documented (Liang *et al.*, 2001).

Crystal data

$[Co(C_7H_4NO_4)_2(H_2O)_2]$
$M_r = 427.19$
Triclinic, $P\overline{1}$
$a = 5.0699$ (1) Å
$b = 6.6184$ (1) Å
$c = 12.3638$ (7) Å
$\alpha = 94.71$ (3)°
$\beta = 98.50$ (3)°
$\gamma = 110.185$ (16)°
$V = 381.12$ (4) Å^3

$Z = 1$
$D_x = 1.861$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 792 reflections
$\theta = 1.7$–25.0°
$\mu = 1.19$ mm^{-1}
$T = 293$ (2) K
Plate, pale yellow
0.20 × 0.10 × 0.03 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
$T_{min} = 0.764$, $T_{max} = 0.960$
2356 measured reflections

1319 independent reflections
1152 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$
$h = -4 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.124$
$S = 1.20$
1319 reflections
132 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O4	2.074 (2)	N1—C5	1.346 (5)
O4—C7	1.266 (5)	C5—C7	1.521 (5)
O4—Co1—O4^{i}	180	O5—Co1—N1^{i}	91.41 (13)
O4—Co1—O5^{i}	89.55 (12)	O4—Co1—N1	78.83 (11)
O4—Co1—O5	90.45 (12)	O5—Co1—N1	88.59 (13)
O5^{i}—Co1—O5	180	N1^{i}—Co1—N1	180
O4—Co1—N1^{i}	101.17 (11)		

Symmetry code: (i) $1 - x, 2 - y, 1 - z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.82	2.643 (4)	177
O5—H51···O3^{ii}	0.78 (5)	1.93 (5)	2.688 (4)	165 (5)
O5—H52···O4^{iii}	0.78 (5)	1.96 (5)	2.712 (4)	160 (5)

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

The organic H atoms were positioned geometrically, with C—H = 0.93 Å and O—H = 0.82 Å, and were constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}$(parent atom). The aqua H atoms were located in difference Fourier maps, and refined with O—H distances restrained at 0.78 (5) Å and isotropic displacement parameters.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

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