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

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A mononuclear cobalt(II) coordination complex, [Co(Hpydc)$_2$(H$_2$O)$_2$] (pydc = 2,5-pyridinedicarboxylate, $C_7H_4NO_4$), has been prepared from the hydrothermal reaction of Co(CH$_3$COO)$_2$·4H$_2$O and H$_2$pydc in water. Cobalt(II) is coordinated by four O atoms, two from pydc ligand, two from water molecules, and two N atoms from the pydc ligands, to form a slightly distorted octahedral geometry. The Co–O and Co–N distances range from 2.055 (2) to 2.169 (2) Å. The discrete structure is further extended to form a three-dimensional structure involving weak hydrogen bonds.

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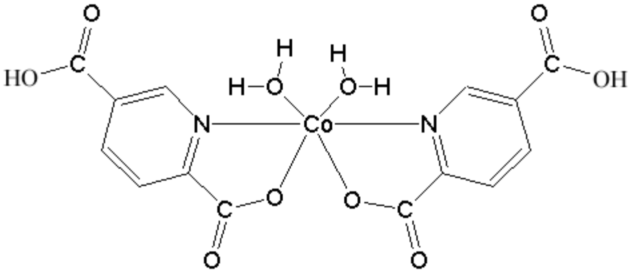
Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.078
Data-to-parameter ratio = 10.7

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

Comment

Research into transition metal complexes has been rapidly expanding because of their fascinating structural diversity and potential applications as functional materials and enzymes (Li *et al.*, 1998, 1999). The selection of a suitable ligand is essential in the design of transition metal complexes. Although some complexes containing the pyridine-2,5-dicarboxylic acid ligand have been reported (Plater *et al.*, 1998), we still chose it as the ligand. It reacts with transition metals or rare earths; a series of novel complexes having infinite or discrete structures has been obtained and reported (Liang *et al.*, 2000*a*,*b*, 2001). We report here the synthesis and crystal structure of the mononuclear cobalt(II) compound [Co(Hpydc)$_2$(H$_2$O)$_2$] (pydc = pyridine-2,5-dicarboxylate), (I).



(I)

The coordination complex (I) was prepared by the hydrothermal reaction of Co(CH$_3$COO)$_2$·4(H$_2$O) and H$_2$pydc in H$_2$O. The crystallographic analysis reveals that the compound is a discrete molecule [Co(Hpydc)$_2$(H$_2$O)$_2$], in which each Co^{II} atom is coordinated by two N and two O atoms of the two Hpydc ligands to form two five-membered chelating rings, and further coordinated by two water molecules to produce a slightly distorted octahedral geometry, as shown in Fig. 1. The

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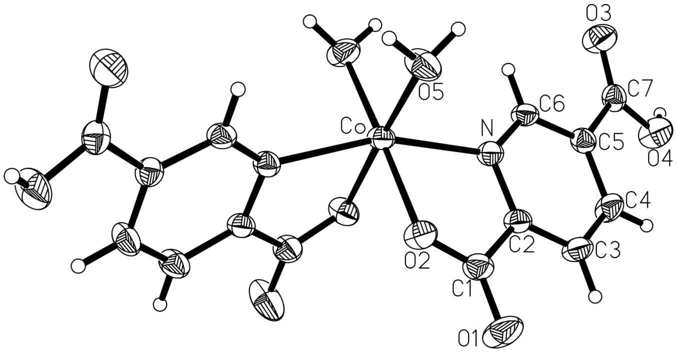

Figure 1
The structure of $[Co(Hpydc)_2(H_2O)_2]$. Displacement ellipsoids are plotted at the 50% probability level.

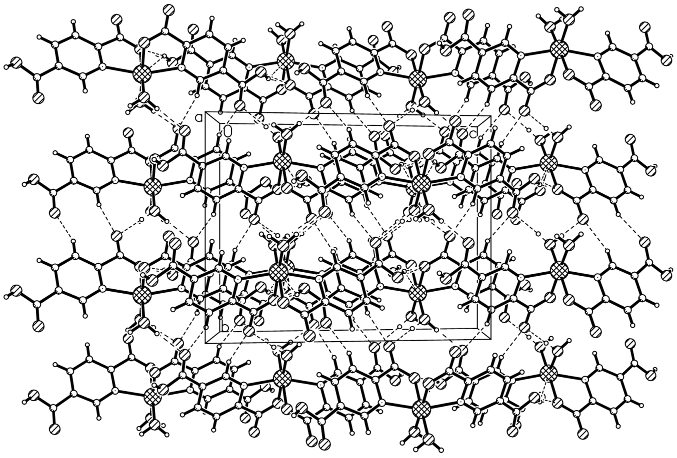

Figure 2
Packing diagram of $[Co(Hpydc)_2(H_2O)_2]$. Dashed lines indicate the hydrogen bonds.

distances and angles around Co are listed in Table 1. The hydrogen bond interactions, having an average O$\cdots$O distance of 2.749 (3) Å, lead to the formation of a three-dimensional network structure, as shown in Fig. 2.

Experimental

A mixture of $Co(CH_3COO)_2 \cdot 4(H_2O)$ (0.225 g), $[H_2pydc] \cdot H_2O$ (0.237 g) and H_2O (15 ml) was sealed in a 25 ml stainless-steel reactor with Teflon liner. The reaction system was heated at 443 K for 72 h. Slow cooling of the system to room temperature yielded orange block-shaped crystals of the complex, which were collected by filtration.

Crystal data

$[Co(C_7H_4NO_4)_2(H_2O)_2]$
$M_r = 427.19$
Monoclinic, $C2/c$
$a = 8.623$ (5) Å
$b = 12.091$ (4) Å
$c = 15.436$ (7) Å
$\beta = 100.59$ (4)°
$V = 1582.0$ (12) Å^3
$Z = 4$

$D_x = 1.794$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 40 reflections
$\theta = 4.3$–20.6°
$\mu = 1.15$ mm^{-1}
$T = 293$ (2) K
Block, orange
0.28 × 0.06 × 0.06 mm

Data collection

SMART CCD diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.723$, $T_{max} = 0.933$
4031 measured reflections
1386 independent reflections

1243 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 10$
$k = -14 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.078$
$S = 1.09$
1386 reflections
130 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 1.4634P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O5	2.0547 (18)	O2—O4^{ii}	2.605 (3)
Co—O2	2.0899 (17)	O2—O5	2.941 (2)
Co—N	2.169 (2)	O3—O5^{iii}	2.802 (3)
O1—O5^{i}	2.649 (2)		
O5^{iv}—Co—O5	93.12 (12)	O2^{iv}—Co—N	87.46 (7)
O5^{iv}—Co—O2	176.44 (7)	O5^{iv}—Co—N^{iv}	92.35 (8)
O5—Co—O2	90.41 (8)	N—Co—N^{iv}	160.30 (10)
O2—Co—O2^{iv}	86.08 (10)	C6—N—Co	131.59 (15)
O5^{iv}—Co—N	101.21 (7)	C2—N—Co	110.27 (14)
O5—Co—N	92.35 (7)	C1—O2—Co	115.50 (14)
O2—Co—N	78.12 (7)		

Symmetry codes: (i) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $\frac{1}{2}+x, \frac{3}{2}-y, z-\frac{1}{2}$; (iii) $-x, 1-y, 1-z$; (iv) $-x, y, \frac{1}{2}-z$.

The organic H atoms were positioned geometrically (C—H bond fixed at 0.96 Å), and allowed to ride on their parent C atoms before the final cycle of refinement. The aqua H atoms were located from difference maps, the O—H distance fixed at 0.94 Å and refined using isotropic displacement parameters.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *XPREP* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97.

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