Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

trans-Diaquabis(pyridine-4-carboxylato)cobalt(II) dihydrate

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Received 28 November 2003
Accepted 15 December 2003
Online 24 December 2003

Key indicators

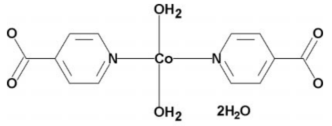
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.114
Data-to-parameter ratio = 9.9

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

By the hydrothermal method, a four-coordinate monomeric Co^{II} complex with two isonicotinate ($C_6H_4NO_2$) ligands, $[Co(L)_2(H_2O)_2]\cdot 2H_2O$, where H*L* is isonicotinic acid, has been synthesized; it has been characterized by elemental analysis and X-ray diffraction techniques. The crystal structure reveals that the Co^{II} atom, on an inversion center, has a CoN_2O_2 square-planar primary coordination environment and weak axial interactions with two more water molecules. Isonicotinate is bonded through nitrogen. A striking structural feature is the formation of a three-dimensional supramolecular architecture through intermolecular O—H···O hydrogen bonds.

Comment

The synthesis and design of supramolecular compounds with special geometric and topological character have attracted much attention in recent decades, because they display recognition, transformation and self-assembly (Zhu *et al.*, 2001; Braga, 2000). Among the various non-covalent interactions, hydrogen bonds are especially important, because they best combine both moderate strength and directionality (Aakeröy & Seddon, 1993). For this reason, we have synthesized and characterized the compound $[Co(L)_2(H_2O)_2](H_2O)_2$, (I), where H*L* = isonicotinic acid.



(I)

X-ray structure analysis reveals that (I) is a monomeric Co^{II} complex (Fig. 1). The coordination geometry around the Co^{II} atom, which lies on an inversion center, is square planar, with Co—O and Co—N distances of 1.989 (3) and 2.008 (3) Å, respectively. Square-planar coordination of Co^{II} is rather unusual, the geometry usually being tetrahedral. By contrast

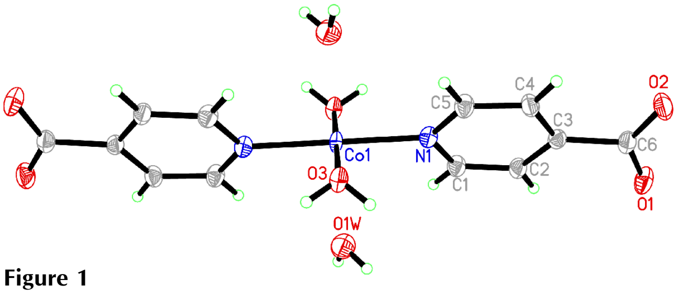


Figure 1
View of the title compound, with displacement ellipsoids drawn at the 30% probability level.

with the previously reported six-coordinate *trans*-tetraaquabis(pyridine-4-carboxylato)cobalt(II) (Jia *et al.*, 2002; Waizumi *et al.*, 1998), an uncoordinated water molecule is included in the asymmetric unit of complex (I); this, and its centrosymmetrically related partner, lie in axial sites 2.454 (2) Å from the Co^{II} atom, representing only weak interactions.

A striking structural feature of (I) is the formation of a three-dimensional supramolecular architecture through intermolecular O—H···O hydrogen-bonding interactions (Table 2).

Experimental

The title complex was prepared by reacting a 15 ml aqueous solution of cobalt(II) nitrate with pyridine-4-carboxylic acid in a 1:2 ratio. NaOH was added to this solution to give a pH of 6.5, and it was stirred at room temperature for 5 h until a homogeneous solution was obtained. Then it was sealed in a 20 ml acid digestion bomb at 413 K for 3 d. Red block-shaped crystals were recovered by filtration and dried in air. The yield was *ca* 58% (based on Co). Analysis calculated for $C_{12}H_{12}CoN_2O_6.2H_2O$: C 38.40, H 4.30, N, 7.47%; found: C 38.85, H 4.55, N 7.23%.

Crystal data

$[Co(C_6H_4NO_2)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 375.20$
Triclinic, $P\overline{1}$
$a = 6.3367$ (8) Å
$b = 6.8936$ (9) Å
$c = 9.1801$ (12) Å
$\alpha = 99.396$ (2)°
$\beta = 105.286$ (2)°
$\gamma = 108.178$ (2)°
$V = 354.09$ (8) Å^3
$Z = 1$
$D_x = 1.760$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 642 reflections
$\theta = 3.2$–23.0°
$\mu = 1.26$ mm^{-1}
$T = 293$ (2) K
Block, red
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.711$, $T_{max} = 0.777$
1810 measured reflections
1217 independent reflections
1118 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.1°$
$h = -7 \rightarrow 7$
$k = -5 \rightarrow 8$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.114$
$S = 1.07$
1217 reflections
123 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.5683P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.122 (14)

Table 1
Selected geometric parameters (Å, °).

Co1—O3	1.989 (3)	Co1—N1	2.008 (3)
O3—Co1—N1	90.22 (12)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2^{i}	0.825 (11)	1.914 (16)	2.730 (4)	169 (6)
O3—H3*B*···O1^{ii}	0.827 (10)	1.804 (16)	2.621 (4)	169 (6)
O1*W*—H1*WA*···O1^{iii}	0.825 (11)	2.014 (17)	2.828 (5)	169 (6)
O1*W*—H1*WB*···O2^{ii}	0.824 (10)	2.141 (18)	2.957 (5)	171 (8)

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

C-bound H atoms were placed at calculated positions and allowed to ride on their parent atoms [C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C)]. H atoms of the water molecules were located in a difference map and were refined isotropically, with O—H distances restrained to 0.82 (1) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

ZQY gratefully acknowledges the financial support of the Science Foundation of Hennan State Education Commission in China (No. 97150016).

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