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Tris(pyridine-2-carboxylato-κ^2O,N)cobalt(III) monohydrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.050
wR factor = 0.066
Data-to-parameter ratio = 11.4

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

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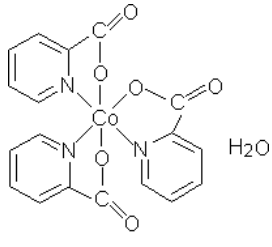
In the title complex, $[Co(C_6H_4O_2N)_3]\cdot H_2O$, the cobalt(III) ion shows a distorted octahedral coordination, comprising three N-atom donors and three O-atom donors from three bidentate pyridine-2-carboxylate ligands. The uncoordinated water molecule interacts with nearby carboxyl groups of the pyridine-2-carboxylate ligands by way of O—H···O hydrogen bonds.

Comment

In the title compound, (I), the cobalt(III) atom shows a distorted octahedral coordination, comprising three N-atom donors and three O-atom donors from three bidenate pyridine-2-carboxylato ligands, as shown in Fig. 1. If the coordinating atoms are considered in isolation, this represents a meridional CoO_3N_3 geometric isomer. The *cis* bond angles in the Co1 octahedron span the range 80.27 (11)–99.48 (11)°. The mean Co—O bond length of 1.876 (2) Å is shorter than the mean Co—N bond length of 1.911 (3) Å (Table 1). In (I), each pyridine-2-carboxylate ligand coordinates to the Co^{III} atom *via* an O atom and an N atom, thus forming five-membered chelate rings, denoted *R*1, *R*2 and *R*3, containing atoms N1, N2 and N3, respectively. The pyridine rings, denoted py1, py2 and py3 containing atoms N1, N2, and N3, respectively, are approximately parallel to their respective chelate-ring planes [dihedral angles = 1.51 (18), 2.13 (16) and 1.60 (4)° for *R*1/py1, *R*2/py2 and *R*3/py3, respectively]. The dihedral angles between pairs of pyridine rings are 80.54 (10), 85.27 (12) and 85.04 (13)° for py1/py2, py1/py3, and py2/py3, respectively.



(I)

The uncoordinated water molecule in (I) forms O—H···O hydrogen bonds (Table 2) to nearby carboxyl O atoms, resulting in an infinite chain along the *a* direction.

Experimental

$CoCl_2\cdot 6H_2O$ (0.5 mmol) was dissolved in distilled water (10 ml), to which an aqueous mixture (20 ml) of pyridine-2-carboxylic acid (1.5 mmol) and NaOH (1.5 mmol) was added dropwise at 333 K. The

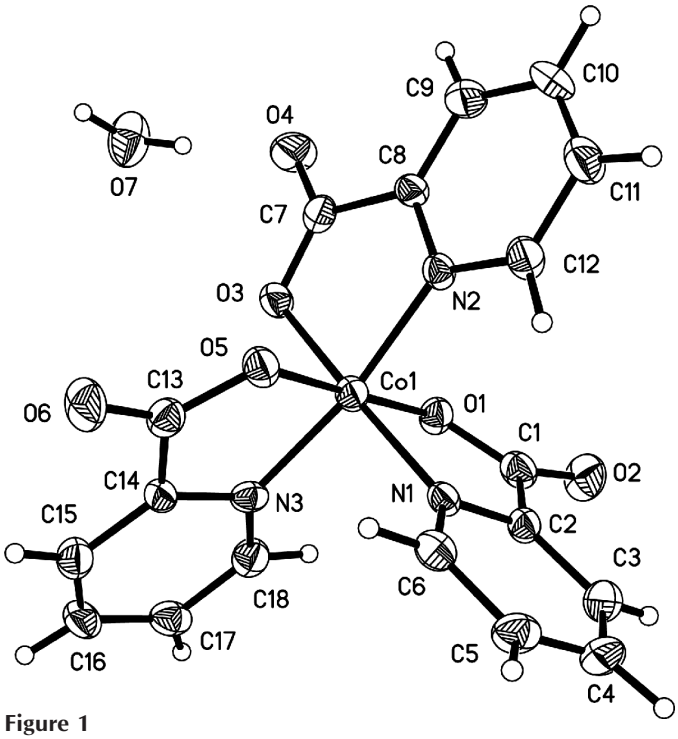


Figure 1
View of (I), showing 50% probability displacement ellipsoids and arbitrary spheres for H atoms.

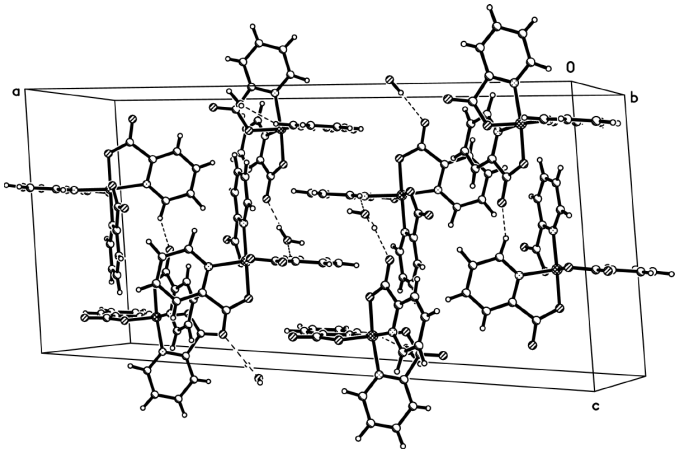


Figure 2
The crystal packing of (I), showing the hydrogen-bond interactions as dashed lines.

mixture was stirred for 6 h and part of the solvent was removed using a rotary vacuum evaporator. The resulting solution was filtered and left in air for 20 d, during which time dark-red prisms of (I) formed. Elemental analysis found: C 48.59, H 3.07, N 9.33; calculated for $C_{18}H_{14}CoN_3O_7$: C 48.78, H 3.18, N 9.48%.

Crystal data

$[Co(C_6H_4NO_2)_3]\cdot H_2O$
M_r = 443.25
Monoclinic, $C2/c$
a = 29.654 (18) Å
b = 8.530 (5) Å
c = 13.801 (8) Å
β = 95.829 (10)°
V = 3473 (4) Å^3
Z = 8
D_x = 1.696 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1193 reflections
θ = 2.5–20.3°
μ = 1.04 mm^{-1}
T = 298 (2) K
Prism, dark red
0.28 × 0.25 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.760, T_{max} = 0.835
9671 measured reflections
3589 independent reflections
2020 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 26.5°
$h = -25 \rightarrow 37$
$k = -10 \rightarrow 10$
$l = -14 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.066
S = 0.95
3589 reflections
315 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.873 (2)	Co1—N3	1.900 (3)
Co1—O5	1.877 (2)	Co1—N2	1.914 (3)
Co1—O3	1.881 (2)	Co1—N1	1.917 (3)
O1—Co1—O5	178.85 (11)	O3—Co1—N2	84.91 (11)
O1—Co1—O3	88.14 (10)	N3—Co1—N2	170.93 (11)
O5—Co1—O3	91.99 (10)	O1—Co1—N1	84.86 (11)
O1—Co1—N3	96.90 (13)	O5—Co1—N1	95.01 (11)
O5—Co1—N3	84.25 (13)	O3—Co1—N1	172.98 (12)
O3—Co1—N3	88.04 (10)	N3—Co1—N1	92.28 (11)
O1—Co1—N2	88.59 (12)	N2—Co1—N1	95.41 (11)
O5—Co1—N2	90.28 (12)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H14···O5^{i}	0.886 (10)	2.012 (15)	2.864 (4)	161 (3)
O7—H13···O4	0.887 (10)	1.966 (12)	2.845 (4)	171 (3)

Symmetry code: (i) $x, -y, z - \frac{1}{2}$.

After the H atoms were located in a difference map, the water O—H distances were restrained to 0.88 (1) Å and their U_{iso}(H) values were allowed to refine freely. All the other H atoms, except H12 (positioned geometrically), were located in difference maps and restrained in their as-found relative positions ±0.01 Å and their U_{iso}(H) values were allowed to refine freely.

Data collection: *SMART* (Bruker, 1997); cell refinement and data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics and preparation of publication material: *SHELXTL* (Sheldrick, 1997*b*).

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