# Poly[di-*μ*-nicotinato-cobalt(II)]

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The title compound, $[Co(C_6H_4NO_2)_2]_n$, contains chiral two-dimensional layers assembled from Co^{2+} cations and nicotinate anions. The Co^{2+} cations lie on twofold rotation axes and are coordinated by two N atoms and two carboxylate groups. Each nicotinate anion links two Co^{2+} cations.

Comment

To date, research on metal–organic frameworks (MOFs) has mostly focused on coordination polymers with rigid organic ligands containing either N- or O-atom donors. Nicotinic acid is one such ligand. A relatively large number of MOF structures containing nicotinate anions have been reported, including copper nicotinates (Chapman *et al.*, 2001; Yu *et al.*, 2002; Kang *et al.*, 2004; Lu & Babb, 2003) and rare-earth nicotinates (Zhang *et al.*, 2005). One cobalt nicotinate MOF has been reported previously (Yeh *et al.*, 2004), which contains chiral two-dimensional layers of stoichiometry $[Co(C_6H_4NO_2)_2]_n$, with water molecules occupying voids within these layers. We describe here the comparable anhydrous framework $[Co(C_6H_4NO_2)_2]_n$, (I), prepared by hydrothermal synthesis.

(I)
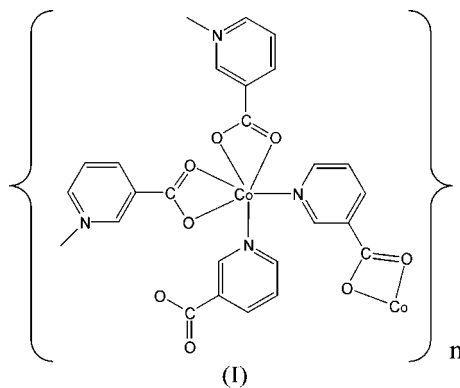
The asymmetric unit of (I) (Fig. 1) comprises one Co^{2+} ion lying on a twofold rotation axis, and one nicotinate anion. Atom Co1 is coordinated by two N atoms in a *cis* arrangement and two carboxylate groups bound in a bidentate manner with one Co—O distance significantly longer than the other (Table 1). Each nicotinate anion links two Co^{2+} ions to generate square two-dimensional layers parallel to the (001) plane (Fig. 2). These layers are chiral and are essentially identical to those in the hydrated structure $[Co(C_6H_4NO_2)_2]\cdot H_2O$ reported by Yeh *et al.* (2004). The shortest Co$\cdots$Co distance within the layer is 7.86 (5) Å. The layers are arranged so that the benzene rings of the nicotinate anions project into the square voids within adjacent layers (Fig. 3).
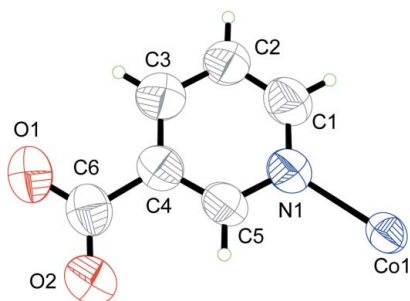
doi:10.1107/S1600536806029400

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Figure 1
The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 70% probability level and H atoms are shown as spheres of arbitrary radii.
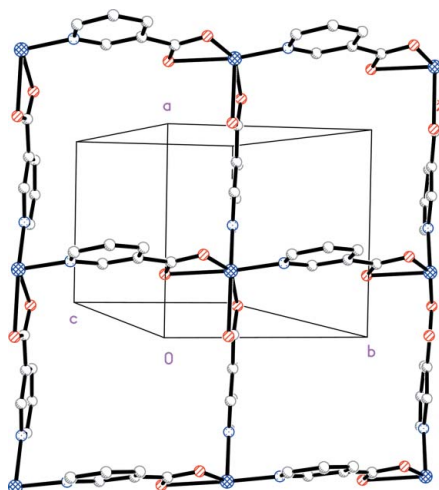

Figure 2
The structure of one chiral $[Co(C_6H_4NO_2)_2]_n$ layer. H atoms have been omitted.

Figure 3
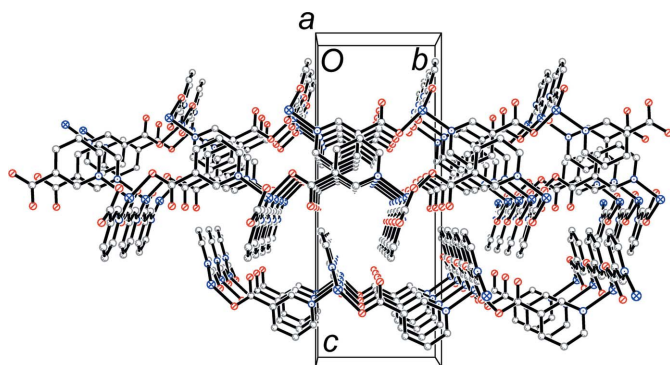Projection along a, showing the arrangement of adjacent $[Co(C_6H_4NO_2)_2]_n$ layers. H atoms have been omitted.

Experimental

Red block-shaped crystals were synthesized hydrothermally from a mixture of $CoCl_2 \cdot 5H_2O$, H_3BO_3, H_2O, nicotinic acid and HCl. In a typical synthesis, $CoCl_2 \cdot 5H_2O$ (0.0475 g), H_3BO_3 (0.0420 g) and nicotinic acid (0.267 g) were dissolved in water (8 ml), followed by addition of 36% aqueous HCl (0.165 g). The mixture was kept in a 25 ml Teflon-lined steel autoclave at 443 K for 7 d. The autoclave was slowly cooled to room temperature, and the product was filtered off, washed with distilled water and dried in air.

Crystal data

$[Co(C_6H_4NO_2)_2]$	$D_x = 1.558$ Mg m^{-3}
$M_r = 303.13$	Mo $K\alpha$ radiation
Tetragonal, $P4_12_12$	$\mu = 1.34$ mm^{-1}
$a = 7.861$ (13) Å	$T = 293$ (2) K
$c = 20.92$ (5) Å	Block, red
$V = 1293$ (4) Å^3	$0.12 \times 0.12 \times 0.10$ mm
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	4309 measured reflections
ω scans	1409 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	1159 reflections with $I > 2\sigma(I)$
$T_{min} = 0.856$, $T_{max} = 0.878$	$R_{int} = 0.070$
	$\theta_{max} = 27.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0895P)^2 + 1.6395P]$
$R[F^2 > 2\sigma(F^2)] = 0.061$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.173$	$(\Delta/\sigma)_{max} = 0.010$
$S = 1.07$	$\Delta\rho_{max} = 1.02$ e Å^{-3}
1409 reflections	$\Delta\rho_{min} = -0.69$ e Å^{-3}
87 parameters	Absolute structure: Flack (1983), 517 Friedel pairs
H-atom parameters constrained	Flack parameter: -0.07 (7)

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.113 (6)	Co1—O2^i	2.441 (6)
Co1—O1^i	2.054 (6)		
O1^{ii}—Co1—O1^i	150.1 (3)	O1^i—Co1—O2^i	58.9 (2)
O1^i—Co1—N1	95.3 (2)	O1^{ii}—Co1—O2^i	97.8 (2)
O1^{ii}—Co1—N1	105.0 (2)	N1^{iii}—Co1—O2^i	96.2 (2)
N1^{iii}—Co1—N1	94.3 (3)	N1—Co1—O2^i	153.89 (18)

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

The low precision of the lattice parameters reflects a crystal of relatively low quality. During refinement, H atoms were placed in calculated positions and allowed to ride, with C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C). The highest peak in the difference map is located 0.93 Å from Co1.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Version 1.27. Bruker AXS Inc., Madison, Wisconsin, USA.
Chapman, M. E., Ayyappan, P., Foxman, B. M., Yee, G. T. & Lin, W. (2001). *Cryst. Growth Des.* **1**, 159–163.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Kang, Y., Yao, Y., Qin, Y., Zhang, J., Chen, Y., Li, Z., Wen, Y., Cheng, J. & Hu, R. (2004). *Chem. Commun.* pp. 1046–1047.

Lu, J. Y. & Babb, A. M. (2003). *Chem. Commun.* pp. 1346–1347.

Sheldrick, G. M. (2003). *SADABS.* University of Göttingen, Germany.

Yeh, C., Suen, M., Hu, H., Chen, J. & Wang, J. (2004). *Polyhedron*, **23**, 1947–1952.

Yu, J., Xu, J., Ye, L., Ding, H., Jing, W., Wang, T., Xu, J., Jia, H., Mu, Z. & Yang, G. (2002). *Inorg. Chem. Commun.* **5**, 572–576.

Zhang, M., Zhang, J., Zheng, S. & Yang, G. (2005). *Angew. Chem. Int. Ed.* **44**, 1385–1388.