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A coordination polymer of Co^{II} with 1,1′-(1,4-butanediyl)bis(imidazole)

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Key indicators

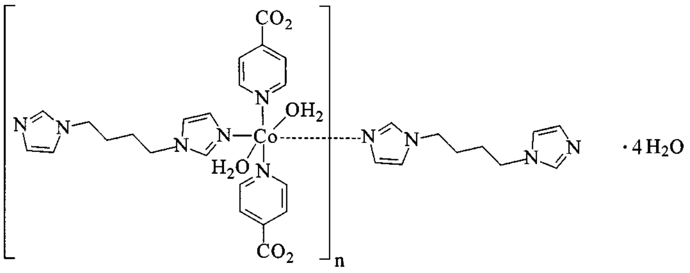
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.077
Data-to-parameter ratio = 17.4

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

In the title compound, *catena*-poly[[[diaquaisonicotinatocobalt(II)]-di-μ-1,1′-(1,4-butanediyl)bis(imidazole] tetrahydrate], $\{[Co(IN)_2L(H_2O)_2]\cdot 4H_2O\}_n$, where L is 1,1′-(1,4-butanediyl)bis(imidazole) ($C_{10}H_{14}N_4$) and IN is the isonicotinate anion ($C_6H_4NO_2$), the cobalt(II) cation, which is at an inversion center, is hexacoordinated by two water molecules and four N atoms from two L ligands and two isonicotinate anions. Each ligand L coordinates to two cobalt(II) cations, acting as a bridge. The cobalt(II) cations are bridged to form an infinite zigzag chain structure along the c axis. The polymeric chains are linked through a variety of hydrogen bonds to form a three-dimensional structure.

Comment

The synthesis and characterization of coordination polymers with infinite one-, two- and three-dimensional structures has been an area of rapid growth in recent years because of the potential of these polymers in various applications, such as catalysis (Fujita *et al.*, 1994), electrical conductivity (Ermer, 1991), host–guest chemistry (Kitazawa *et al.*, 1994) and magnetism (Inoue *et al.*, 1996). Much of the work has so far been focused on coordination polymers with rigid ligands, such as 4,4′-bipyridine (Lu *et al.*, 1997) and pyrazine (Kawata *et al.*, 1998). However, transition metal complexes with flexible ligands have rarely been investigated (Ma, Liu, Xing *et al.*, 2000) and we are interested in coordination polymers containing flexible ligands. Based on its structure, 1,1′-(1,4-butanediyl)bis(imidazole) (L) can be used as a flexible bidentate ligand to fabricate coordination polymers. In this paper, we present the preparation and crystal structure of the compound, (I).



(I)

Compound (I) is isostructural with $[CuL(IN)_2(H_2O)_2]\cdot 4H_2O$ (IN is the isonicotinate anion; Ma *et al.*, 2003). Selected bond lengths and angles for (I) are given in Table 1. Fig. 1 shows the coordination environment of the cobalt(II) cation. Each cobalt(II) cation, which lies at an inversion center, is

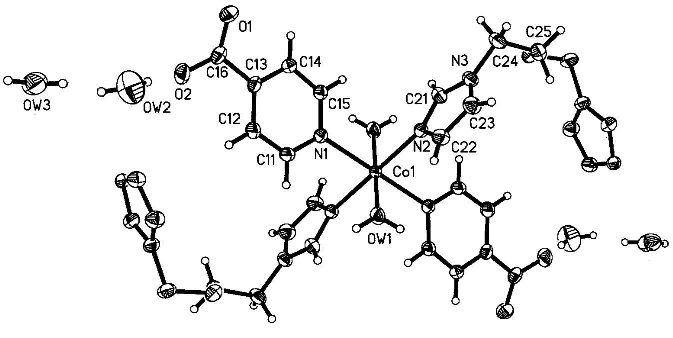


Figure 1
View of the local coordination of Co^{II}, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

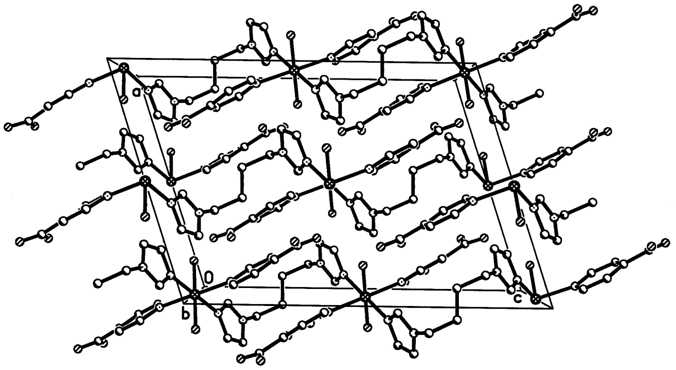


Figure 2
The infinite zigzag polymeric chain of (I) along the *c* axis. (Water molecules and H atoms have been omitted for clarity.)

hexacoordinated by two water molecules and four N atoms from two *L* ligands and two isonicotinate anions. The presence of an uncoordinated carboxylate group is somewhat unexpected, because the carboxylate group of the isonicotinate anion is a better coordinating group than O atoms in water with respect to the cobalt(II) cation. The distance between the cobalt(II) cation and the N atom from ligand *L* is 2.1248 (11) Å, similar to that of the Co—N(IN) distance of 2.1826 (12) Å. The Co—O(water) distance of 2.1223 (10) Å is near to that of a related cobalt(II) complex (Ma, Liu, Liu *et al.*, 2000). The distance between neighboring cobalt(II) cations is 8.742 (1) Å. As shown in Fig. 2, each ligand *L* coordinates to two cobalt(II) cations, acting as a bridging ligand to form an infinite zigzag chain structure.

The polymeric chains of (I) are held together through hydrogen bonds to form a three-dimensional structure. The hydrogen bonds in this study have been considered with liberal distance cut-off criteria of $2.5 < D\cdots A < 3.0$ Å and $120 < D—\text{H}\cdots A < 180°$. The selected hydrogen-bond distances and angles are listed in Table 2. It can be seen that there are six H atoms involved in hydrogen bonding in the asymmetric unit. All of them come from water molecules. The uncoordinated carboxylate O atoms are also involved in hydrogen bonds and play the role of acceptors. The polymeric chains are connected through various hydrogen bonds to form a three-dimensional structure.

Experimental

A mixture of $CoCl_2\cdot6H_2O$ (0.238 g, 1 mmol) and NaOH (0.08 g, 2 mmol) in water was stirred for 10 min at room temperature, then the precipitate was filtered. Isonicotinic acid (0.246 g, 2 mmol) was added to the $Co(OH)_2$ suspension in water with constant stirring. Then *L* (0.380 g, 2 mmol) was added to the mixture with stirring for 1 h and a blue solution was obtained. Pink crystals were obtained from the solution after several days (68% yield based on Co). Analysis calculated for $[CoL(IN)_2(H_2O)_2]\cdot4H_2O$: C 43.89, H 5.65, N 13.97%; found: C 43.95, H 5.44, N 14.08%.

Crystal data

$[Co(C_6H_4NO_2)_2(C_{10}H_{14}N_4)(H_2O)_2]\cdot4H_2O$
$M_r = 601.48$
Monoclinic, $C2/c$
$a = 12.124$ (2) Å
$b = 13.464$ (3) Å
$c = 17.483$ (4) Å
$\beta = 108.55$ (3)°
$V = 2705.6$ (11) Å^3
$Z = 4$

$D_x = 1.477$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12084 reflections
$\theta = 2.3$–27.5°
$\mu = 0.70$ mm^{-1}
$T = 293$ (2) K
Block, pink
0.53 × 0.31 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.770$, $T_{max} = 0.932$
12991 measured reflections

3109 independent reflections
2606 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$
$h = 0 \rightarrow 15$
$k = 0 \rightarrow 17$
$l = -22 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.077$
$S = 1.06$
3109 reflections
179 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O*W*1	2.1223 (10)	Co1—N2	2.1248 (11)
Co1—N1	2.1826 (12)		
O*W*1^{i}—Co1—N1	87.04 (5)	O*W*1—Co1—N2	90.32 (4)
O*W*1—Co1—N1	92.96 (5)	N1—Co1—N2	91.57 (4)
O*W*1^{i}—Co1—N2	89.68 (4)	N1—Co1—N2^{i}	88.43 (4)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O*W*1—H1$\cdots$O2^{ii}	0.84	1.95	2.7819 (15)	170
O*W*1—H2$\cdots$O1^{iii}	0.84	1.83	2.6654 (15)	179
O*W*2—H3$\cdots$O2	0.84	1.99	2.823 (2)	175
O*W*2—H4$\cdots$O*W*2^{iv}	0.84	2.09	2.820 (4)	146
O*W*2—H5$\cdots$O*W*3	0.84	1.95	2.769 (2)	164
O*W*3—H6$\cdots$O1^{v}	0.84	1.97	2.8122 (18)	180
O*W*3—H7$\cdots$O*W*3^{vi}	0.84	1.89	2.729 (3)	175
O*W*3—H8$\cdots$O*W*2	0.84	1.94	2.769 (2)	171

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

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. Water H atoms were locatedin a difference Fourier map and refined freely for H1 and H2; $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$ for the other water H atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL*97.

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