metal-organic papers

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Key indicators

Single-crystal X-ray study T = 292 KMean $\sigma(\text{C}-\text{C}) = 0.008 \text{ Å}$ R factor = 0.074 wR factor = 0.211 Data-to-parameter ratio = 15.3

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

catena-Poly[[[aqua(dipyrido[3,2-a:2',3'-c]phenazine)cobalt(II)]-μ-succinato] monohydrate]

In the title compound, {[$Co(C_4H_4O_4)(C_{18}H_{10}N_4)(H_2O)$]·· H_2O }_n, each Co^{II} atom is six-coordinated by two N atoms from one dipyrido[3,2-*a*:2',3'-*c*]phenazine ligand, and by four O atoms from two succinate anions (one chelating bidentate and one monodentate) and one water molecule in a distorted *cis*-CoN₂O₄ octahedral coordination. The Co^{II} atoms are bridged by the succinate ligands to generate a helical chain structure. The chain motif is consolidated into a layer structure by O-H···O hydrogen bonds involving the water molecules and carboxylate O atoms.

Comment

The rational design and synthesis of metal–organic coordination polymers is of great current interest (Eddaoudi *et al.*, 2001). 1,10-Phenanthroline (phen) or its derivatives, as one type of important organic ligands, have been widely used as components in the construction of metal–organic coordination polymers (Chen & Liu, 2002). The phen derivative dipyrido[3,2-*a*:2',3'-*c*]phenazine, *L*, possesses an extended aromatic system and its coordination polymers have recently been studied (Zhang & Sun, 2006). As a continuation of this work, we have prepared the polymeric title compound, $[Co(suc)(L)(H_2O)]\cdot H_2O$, (I) (Fig. 1), from a combination of Co^{2+} ions, succinic acid (H₂suc) and *L* as a secondary chelating ligand.



Selected bond lengths and angles for (I) are given in Table 1. Each Co^{II} atom is six-coordinated by two N atoms from one L ligand, and by four O atoms from two suc^{2–} anions (one

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Figure 1

The asymmetric unit of (I), expanded to show the metal coordination. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry code: (i) 1 - x, $y - \frac{1}{2}, \frac{3}{2} - z$.]

monodentate and one chelating bidentate) and one water molecule, resulting in a very distorted octahedral coordination. Compound (I) also incorporates an uncoordinated water molecule (Fig. 1). The C–O bond lengths of both carboxylate groups of the suc^{2-} dianion suggest delocalization of the bonding and its carbon backbone adopts a gauche conformation.

The Co^{II} atoms are bridged by the suc²⁻ ligands to generate a helical chain structure propagating along [010] (Fig. 2) generated by the 21 screw axis. This chain motif is consolidated into a layer structure by $O-H \cdots O$ hydrogen bonds involving the water molecules and carboxylate O atoms (Table 2).

Experimental

The ligand L was synthesized according to the method of Che et al. (2006). An ethanolic solution (24 ml) of L (0.5 mmol) was added slowly to an aqueous solution (20 ml) of CoCl₂·2H₂O (0.5 mmol) and H₂suc (1 mmol) with stirring at refluxing temperature. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for one week, yielding red crystals of (I) (61% yield based on Co).

Crystal data

H_2O $Z = 4$	
$M_r = 493.33$ $D_x = 1.569 \text{ Mg m}^{-3}$	
Monoclinic, $P2_1/c$ Mo $K\alpha$ radiation	
$a = 8.6818 (17) \text{ \AA} \qquad \mu = 0.87 \text{ mm}^{-1}$	
b = 7.8022 (16)Å $T = 292 (2) $ K	
c = 30.968 (6) Å Block, red	
$\beta = 95.27 \ (3)^{\circ}$ $0.31 \times 0.27 \times 0.24 \ m$	ım



Figure 2

A view of the one-dimensional chain structure of (I). Uncoordinated water molecules and H atoms have been omitted.

 $R_{\rm int} = 0.074$

 $\theta_{\rm max} = 27.5^\circ$

Data collection

Rigaku R-AXIS RAPID	18973 measured reflections	
diffractometer	4741 independent reflections	
ω scans	3215 reflections with $I > 2\sigma(I)$	

Absorption correction: multi-scan (ABSCOR; Higashi, 1995) $T_{\min} = 0.759, \ T_{\max} = 0.816$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_0^2) + (0.11P)^2]$ $R[F^2 > 2\sigma(F^2)] = 0.074$ wR(F²) = 0.211 + 1.9763*P*] where $P = (F_0^2 + 2F_c^2)/3$ S = 1.04 $(\Delta/\sigma)_{\rm max} = 0.001$ $\Delta \rho_{\rm max} = 3.08 \text{ e } \text{\AA}^{-3}$ 4741 reflections $\Delta \rho_{\rm min} = -0.43 \text{ e} \text{ Å}^{-3}$ 310 parameters H atoms treated by a mixture of

independent and constrained refinement

Table 1

Selected geometric parameters (Å, °).

C1-O2	1.250 (5)	Co1-N2	2.126 (4)
C1-O1	1.267 (5)	Co1-O1	2.067 (3)
C4-O3	1.258 (5)	Co1 - O1W	2.061 (3)
C4-O4	1.277 (6)	Co1-O3 ⁱ	2.177 (3)
Co1-N1	2.115 (4)	Co1-O4 ⁱ	2.147 (3)
N1 - Co1 - N2	77 57 (14)	$O4^{i}-Co1-O3^{i}$	60.43(12)
	(11)	01 001 00	00112 (12)
	(7, 6, (5))		
1 - 02 - 03 - 04	07.6 (5)		
Semi-mature and as (i)	1 1 1 3		

Symmetry code: (i) -x + 1, $y - \frac{1}{2}$, $-z + \frac{3}{2}$

Table 2	_	
Hydrogen-bond geometry	(Å,	°).

$D - H \cdots A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$\begin{array}{c} O1W-H11W\cdots O2\\ O1W-H12W\cdots O4^{ii}\\ O2W-H21W\cdots O1^{iii}\\ O2W-H22W\cdots O2 \end{array}$	0.93 (4)	1.75 (3)	2.612 (5)	154 (5)
	0.92 (4)	1.76 (2)	2.678 (4)	172 (5)
	0.92 (7)	2.14 (8)	3.041 (6)	165 (9)
	0.92 (7)	1.90 (6)	2.815 (6)	173 (10)

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

All C-bound H atoms were generated geometrically and refined as riding atoms, with C-H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecules were located in a difference map and refined with an O-H distance restraint of 0.90 (2) Å. The highest residual electron-density peak is located 0.92 Å from atom H6.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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