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catena-Poly[[*cis*-diaqua(1,10-phenanthroline-κ^2N,N')-cobalt(II)]-μ_2-5-sulfonatosalicylato-$\kappa^2O:O'$]

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In the title one-dimensional chain complex, $[Co(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]_n$, each Co^{II} atom displays an octahedral geometry. Hydrogen-bonding interactions between chains generate a two-dimensional architecture.

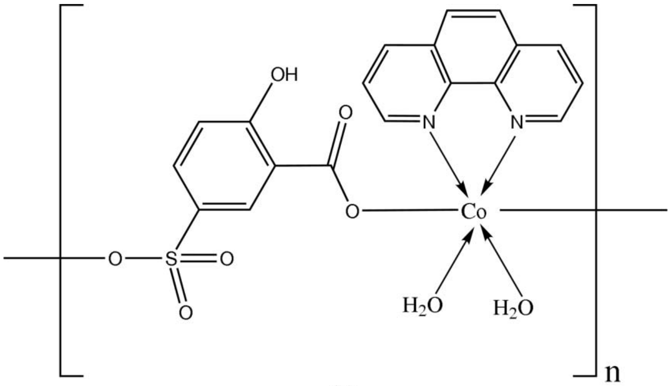
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.067
wR factor = 0.136
Data-to-parameter ratio = 12.8

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

Comment

Recently, three metal complexes with the formula $[M(Hssal)(phen)(H_2O)_2]_n$ (M^{2+} = Cu^{2+}, Zn^{2+} and Mn^{2+}; Hssal^{2-} is the 5-sulfonatosalicylate dianion and phen is 1,10-phenanthroline) have been synthesized and structurally characterized (Chen *et al.*, 2003; Fan & Zhu, 2005). Each metal atom in these complexes adopts an octahedral geometry defined by two N donors from one phen ligand, two O atoms, one from a sulfonyl and one from a carboxyl group of two different Hssal^{2-} ligands, and two O atoms from two *cis*-arranged water molecules. The fourth crystal structure of such a complex containing the Co^{II} atom, *viz.* the title compound, (I), is presented here.



(I)

The coordination environment around the Co^{II} atom is shown in Fig. 1. The molecular structure is a one-dimensional chain assembled by $[Co(Hssal)(phen)(H_2O)_2]$ units through the bridging Hssal^{2-} ligands (Fig. 2). In the chain, intramolecular hydrogen bonds are formed between the hydroxy group and coordinated carboxyl O atom, and between the uncoordinated carboxyl oxygen atom and the water molecule (O2w). Between chains, water molecules and sulfonyl O atoms form intermolecular hydrogen bonds, giving rise to a two-dimensional hydrogen-bonding network (Fig. 3 and Table 2).

Comparison of (I) with analogous complexes (II)–(IV), $[M(Hssal)(phen)(H_2O)_2]_n$ [for (II), M^{2+} = Cu^{2+}; for (III), M^{2+} = Zn^{2+}; for (IV), M^{2+} = Mn^{2+}) shows some interesting features in the coordination geometries of the four complexes (Table 3). The geometry around the Cu^{II} atom in (II) is very distorted

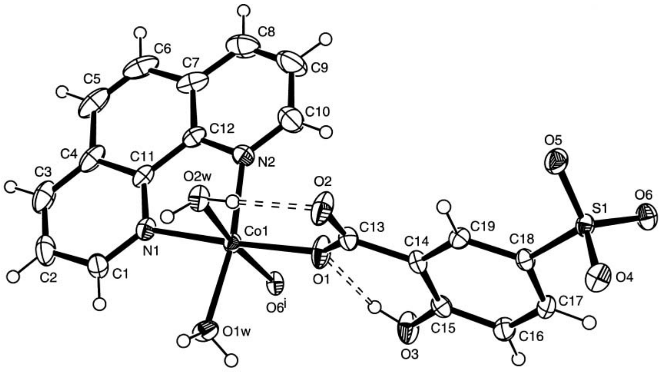


Figure 1
An *ORTEP-3* (Farrugia, 1997) view of a segment of (I). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines [symmetry code: (i) $x, \frac{1}{2} - y, -\frac{1}{2} + z$].

octahedral as a result of the Jahn–Teller effect, while the geometries around the Co^{II} and Zn^{II} atoms are similar, and associated bond lengths, such as M—O*w*, M—N, M—O (COO^-) and M—O (SO_3^-) in (IV), are longer than those in (I) and (III). Therefore, further investigation of $[M(Hssal)(phen)(H_2O)_2]_n$ complexes (M^{2+} = Ni^{2+}, Fe^{2+} and Cr^{2+}) will provide much information on coordination geometries.

Experimental

A mixture of $CoCl_2 \cdot 6H_2O$ (0.238 g, 1.0 mmol), 5-sulfosalicylic acid dihydrate (0.051 g, 0.20 mmol), and pyridine (1 ml, 4%) in water (20 ml) was stirred at room temperature for 12 h. 1,10-Phenanthroline (0.041 g, 0.20 mmol) was then added. The resulting solution was put aside and the solvent allowed to evaporate. Red block-shaped crystals of (I) were obtained after four weeks.

Crystal data

$[Co(C_7H_4O_6S)(C_{12}H_8N_2)(H_2O)_2]$
M_r = 491.33
Monoclinic, $P2_1/c$
a = 14.3102 (8) Å
b = 7.6342 (4) Å
c = 18.5783 (10) Å
β = 107.637 (1)°
V = 1934.22 (18) Å^3
Z = 4
D_x = 1.687 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4391 reflections
θ = 2.3–28.2°
μ = 1.05 mm^{-1}
T = 295 (2) K
Block, red
0.26 × 0.22 × 0.13 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.772, T_{max} = 0.876
10606 measured reflections
3786 independent reflections
3674 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°
$h = -17 \rightarrow 17$
$k = -8 \rightarrow 9$
$l = -22 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.136
S = 1.30
3786 reflections
295 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0326P)^2 + 5.8354P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

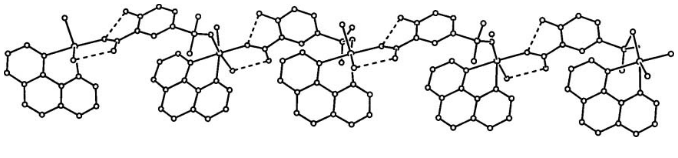


Figure 2
A view of the one-dimensional chain in (I). Hydrogen bonds are shown as dashed lines and H atoms have been omitted for clarity.

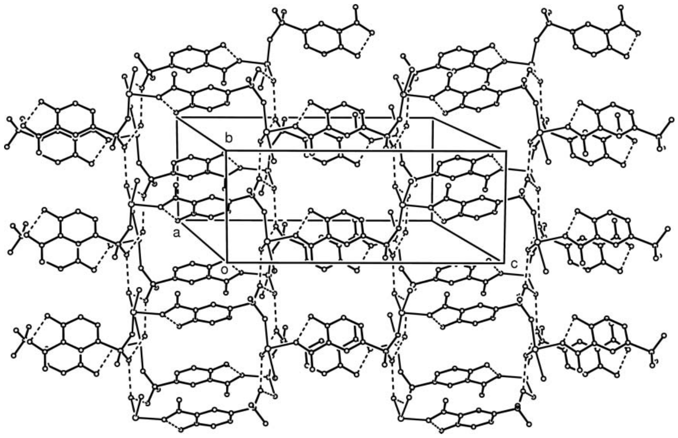


Figure 3
A view of the two-dimensional hydrogen-bonding (dashed lines) network for (I). The phen and H atoms have been omitted for clarity.

Table 1
Selected interatomic distances (Å).

Co1—O1	2.047 (3)	Co1—N2	2.113 (4)
Co1—O6^{i}	2.151 (3)	S1—O5	1.446 (3)
Co1—O1*w*	2.032 (3)	S1—O6	1.450 (3)
Co1—O2*w*	2.151 (3)	S1—O4	1.464 (3)
Co1—N1	2.132 (4)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H1*w*1···O4^{ii}	0.85 (1)	1.87 (1)	2.712 (4)	177 (5)
O1*w*—H2*w*1···O4^{iii}	0.85 (4)	1.87 (4)	2.724 (4)	178 (5)
O2*w*—H1*w*2···O5^{ii}	0.84 (4)	2.00 (4)	2.828 (4)	166 (4)
O2*w*—H2*w*2···O2	0.85 (1)	1.89 (2)	2.698 (4)	160 (5)
O3—H3*A*···O1	0.84 (4)	1.80 (3)	2.579 (5)	152 (6)

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

Table 3
Comparative geometrical parameters (Å) for $[M(Hssal)(phen)(H_2O)_2]_n$ complexes.

Bond length	(II)	(III)	(IV)
M—O*w*	1.9537 (19)	2.0361 (14)	2.2316 (14)
M—O*w*	2.418 (2)	2.1615 (14)	2.1255 (14)
M—N	2.010 (2)	2.1288 (16)	2.2659 (15)
M—N	2.017 (2)	2.1438 (16)	2.2447 (15)
M—O(COO^-)	1.9529 (17)	2.0373 (13)	2.1174 (13)
M—O(SO_3^-)	2.3791 (17)	2.1754 (13)	2.1835 (12)

All aromatic H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The water and hydroxy H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.85 (1) Å and a fixed isotropic displacement parameter of $U_{\rm iso}$(H) = 0.05 Å^2.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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