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Poly[[[(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ_3-5-hydroxyisophthalato-$\kappa^4O,O':O'':O'''$] monohydrate]

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Key indicators

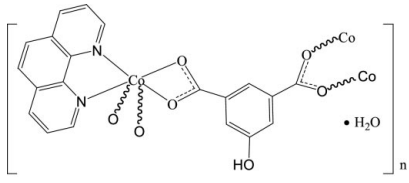
Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.089
Data-to-parameter ratio = 15.7

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

The title compound, $\{[Co(C_8H_4O_5)(C_{12}H_8N_2)]\cdot H_2O\}_n$, is isostructural with its manganese analog [Skakle, Foreman & Plater (2001). *Acta Cryst.* E**57**, m373–m375]. The asymmetric unit consists of one Co atom, one 1,10-phenanthroline ligand bound in a bidentate manner, one hydroxyisophthalate ligand and one water molecule. The Co coordination is completed by two further O atoms from two symmetry-related hydroxyisophthalate ligands, giving a grossly distorted octahedral geometry.

Comment

The title compound, (I), was synthesized by the hydrothermal reaction of 5-hydroxyisophthalic acid with 1,10-phenanthroline (phen) and cobalt acetate. The asymmetric unit consists of one Co atom, one phen ligand bound in a bidentate manner, one hydroxyisophthalate ligand and one water molecule. The Co coordination is completed by two further O atoms from two symmetry-related hydroxyisophthalate ligands, giving a grossly distorted octahedral geometry. 5-Hydroxyisophthalate acts as a tetradentate ligand in this structure, with one carboxylate group acting as bidentate to one Co atom and the two remaining O atoms acting as monodentate to two further Co atoms. The Co—O distances range from 2.0421 (12) to 2.2523 (13) Å and the Co—N distances are 2.1044 (13) and 2.1161 (13) Å.



(I)

In the structure of (I), one-dimensional chains are formed by the cobalt cations and the carboxylate ligands; these chains are linked by a hydrogen-bonding network consisting of the phenol OH group, carboxylate O atoms and the water molecule, forming two-dimensional sheets. This arrangement is also seen in the isostructural manganese analog (Skakle *et al.*, 2001) and the related $[Mn(C_8H_4O_5)(2,2'\text{-bipyridyl})]_n\cdot nH_2O$ structure (Plater *et al.*, 2001).

Experimental

5-Hydroxyisophthalic acid (0.091 g, 0.5 mmol), cobalt(II) acetate tetrahydrate (0.125 g, 0.5 mmol), 1,10-phenanthroline (0.102 g, 0.57 mmol), sodium carbonate (0.081 g, 0.76 mmol) and water (16 ml) were sealed in a 25 ml stainless-steel reactor with a Teflon liner. The reaction system was heated at 433 K for 60 h. Slow cooling of the system to room temperature yielded red prismatic crystals of the complex, which were collected by filtration.

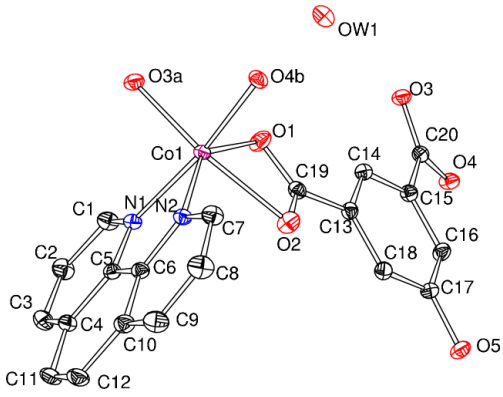


Figure 1
The structure of (I). Displacement ellipsoids are plotted at the 50% probability level. H atoms have been omitted for clarity [symmetry codes: (*a*) $2-x, 1-y, 2-z$; (*b*) $x-\frac{1}{2}, 1-y, z-\frac{1}{2}$].

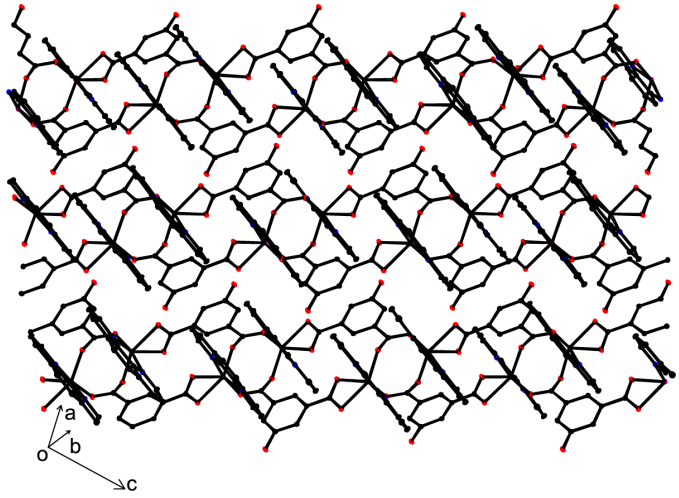


Figure 2
Drawing showing the one-dimensional chains of (I). H atoms and solvent water molecules have been omitted for clarity.

Crystal data

$[Co(C_8H_4O_5)(C_{12}H_8N_2)]\cdot H_2O$	$D_x = 1.697$ Mg m^{-3}
$M_r = 437.26$	Mo $K\alpha$ radiation
Monoclinic, $P2/n$	Cell parameters from 4790 reflections
$a = 8.5218$ (10) Å	$\theta = 1.7$–$28.3°$
$b = 12.0440$ (10) Å	$\mu = 1.05$ mm^{-1}
$c = 17.028$ (2) Å	$T = 130$ (2) K
$\beta = 101.599$ (5)°	Prism, red
$V = 1712.0$ (3) Å^3	0.40 × 0.30 × 0.20 mm
$Z = 4$	

Data collection

Siemens SMART CCD area-detector diffractometer	4248 independent reflections
ω scans	4069 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.021$
$T_{min} = 0.734$, $T_{max} = 0.811$	$\theta_{max} = 28.3°$
13723 measured reflections	$h = -11 \rightarrow 11$
	$k = -16 \rightarrow 16$
	$l = -13 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 1.0992P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.034$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.089$	$\Delta\rho_{max} = 0.57$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -0.64$ e Å^{-3}
4248 reflections	Extinction correction: *SHELXL*97
270 parameters	Extinction coefficient: 0.00015 (3)
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Co1—O3^{i}	2.0421 (12)	Co1—N1	2.1161 (13)
Co1—O4^{ii}	2.0801 (11)	Co1—O1	2.1654 (12)
Co1—N2	2.1044 (13)	Co1—O2	2.2523 (13)
O3^{i}—Co1—O4^{ii}	91.66 (5)	N2—Co1—O1	144.49 (5)
O3^{i}—Co1—N2	121.69 (5)	N1—Co1—O1	95.85 (5)
O4^{ii}—Co1—N2	96.52 (5)	O3^{i}—Co1—O2	150.24 (5)
O3^{i}—Co1—N1	84.19 (5)	O4^{ii}—Co1—O2	97.08 (5)
O4^{ii}—Co1—N1	169.67 (5)	N2—Co1—O2	85.59 (5)
N2—Co1—N1	77.81 (5)	N1—Co1—O2	91.13 (5)
O3^{i}—Co1—O1	91.78 (5)	O1—Co1—O2	59.39 (4)
O4^{ii}—Co1—O1	93.73 (5)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···*OW*1^{i}	0.82	2.10	2.6302 (18)	122
*OW*1—H*W*1*B*···O1	0.75 (3)	2.30 (3)	2.8988 (19)	138 (3)
*OW*1—H*W*1*A*···O4^{ii}	0.87 (4)	1.92 (4)	2.7740 (19)	165 (3)

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

H atoms bonded to C atoms and the phenolic H were placed in calculated positions and included as part of a riding model, with U_{iso}(H) values set at $1.2U_{eq}$ of the parent atoms. Water H atoms were located from difference maps and refined freely.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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