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**Key indicators**

Single-crystal X-ray study  
 T = 298 K  
 Mean  $\sigma(C-C)$  = 0.004 Å  
 R factor = 0.029  
 wR factor = 0.076  
 Data-to-parameter ratio = 13.4

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

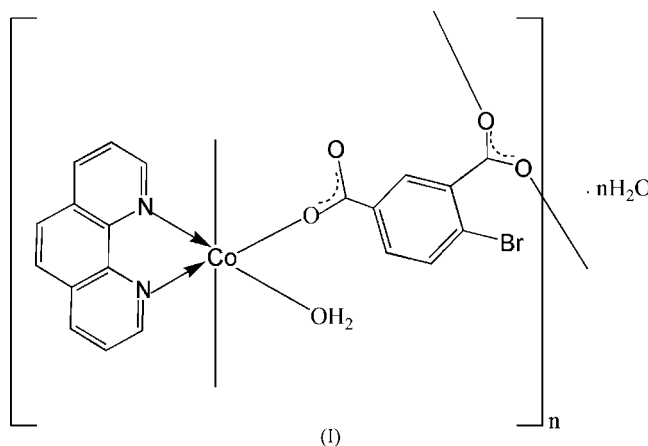
**Poly[[[aqua(1,10-phenanthroline)cobalt(II)]-  
 $\mu_3$ -4-bromoisophthalato] monohydrate]**

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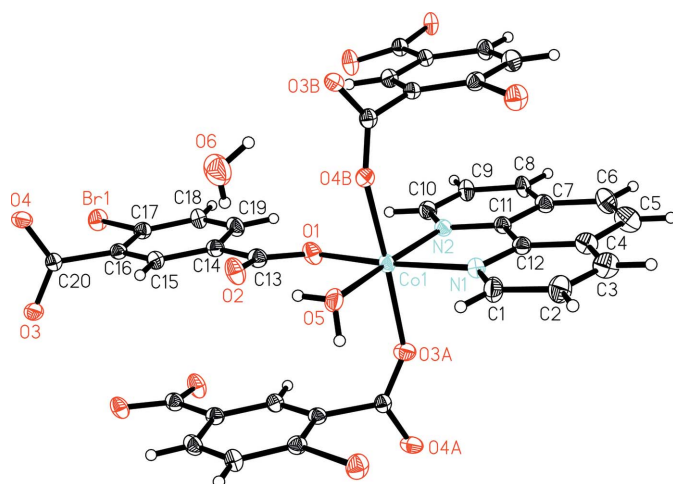
In the title compound,  $\{[Co(C_8H_3BrO_4)(C_{12}H_8N_2)(H_2O)] \cdot H_2O\}_n$ , each  $Co^{II}$  ion is six-coordinated by three O atoms from three carboxylate groups of three 4-bromoisophthalate dianions, one water molecule, and two N atoms from a 1,10-phenanthroline ligand. The coordination geometry around the  $Co^{II}$  cation is octahedral. Whereas the 1,10-phenanthroline ligand chelates to just one  $Co^{II}$  cation, the 4-bromoisophthalate dianions are bonded to three  $Co^{II}$  cations. The crystal structure is stabilized by several hydrogen bonds.

**Comment**

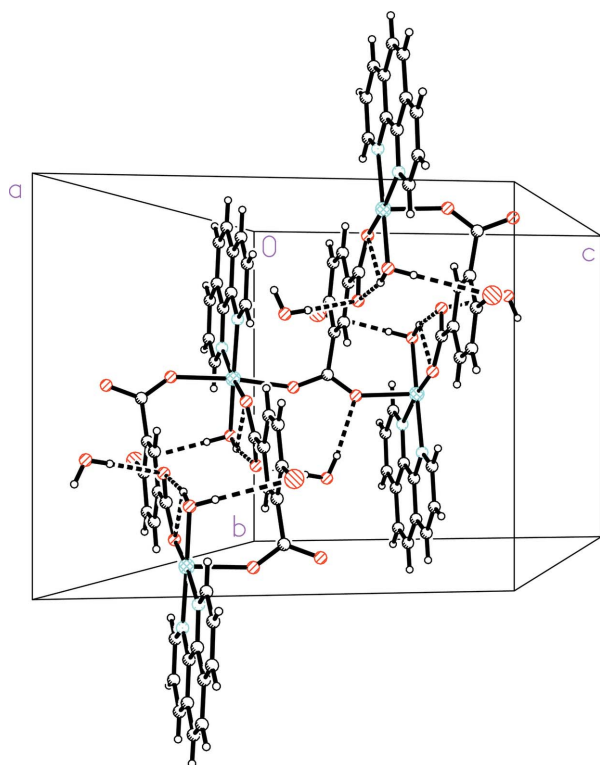
In recent years, the use of crystal engineering concepts has produced a variety of coordination networks (Hagman *et al.*, 1999; Moulton & Zaworotko, 2001; Munakata *et al.*, 1999; Zaworotko, 2001). The design of suitable ligands and the choice of metal ions required to generate well defined architectures in a controlled fashion constitute an extremely active field of research (Cotton *et al.*, 2001; Evans & Lin, 2002). 4-Bromoisophthalic acid is an interesting ligand, since both carboxylate groups are potential coordinating groups. Against this background, we present here the crystal structure of the title compound, (I).



In compound (I), the  $Co^{II}$  cations are hexacoordinated, in octahedral geometry, by three O atoms of the 4-bromoisophthalate dianions, two N atoms from one chelating 1,10-phenanthroline ligand and a water molecule (Fig. 1 and Table 1). Only three of the four O atoms of the 4-bromoisophthalate dianions coordinate to a  $Co^{II}$  cation. The bidentate carboxylate group, adjacent to the Br group, is almost perpendicular to the aromatic ring (Table 1), and the other carboxylate group, which is monodentate, is almost coplanar with the aromatic ring.


**Figure 1**

The coordination environment of the  $\text{Co}^{\text{II}}$  cation in (I), with the atom-numbering scheme, showing displacement ellipsoids at the 50% probability level. Atoms labelled with the suffixes A and B, and their respective unlabelled atoms, are generated by the symmetry operators  $(\frac{1}{2} - x, \frac{3}{2} - y, -z)$  and  $(\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z)$ , respectively.


**Figure 2**

A packing diagram for (I), with hydrogen bonds shown as dashed lines.

Each  $\text{Co}^{\text{II}}$  ion is bridged by three 4-bromoisophthalate dianions, forming a network structure (Fig. 2). A solvent water molecule is connected to the polymeric structure via  $\text{O} \cdots \text{H} \cdots \text{O}$  and  $\text{O} \cdots \text{H} \cdots \text{Br}$  hydrogen bonds (Table 2).

## Experimental

The title compound was synthesized by adding a dimethylformamide solution (10 ml) of 1,10-phenanthroline (0.04 g, 0.2 mmol) and 4-

bromoisophthalic acid (0.05 g, 0.2 mmol) dropwise to a stirred aqueous solution (10 ml) of cobalt(II) sulfate heptahydrate (0.06 g, 0.2 mmol) at 298 K. The reaction mixture was then filtered and the filtrate allowed to stand for about six weeks until red crystals were obtained. Block-shaped crystals of (I) suitable for X-ray diffraction were collected by filtration, washed with water and ethanol and dried in air.

### Crystal data

$[\text{Co}(\text{C}_8\text{H}_3\text{BrO}_4)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$	$D_x = 1.861 \text{ Mg m}^{-3}$
$M_r = 518.18$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 4543 reflections
$a = 28.8790 (18) \text{ \AA}$	$\theta = 2.5\text{--}28.0^\circ$
$b = 10.8803 (7) \text{ \AA}$	$\mu = 3.13 \text{ mm}^{-1}$
$c = 12.8559 (8) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 113.685 (1)^\circ$	Block, red
$V = 3699.2 (4) \text{ \AA}^3$	$0.32 \times 0.29 \times 0.25 \text{ mm}$
$Z = 8$	

### Data collection

Bruker SMART CCD area-detector diffractometer	3620 independent reflections
$\varphi$ and $\omega$ scans	3104 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.020$
$T_{\text{min}} = 0.381, T_{\text{max}} = 0.453$	$\theta_{\text{max}} = 26.0^\circ$
10220 measured reflections	$h = -35 \rightarrow 28$
	$k = -13 \rightarrow 13$
	$l = -15 \rightarrow 15$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 2.1039P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.076$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
3620 reflections	$\Delta\rho_{\text{min}} = -0.40 \text{ e \AA}^{-3}$
271 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Co1—O1	2.0347 (16)	Co1—O3 <sup>i</sup>	2.1382 (16)
Co1—N2	2.1122 (18)	Co1—O4 <sup>ii</sup>	2.1489 (16)
Co1—N1	2.1223 (19)	Co1—O5	2.1565 (16)
O1—Co1—N2	93.08 (7)	N1—Co1—O4 <sup>ii</sup>	90.00 (7)
O1—Co1—N1	171.55 (7)	O3 <sup>i</sup> —Co1—O4 <sup>ii</sup>	171.21 (7)
N2—Co1—N1	78.49 (7)	O1—Co1—O5	94.02 (7)
O1—Co1—O3 <sup>i</sup>	92.87 (7)	N2—Co1—O5	172.41 (7)
N2—Co1—O3 <sup>i</sup>	88.99 (7)	N1—Co1—O5	94.38 (7)
N1—Co1—O3 <sup>i</sup>	87.59 (7)	O3 <sup>i</sup> —Co1—O5	93.33 (6)
O1—Co1—O4 <sup>ii</sup>	90.76 (7)	O4 <sup>ii</sup> —Co1—O5	78.41 (6)
N2—Co1—O4 <sup>ii</sup>	98.82 (7)		

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

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{---}H \cdots A$	$D\text{---}H$	$H \cdots A$	$D \cdots A$	$D\text{---}H \cdots A$
O6—H6B $\cdots$ O3 <sup>ii</sup>	0.85	2.20	3.045 (3)	174
O6—H6A $\cdots$ O2	0.85	2.12	2.963 (3)	171
O5—H5B $\cdots$ Br1 <sup>i</sup>	0.85	2.60	3.4486 (17)	180
O5—H5A $\cdots$ O2	0.85	1.78	2.613 (2)	166

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

All H atoms were positioned geometrically and allowed to ride on their parent atoms, at distances of C–H = 0.93 Å and O–H = 0.85 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{O})$ .

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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