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## Key indicators

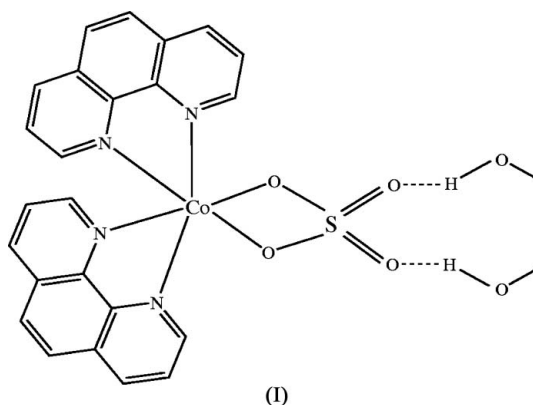
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
H-atom completeness 94%  
Disorder in solvent or counterion  
 $R$  factor = 0.036  
 $wR$  factor = 0.107  
Data-to-parameter ratio = 16.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(1,10-phenanthroline- $\kappa^2\text{N},\text{N}'$ )(sulfato- $\kappa^2\text{O},\text{O}'$ )-  
cobalt(II) 1,2-ethanediol solvate

In the title compound,  $[\text{Co}(\text{SO}_4)(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_2\text{H}_6\text{O}_2$ , a twofold rotation axis passes through the Co and S atoms, and through the mid-point of the solvent C—C bond. The coordination environment of the  $\text{Co}^{\text{II}}$  centre is a distorted  $\text{CoN}_4\text{O}_2$  octahedron, with four N atoms from two chelating 1,10-phenanthroline ligands and two O atoms from a bidentate sulfate ligand. The two chelating  $\text{N}_2\text{C}_2$  groups are oriented at  $70.16(6)^\circ$  to each other. Intermolecular  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bonds help to stabilize the structure.

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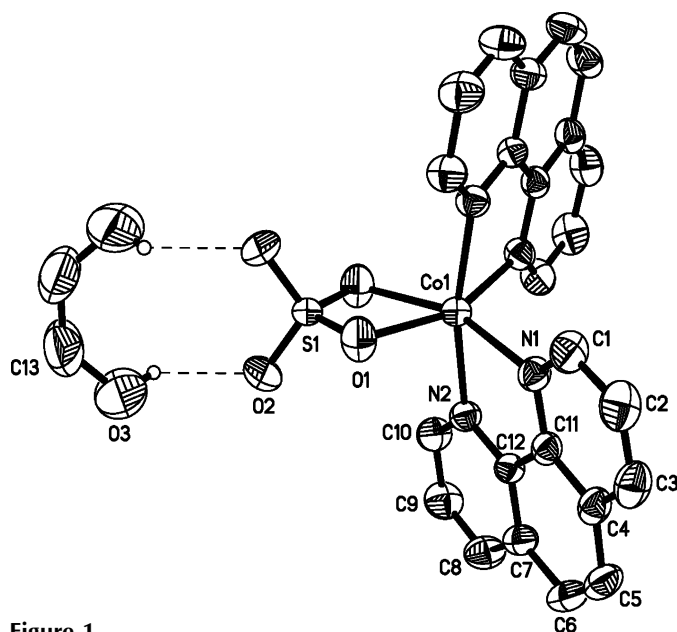
## Comment

Some cobalt complexes are potent antiviral agents (Bottcher *et al.*, 1995) and 1,10-phenanthroline (phen) also has biological activity, *e.g.* as a sterilizing agent (Husseini, 1981). 1,10-Phenanthroline has also been widely employed as a bidentate ligand in coordination reactions and in the construction of networks involving the cobalt metal ion (Bulut *et al.*, 2003; Zhu *et al.*, 2004; Zhang *et al.*, 2000). Recently, we have utilized polydentate and mixed ligands for the design of coordination networks (Lu *et al.*, 2002). The title compound, (I), was obtained unintentionally during an attempt to synthesize a mixed-ligand complex of  $\text{Co}^{\text{II}}$  with phen and 1,2-bis(2-pyridyl)ethylene *via* a solvothermal reaction.



Solvent-free Co–phen complexes with bidentate sulfate ligands (Palade *et al.*, 1973; Hennig *et al.*, 1975), with monodentate sulfate ligands (Li *et al.*, 1987), and with bidentate bridging sulfate ligands (Palade *et al.*, 1976) have been synthesized. The crystal structure of the title complex, (I), has not hitherto been reported.

A twofold rotation axis passes through the Co and S atoms, also through the mid-point of the solvent C—C bond. In the complex molecule, the  $\text{Co}^{\text{II}}$  centre is coordinated by four N atoms from two chelating phen ligands and two O atoms from


**Figure 1**

The structure of (I), showing the atom-numbering scheme and probability displacement ellipsoids drawn at the 50% level. The dashed lines represent O—H...O interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. Unlabelled atoms are related to labelled atoms by  $(1-x, y, \frac{1}{2}-z)$ .

a bidentate sulfate ligand, in a distorted octahedral geometry (Table 1). The Co—O bond distance is 2.1313 (14) Å, and the O—Co—O bite angle is 66.32 (7)°. The geometry of the phen ligand is in good agreement with those observed in many cobalt complexes (Li *et al.*, 1987). The Co—N distances [2.1261 (15)–2.1368 (15) Å] are in good accord with those reported in other six-coordinate Co—phen complexes, *e.g.* [Co(phen)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]·2C<sub>5</sub>H<sub>3</sub>N<sub>2</sub>O<sub>4</sub>·2.25H<sub>2</sub>O, (II) [2.1216 (15)–2.1300 (14) Å; Bulut *et al.*, 2003]. The N—Co—N bite angle of 78.10 (6)° is similar to that found in (II), *viz.* 78.06 (5)°. The dihedral angle between the two chelating N<sub>2</sub>C<sub>2</sub> groups is 70.16 (6)°; this is smaller than that found in (II) [75.33 (2)°], probably because of the replacement of the sulfate ligand by water.

The solvent molecule is disordered over three positions and was refined as three CO groups with occupancies of 0.30 0.30 and 0.40 for atom O3, sharing a common C13 atom. No attempt was made to find more than one position for each hydroxyl H atom. A pair of symmetry-related intermolecular O—H...O hydrogen bonds stabilizes the structure (Table 2 and Fig. 1).

## Experimental

The title compound was obtained unintentionally during an attempt to synthesize a mixed-ligand complex of Co(II) with phen and 1,2-bis(2-pyridyl)ethylene *via* a solvothermal reaction. A mixture of phen·H<sub>2</sub>O (0.2 mmol), 1,2-bis(2-pyridyl)ethylene (0.1 mmol), Co(SO<sub>4</sub>)<sub>2</sub>·7H<sub>2</sub>O (0.1 mmol), 1,2-ethanediol (2.0 ml) and water (1.0 ml) were placed in a thick Pyrex tube. The tube was sealed and heated at 453 K for 3 d to give red block-like crystals of (I). Analysis

found: C 54.10, H 3.92, N 10.10%; calculated for C<sub>26</sub>H<sub>22</sub>CoN<sub>4</sub>O<sub>6</sub>S: C 54.08, H 3.84, N 9.70%. FT-IR data (KBr, cm<sup>-1</sup>) 3360 (*m*, *b*), 3061 (*w*), 1606 (*m*), 1582 (*w*), 1513 (*s*), 1422 (*m*), 1430 (*w*), 1113 (*s*).

## Crystal data

[Co(SO<sub>4</sub>)(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]·C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>  
 $M_r = 577.47$   
 Monoclinic, C2/c  
 $a = 18.500$  (2) Å  
 $b = 11.8612$  (12) Å  
 $c = 12.8230$  (14) Å  
 $\beta = 119.052$  (2)°  
 $V = 2459.8$  (5) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.559$  Mg m<sup>-3</sup>  
 Mo- $K\alpha$  radiation  
 Cell parameters from 4704 reflections  
 $\theta = 3.2$ –28.0°  
 $\mu = 0.83$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, red  
 0.61 × 0.46 × 0.41 mm

## Data collection

Bruker SMART CCD 1K area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.630$ ,  $T_{\max} = 0.726$   
 8438 measured reflections

3065 independent reflections  
 2656 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.052$   
 $\theta_{\text{max}} = 28.3^\circ$   
 $h = -24 \rightarrow 11$   
 $k = -15 \rightarrow 15$   
 $l = -14 \rightarrow 17$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.107$   
 $S = 1.07$   
 3065 reflections  
 191 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.6033P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.55$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.52$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Co1—N2	2.1261 (15)	S1—O1	1.4865 (14)
Co1—O1	2.1313 (14)	C13—O3	1.320 (6)
Co1—N1	2.1368 (15)	C13—C13 <sup>i</sup>	1.386 (7)
S1—O2	1.4483 (14)		
O1 <sup>i</sup> —Co1—O1	66.32 (7)	O1—S1—O1 <sup>i</sup>	103.31 (11)
N2—Co1—N1	78.10 (6)	O3—C13—C13 <sup>i</sup>	128.1 (6)
O2 <sup>i</sup> —S1—O2	110.38 (14)		

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

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O3—H3...O2	0.82	2.01	2.709 (8)	143

The H atoms of phen were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atoms of 1,2-ethanediol were located in a difference map and then allowed to ride on their parent atoms, with C—H = 0.97 and O—H = 0.82 Å;  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $1.5U_{\text{eq}}(\text{O})$ . Only one H atom was included for each OH group. The 1,2-ethanediol is disordered over three positions, and this was refined as three CO groups, of 0.30 0.30 and 0.40 site occupancies, sharing a common C13 atom.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

X-ray data were collected at the Chinese University of Hong Kong.

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