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catena-Poly[[diaqua(2,2′-bipyridine-κ^2N,N')-cobalt(II)]-μ-sulfato]

Xin-Hua Li[a]* and Xian-Xing Chi[b]

[a]School of Chemistry and Materials Science, Wenzhou Normal College, Zhejiang, Wenzhou 325027, People's Republic of China, and [b]School of Physics and Electronic Information Science, Wenzhou Normal College, Zhejiang, Wenzhou 325027, People's Republic of China

Correspondence e-mail: xhli@wznc.zj.cn

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Key indicators

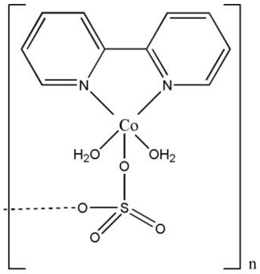
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.027
wR factor = 0.071
Data-to-parameter ratio = 11.9

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

By reaction of cobalt(II) sulfate with 5-hydroxyisophthalic acid and 2,2′-bipyridine in a water–dimethylformamide solution, the title novel sulfate-anion-bridged inorganic–organic hybrid, $[Co(C_{10}H_8N_2)(H_2O)_2SO_4]_n$, has been synthesized. Structural characterization of the complex shows that it displays a polymeric linear structure, formed by sulfate bridges between six-coordinate Co^{II} ions that lie on twofold rotation axes. Hydrogen bonding between chains results in a two-dimensional framework stucture.

Comment

The synthesis of hybrid organic–inorganic compounds is a very fruitful tool for obtaining frameworks with porous properties (Banglin *et al.*, 2001; Ferey, 2001; Snejko *et al.*, 2002). Weak interactions play an important role in these compounds and many frameworks are linked by different kinds of weak interactions, such as hydrogen bonds. We report here the preparation and crystal structure of the title cobalt(II) complex, (I) (Fig. 1).



(I)

The 5-hydroxyisophthalic acid starting material does not coordinate to the metal ion, but it affects the manner of coordination of the Co^{II} ion. A linear sulfate-anion-bridged polymeric Co^{II} complex was obtained which is different from the reference structure (Li & Zhou, 1987), where the sulfate anion is monodentate instead of bridging.

In the repeat unit of (I), the geometry around the Co^{II} ion is octahedral, with the metal chelated by the heterocycle and also bonded to two water molecules (Fig. 1), with Co—N distances of 2.102 (2) Å and Co—O distances of 2.088 (2) Å (Table 1), forming a distorted square plane. The sulfate anion is present in a μ_2-bridging mode (Fig. 2) and binds to each Co atom through one O atom, with Co—O distances of 2.166 (2) Å, forming a linear structure. The Co atom lies on a twofold rotation axis.

O—H···O hydrogen bonding links coordinated water molecules and sulfate anions, both within the repeat unit and between adjacent polymer chains (Table 2), generating a two-dimensional framework structure.

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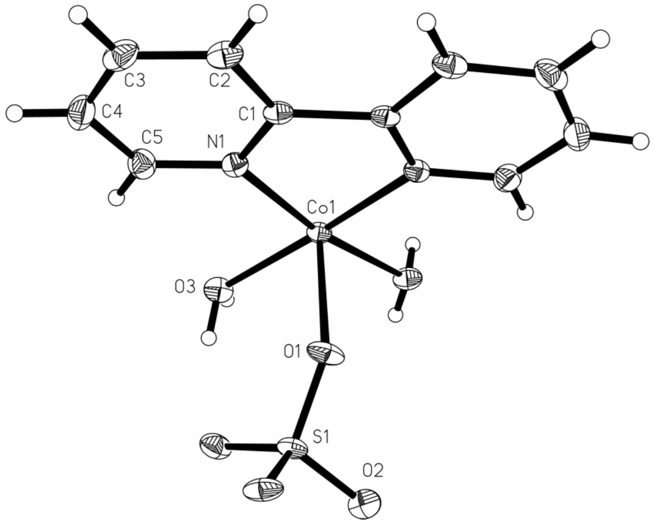

Figure 1
A view of the repeat unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

Experimental

Cobalt(II) sulfate heptahydrate (0.28 g, 1 mmol) was dissolved in water (10 ml). A dimethylformamide solution (10 ml) of 2,2′-bipyridine (0.16 g, 1 mmol) and 5-hydroxyisophthalic acid (0.18 g, 1 mmol) was then added dropwise with stirring at 298 K. The reaction mixture was filtered and the filtrate allowed to stand for about five weeks until pink single crystals of (I) were obtained. Prism-shaped crystals suitable for X-ray diffraction were collected by filtration, washed with water and ethanol, and dried in air.

Crystal data

$[Co(C_{10}H_8N_2)(H_2O)_2SO_4]$
$M_r = 347.21$
Monoclinic, $C2/c$
$a = 15.524$ (12) Å
$b = 12.802$ (10) Å
$c = 6.601$ (5) Å
$\beta = 102.56$ (3)°
$V = 1280.5$ (17) Å^3
$Z = 4$
$D_x = 1.801$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1150 reflections
$\theta = 2.8$–25.2°
$\mu = 1.53$ mm^{-1}
$T = 298$ (2) K
Prism, pink
$0.30 \times 0.10 \times 0.08$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.629$, $T_{max} = 0.885$
3266 measured reflections
1150 independent reflections
1116 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.2°$
$h = -18 \rightarrow 17$
$k = -15 \rightarrow 15$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.071$
$S = 1.13$
1150 reflections
97 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 1.982P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

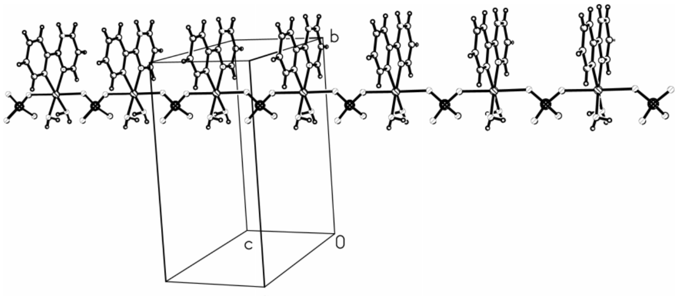

Figure 2
The linear structure of (I), bridged by sulfate anions.

Table 1
Selected geometric parameters (Å, °).

Co1—O3	2.088 (2)	Co1—O1	2.166 (2)
Co1—N1	2.102 (2)		
O3^i—Co1—O3	93.11 (12)	N1—Co1—O1	90.96 (7)
O3^i—Co1—N1	171.24 (7)	N1^i—Co1—O1	88.23 (7)
O3—Co1—N1	94.76 (9)	O1—Co1—O1^i	178.95 (8)
N1—Co1—N1^i	77.67 (12)	C5—N1—Co1	125.59 (16)
O3^i—Co1—O1	93.24 (7)	C1—N1—Co1	116.00 (16)
O3—Co1—O1	87.49 (7)	S1—O1—Co1	137.71 (10)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1···O2^{ii}	0.74 (3)	2.01 (3)	2.735 (3)	169 (3)
O3—H3···O2^{iii}	0.82	1.88	2.674 (3)	163

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

The water H atoms were positioned geometrically and refined subject to the restraint O—H = 0.82 (1) Å. The other H atoms were positioned geometrically and were allowed to ride on their parent atoms at C—H distances of 0.93 Å, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976) and *XP* in *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL*97.

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