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catena-Poly[[[diaquahexapyridine-μ-sulfato-dicobalt(II)]-μ-sulfato] tetrahydrate]

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In the crystal structure of the title compound, $[Co_2(SO_4)_2(C_5H_5N)_6(H_2O)_2]\cdot4H_2O$, the sulfate dianion bridges a $(C_5H_5N)_4Co$ unit to a $(C_5H_5N)_2(H_2O)_2Co$ unit, forming a chain that runs along the *a* axis of the monoclinic unit cell. The Co atoms of the units lie on special positions, each of $\overline{1}$ site symmetry. Adjacent chains are linked through the uncoordinated water molecules into layers.

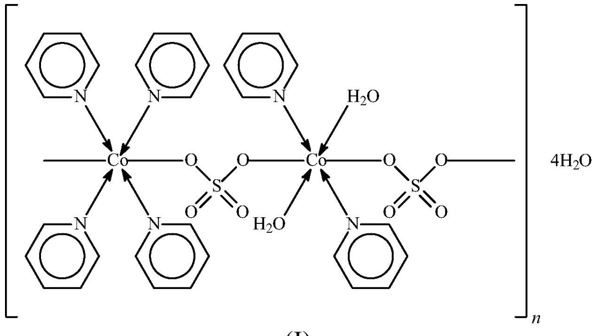
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.111
Data-to-parameter ratio = 15.6

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

Comment

Cobalt(II) sulfate crystallizes from pyridine as the μ_2-sulfato-bridged pyridine-coordinated triaqua compound, (I). The compound adopts a six-coordinate chain structure and the O atoms of the sulfate groups are *cis* to each other in an octahedral geometry (Zhang, 2004). The formulation of the title compound, expressed as $[(C_5H_5N)_3(SO_4)(H_2O)Co]\cdot2H_2O$, has two of the three water molecules in outer-sphere coordination. There are two cobalt(II) atoms, and both lie on special positions of $\overline{1}$ site symmetry. The sulfate dianion bridges a $(C_5H_5N)_4Co$ unit to a $(C_5H_5N)_2(H_2O)_2Co$ unit, forming a chain that runs along the *a* axis of the monoclinic unit cell (Fig. 1). The manner of bridging leads to a *trans* alignment of the O atoms of the dianion. Adjacent chains are linked by hydrogen bonds (Table 2) into layers.



(I)

Experimental

4-Methylmercaptobenzaldehyde (0.33 g, 2.17 mmol) and *N*-phenylthiourea (0.32 g, 2.17 mmol) were heated with cobalt(II) acetate tetrahydrate (0.27 g, 1.09 mmol) in ethanol (30 ml) for several hours. Several drops of triethylamine were also added. The solvent was then removed and the product recrystallized from pyridine to furnish pale-pink crystals. The sulfur in the compound is probably derived from the decomposition of the thiourea; the mechanism of formation was not investigated further.

Crystal data

$[Co_2(SO_4)_2(C_5H_5N)_6(H_2O)_2]\cdot 4H_2O$
$M_r = 892.68$
Monoclinic, $P2_1/n$
$a = 12.486$ (2) Å
$b = 9.443$ (1) Å
$c = 16.839$ (2) Å
$\beta = 108.289$ (2)°
$V = 1885.1$ (4) Å^3
$Z = 2$
$D_x = 1.573$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 837 reflections
$\theta = 1.8$–27.5°
$\mu = 1.06$ mm^{-1}
$T = 298$ (2) K
Block, pink
0.26 × 0.19 × 0.13 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.769$, $T_{max} = 0.874$
10 748 measured reflections
4221 independent reflections
3588 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$
$h = -16 \rightarrow 13$
$k = -11 \rightarrow 12$
$l = -21 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.111$
$S = 1.14$
4221 reflections
271 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.7327P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.096 (2)	Co2—O2	2.124 (2)
Co1—N1	2.152 (2)	Co2—O1*w*	2.134 (2)
Co1—N2	2.223 (2)	Co2—N3	2.148 (2)
O1—Co1—O1^{i}	180	O2—Co2—O2^{ii}	180
O1—Co1—N1	89.12 (8)	O2—Co2—O1*w*	88.51 (7)
O1—Co1—N1^{i}	90.88 (8)	O2—Co2—O1*w*^{ii}	91.49 (7)
O1—Co1—N2	84.94 (8)	O2—Co2—N3^{ii}	88.86 (8)
O1—Co1—N2^{i}	95.06 (8)	O2—Co2—N3	91.14 (8)
N1—Co1—N1^{i}	180	O1*w*—Co2—O1*w*^{ii}	180
N1—Co1—N2	92.06 (8)	O1*w*—Co2—N3^{ii}	92.23 (9)
N1—Co1—N2^{i}	87.94 (8)	O1*w*—Co2—N3	87.77 (9)
N2—Co1—N2^{i}	180	N3^{ii}—Co2—N3	180

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O3^{ii}	0.85 (1)	1.80 (1)	2.644 (3)	170 (3)
O1*w*—H1*w*2···O2*w*	0.85 (1)	2.05 (1)	2.891 (3)	175 (3)
O2*w*—H2*w*1···O4^{iii}	0.85 (1)	1.92 (1)	2.759 (3)	168 (4)
O2*w*—H2*w*2···O3*w*	0.85 (1)	1.97 (2)	2.742 (4)	150 (4)
O3*w*—H3*w*1···O2^{iii}	0.85 (1)	1.98 (1)	2.821 (3)	173 (4)
O3*w*—H3*w*2···O2*w*^{iii}	0.85 (1)	1.95 (1)	2.787 (4)	168 (4)

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

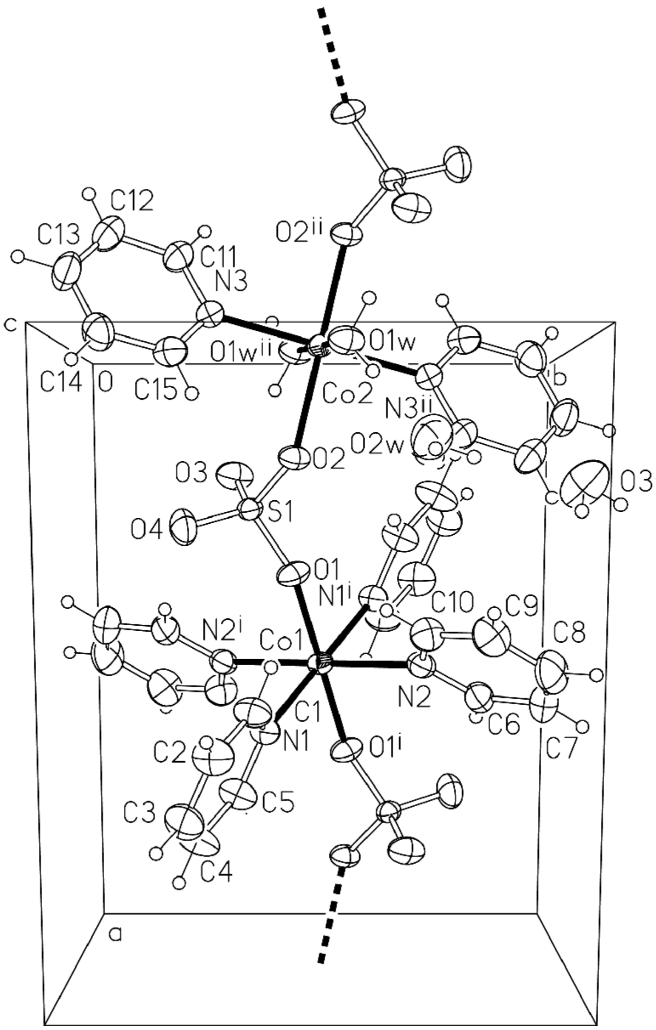


Figure 1
ORTEPII plot (Johnson, 1976) of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $-x, 1-y, 1-z$.]

The carbon-bound H atoms were placed in calculated positions (C—H = 0.93 Å) and were treated as riding, with U_{iso}(H) values set at 1.2 times U_{eq}(C). The water H atoms were located and refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å.

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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Acta Cryst. (2005). E**61**, m474–m475 Ali *et al.* • $[Co_2(SO_4)_2(C_5H_5N)_6(H_2O)_2]\cdot 4H_2O$ **m475**