Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

A one-dimensional coordination polymer: *catena*-poly[[triaquapyridinecobalt(II)]-μ-sulfato]

Yu-Xia Zhang

Department of Chemistry, Xinyang Normal University, Henan 464000, People's Republic of China

Correspondence e-mail: yuxiazhang@eyou.com

Received 21 November 2003
Accepted 1 December 2003
Online 12 December 2003

Key indicators

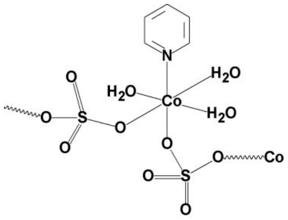
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.023
wR factor = 0.053
Data-to-parameter ratio = 12.3

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

In the structure of $[Co(C_5H_5N)(H_2O)_3SO_4]_n$, a one-dimensional coordination polymer, each Co^{II} atom is octahedrally coordinated by two O atoms of two different sulfate ions, a pyridine molecule and three water molecules. The polymeric chains are connected by weak intermolecular O—H···O hydrogen-bonding interactions to give a two-dimensional structure.

Comment

The most important driving forces in crystal engineering include coordination bonding and hydrogen-bonding interactions. Networks assembled from mono- or polynuclear metal complexes *via* hydrogen-bonding interactions have been reported recently (Aakeröy *et al.*, 1998). The unique strength, directionality, and complementarity of non-covalent hydrogen bonds play a central role in the creation of a variety of architectures for molecular self-assembly and recognition in chemical, physical and biological sciences (Lehn, 1995; Whitesides *et al.*, 1991; Rebek, 1990). Here, the structure of a one-dimensional coordination polymer, $[Co(C_5H_5N)(H_2O)_3SO_4]_n$, (I), which features a two-dimensional hydrogen-bonded network resulting from inter-polymer O—H···O hydrogen-bonding interactions, is reported.



(I)

The X-ray structure determination reveals that (I) is a one-dimensional coordination polymer (Fig. 1). The coordination geometry around the Co^{II} atom is octahedral; one of the

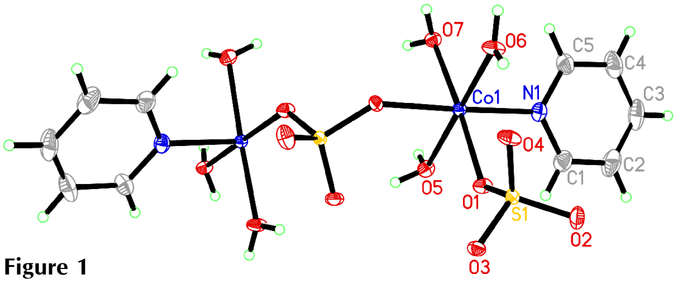


Figure 1
A part of the polymeric chain, showing 30% probability displacement ellipsoids and the atom-numbering scheme for the contents of the asymmetric unit.

sulfate O atoms (O1) and the three water O atoms (O5, O6 and O7) occupy the basal plane, with Co—O distances in the normal range of 2.0762 (16)–2.1358 (14) Å. An O atom of another sulfate ion, $O3^{ii}$ [symmetry code: (ii) $1 - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$], and the N atom of the pyridine ligand, N1, occupy the two apices of the octahedron, with Co—O and Co—N distances of 2.1114 (14) and 2.1056 (18), respectively.

In the crystal structure, the polymeric chains are arranged parallel to the *b* axis. In each polymeric chain, O6—H6*A*···O4, O5—H5*B*···$O2^{i}$, O5—H5*C*···$O4^{ii}$ and O7—H7*A*···$O4^{i}$ hydrogen bonds involving the water molecules and sulfate O atoms are observed [symmetry code: (i) x, $y - 1$, z]. Adjacent polymeric chains are inter-linked through O6—H6*B*···$O1^{iii}$ and O7—H7*B*···$O3^{iii}$ hydrogen bonds to form a two-dimensional network [symmetry code: (iii) x, $\frac{1}{2} - y$, $z + \frac{1}{2}$]. The geometry of these O—H···O hydrogen bonds and the symmetry codes are given in Table 2.

Experimental

The title compound was synthesized by the reaction of $Co(SO_4)_2 \cdot 3H_2O$ and pyridine (molar ratio 1:2) in water. The concentrated solution was left undisturbed for slow evaporation of the solvent to give red crystals. Analysis found: C 20.54, H 3.63, N 4.99%; calculated for $C_5H_{11}CoNO_7S$: C 20.84, H 3.85, N 4.86%.

Crystal data

$[Co(SO_4)(C_5H_5N)(H_2O)_3]$
$M_r = 288.14$
Monoclinic, $P2_1/c$
$a = 11.951$ (4) Å
$b = 7.639$ (2) Å
$c = 11.507$ (4) Å
$\beta = 110.711$ (4)°
$V = 982.7$ (5) Å^3
$Z = 4$

$D_x = 1.948$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 642 reflections
$\theta = 3.2$–19.9°
$\mu = 1.98$ mm^{-1}
$T = 293$ (2) K
Block, red
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.599$, $T_{max} = 0.674$
5362 measured reflections

1988 independent reflections
1710 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.4$°
$h = -14 \rightarrow 14$
$k = -9 \rightarrow 8$
$l = -9 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.053$
$S = 1.04$
1988 reflections
161 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2 + 0.4534P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0271 (15)

Table 1
Selected geometric parameters (Å, °).

Co1—O6	2.0762 (16)	Co1—$O3^{ii}$	2.1114 (14)
Co1—O7	2.1050 (15)	Co1—O5	2.1144 (16)
Co1—N1	2.1056 (18)	Co1—O1	2.1358 (14)
O6—Co1—O7	88.73 (6)	N1—Co1—O5	90.25 (7)
O6—Co1—N1	91.15 (7)	$O3^{i}$—Co1—O5	91.01 (6)
O7—Co1—N1	91.26 (6)	O6—Co1—O1	92.37 (6)
O6—Co1—$O3^{ii}$	87.63 (6)	O7—Co1—O1	176.61 (6)
O7—Co1—$O3^{ii}$	87.19 (5)	N1—Co1—O1	91.92 (6)
N1—Co1—$O3^{ii}$	178.05 (6)	$O3^{i}$—Co1—O1	89.65 (5)
O6—Co1—O5	177.86 (6)	O5—Co1—O1	85.96 (6)
O7—Co1—O5	92.86 (6)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*B*···$O2^{i}$	0.82 (1)	1.95 (2)	2.777 (2)	176 (3)
O5—H5*C*···$O4^{ii}$	0.82 (1)	2.12 (2)	2.848 (3)	148 (3)
O6—H6*A*···O4	0.81 (1)	1.97 (2)	2.709 (2)	151 (3)
O6—H6*B*···$O1^{iii}$	0.82 (1)	2.01 (2)	2.828 (2)	172 (2)
O7—H7*A*···$O4^{i}$	0.81 (1)	2.07 (2)	2.875 (2)	171 (2)
O7—H7*B*···$O3^{iii}$	0.81 (1)	1.97 (1)	2.781 (2)	174 (2)

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

C-bound H atoms were placed at calculated positions and allowed to ride on the atom to which they are bonded [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. H atoms of the water molecules were located in a difference map and their positional and U_{iso} parameters were refined. O—H distances were restrained to 0.82 (1) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

YXZ gratefully acknowledges the financial support of the Science Foundation of Henan State Education Commission in China (No. 2001150006).

References

Aakeröy, C. B., Beatty, A. M. & Leinen, D. S. (1998). *J. Am. Chem. Soc.* **120**, 7383–7384.
Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Lehn, J. M. (1995). *Supramolecular Chemistry*. Weinheim: VCH.
Rebek, J. (1990). *Angew. Chem. Int. Ed. Engl.* **29**, 102–103.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Whitesides, G. M., Mathias, J. P. & Seto, C. T. (1991). *Science*, **254**, 1312–1313.