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catena-Poly[[silver(I)-[μ-4-(2-pyridyl)-pyrimidine-2-sulfonato]] monohydrate]

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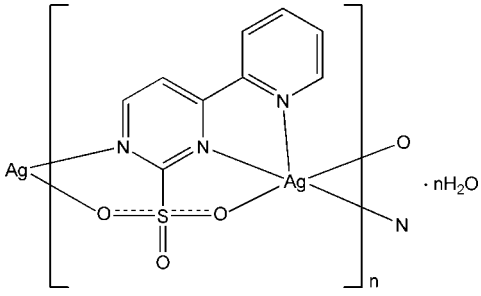
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.024; wR factor = 0.071; data-to-parameter ratio = 15.5.

In the title compound, $\{[Ag(C_9H_6N_3O_3S)]\cdot H_2O\}_n$, the Ag^I atom is coordinated by three N atoms and two sulfonate O atoms from two different 4-(2-pyridyl)pyrimidine-2-sulfonate ligands. The ligand bridges two Ag^I atoms, forming a polymeric zigzag chain propagating parallel to [001]. The uncoordinated water molecule is involved in hydrogen bonds with sulfonate O atoms.

Related literature

For our previous work with the 4-(2-pyridyl)pyrimidine-2-sulfonate ligand, see: Zhu *et al.* (2007).



Experimental

Crystal data

$[Ag(C_9H_6N_3O_3S)]\cdot H_2O$
M_r = 362.12
Monoclinic, $P2_1/c$
a = 6.9020 (3) Å
b = 13.6228 (6) Å
c = 12.1337 (5) Å
β = 99.975 (2)°
V = 1123.62 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.99 mm^{-1}
T = 298 K
0.18 × 0.15 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.706, T_{max} = 0.788
6630 measured reflections
2533 independent reflections
2160 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.071
S = 1.02
2533 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag1—N1^{i}	2.279 (2)	Ag1—O1^{i}	2.668 (2)
Ag1—N2	2.393 (2)	Ag1—O3	2.693 (2)
Ag1—N3	2.337 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H2···O3	0.85	1.95	2.793 (4)	173
O4—H1···O2^{ii}	0.85	2.07	2.913 (4)	173

Symmetry code: (ii) $-x+2, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2295).

References

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhu, H.-B., Dong, H.-Z., Huang, W. & Gou, S.-H. (2007). *J. Mol. Struct.* **831**, 55–60.

supporting information

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catena-Poly[[silver(I)-[μ-4-(2-pyridyl)pyrimidine-2-sulfonato]] monohydrate]

Hai-Bin Zhu

S1. Comment

In our previous work, we have reported several divalent transition metal coordination compounds with 4-(2-pyridyl)-pyrimidine-2-sulfonate (*L*) ligand (Zhu *et al.*, 2007). Herein, we present a new silver(I) coordination polymer with *L*.

The title compound has a polymeric zigzag chain structure, where the Ag^{I} atom is penta-coordinated by three N atoms and two sulfonate O atoms from two *L* ligands (Fig. 1). The Ag—N bond lengths vary between 2.279 (2) and 2.393 (2) Å, and the Ag—O distances are in the range of 2.668 (2) and 2.693 (2)Å (Table 1). The uncoordinated water molecule is involved in hydrogen bonds with sulfonate O atoms (Table 2).

S2. Experimental

A colorless solution of $AgNO_3$ (0.017 g, 0.1 mmol) in CH_3CN (5 ml) was carefully layered onto a solution of 4-(2-pyridyl)pyrimidine-2-sulfonic acid (0.026 g, 1 mmol) in H_2O (5 ml). Diffusion between the two phases over a period of 5 d produced light-yellow crystals (yield: 0.026 g, 72% based on silver nitrate).

S3. Refinement

H atoms bounded to C atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H =0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). The positions of the water H atoms were found from a difference Fourier map and refined as riding with O—H = 0.85 Å and U_{iso}(H) = 1.2U_{eq}(O).

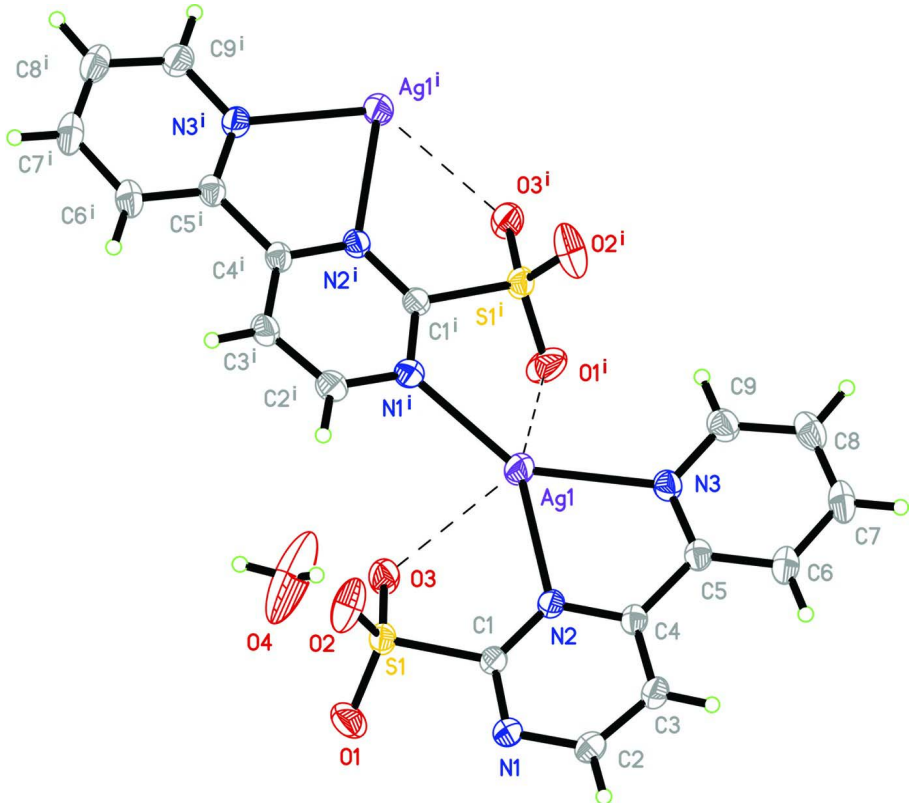

Figure 1

The coordination environment around Ag^{I} in the title complex. Displacement ellipsoids are drawn at the 30% probability level. The Ag···O bonds are shown as dashed lines. [Symmetry code: (i) x, 1/2-y, 1/2+z.]

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Crystal data

$[Ag(C_9H_6N_3O_3S)]\cdot H_2O$
$M_r = 362.12$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.9020\ (3)$ Å
$b = 13.6228\ (6)$ Å
$c = 12.1337\ (5)$ Å
$\beta = 99.975\ (2)°$
$V = 1123.62\ (8)$ Å^3
$Z = 4$
$F(000) = 712$
$D_x = 2.147$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2533 reflections
$\theta = 2.3–27.5°$
$\mu = 1.99$ mm^{-1}
$T = 298$ K
Block, colorless
0.18 × 0.15 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.706$, $T_{max} = 0.788$
6630 measured reflections
2533 independent reflections
2160 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -8\rightarrow8$
$k = -17\rightarrow15$
$l = -15\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.071$
$S = 1.02$
2533 reflections
163 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.5886P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.81252 (4)	0.174975 (15)	0.078449 (17)	0.04992 (10)
N2	0.7873 (3)	0.14417 (14)	−0.11767 (17)	0.0335 (4)
N3	0.7593 (3)	0.00808 (15)	0.04023 (18)	0.0389 (4)
C3	0.7075 (4)	0.03190 (19)	−0.2672 (2)	0.0420 (6)
H3A	0.6753	−0.0311	−0.2936	0.050*
C4	0.7418 (3)	0.05178 (16)	−0.1536 (2)	0.0333 (5)
C6	0.6871 (4)	−0.1210 (2)	−0.0934 (3)	0.0480 (6)
H6A	0.6683	−0.1416	−0.1675	0.058*
C9	0.7459 (4)	−0.0571 (2)	0.1213 (3)	0.0477 (6)
H9A	0.7662	−0.0355	0.1950	0.057*
C8	0.7034 (4)	−0.1546 (2)	0.1002 (3)	0.0527 (7)
H8A	0.6952	−0.1977	0.1586	0.063*
C7	0.6733 (4)	−0.1873 (2)	−0.0083 (3)	0.0544 (8)
H7A	0.6440	−0.2529	−0.0246	0.065*
C5	0.7293 (3)	−0.02331 (18)	−0.0662 (2)	0.0359 (5)
S1	0.85817 (10)	0.33521 (4)	−0.14563 (5)	0.04032 (15)
N1	0.7693 (3)	0.19927 (16)	−0.30431 (18)	0.0410 (5)
C1	0.7996 (3)	0.21175 (17)	−0.1937 (2)	0.0338 (5)
O2	0.6717 (4)	0.38366 (17)	−0.1628 (2)	0.0786 (8)
C2	0.7221 (4)	0.1074 (2)	−0.3396 (2)	0.0463 (6)
H2B	0.6986	0.0947	−0.4160	0.056*
O1	0.9932 (4)	0.36957 (18)	−0.21511 (19)	0.0694 (7)
O3	0.9460 (3)	0.32665 (13)	−0.02960 (17)	0.0521 (5)
O4	1.2896 (6)	0.4143 (3)	0.0834 (5)	0.189 (3)
H2	1.1797	0.3920	0.0504	0.226*
H1	1.3116	0.4722	0.1086	0.226*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.07851 (18)	0.03703 (13)	0.03468 (13)	0.00054 (9)	0.01113 (10)	−0.00254 (7)
N2	0.0349 (10)	0.0297 (9)	0.0368 (11)	−0.0010 (8)	0.0082 (8)	−0.0028 (8)
N3	0.0411 (11)	0.0335 (10)	0.0430 (11)	0.0032 (9)	0.0096 (9)	0.0039 (9)
C3	0.0486 (14)	0.0329 (12)	0.0455 (14)	−0.0056 (11)	0.0107 (11)	−0.0092 (10)

C4	0.0272 (11)	0.0300 (11)	0.0432 (13)	0.0012 (8)	0.0076 (9)	−0.0016 (9)
C6	0.0498 (15)	0.0319 (13)	0.0616 (18)	−0.0013 (11)	0.0077 (13)	−0.0046 (11)
C9	0.0497 (15)	0.0428 (14)	0.0526 (16)	0.0047 (12)	0.0144 (12)	0.0088 (12)
C8	0.0436 (15)	0.0419 (14)	0.074 (2)	0.0054 (11)	0.0144 (14)	0.0200 (14)
C7	0.0494 (16)	0.0296 (13)	0.083 (2)	0.0000 (11)	0.0094 (15)	0.0069 (13)
C5	0.0283 (11)	0.0305 (11)	0.0496 (14)	0.0021 (9)	0.0091 (10)	0.0000 (10)
S1	0.0537 (4)	0.0295 (3)	0.0366 (3)	−0.0036 (3)	0.0045 (3)	−0.0018 (2)
N1	0.0530 (13)	0.0370 (10)	0.0342 (11)	−0.0035 (9)	0.0110 (9)	−0.0035 (8)
C1	0.0352 (11)	0.0318 (11)	0.0354 (12)	−0.0005 (9)	0.0089 (9)	−0.0030 (9)
O2	0.0733 (15)	0.0478 (13)	0.105 (2)	0.0202 (11)	−0.0121 (14)	−0.0218 (13)
C2	0.0590 (16)	0.0432 (14)	0.0368 (13)	−0.0060 (12)	0.0087 (11)	−0.0094 (11)
O1	0.0992 (17)	0.0608 (14)	0.0516 (12)	−0.0412 (13)	0.0224 (12)	−0.0040 (10)
O3	0.0732 (13)	0.0410 (11)	0.0394 (11)	−0.0113 (9)	0.0021 (9)	−0.0044 (8)
O4	0.113 (3)	0.114 (3)	0.304 (7)	0.030 (2)	−0.063 (4)	−0.126 (4)

Geometric parameters (Å, º)

Ag1—N1^{i}	2.279 (2)	C9—C8	1.374 (4)
Ag1—N2	2.393 (2)	C9—H9A	0.9300
Ag1—N3	2.337 (2)	C8—C7	1.370 (5)
Ag1—O1^{i}	2.668 (2)	C8—H8A	0.9300
Ag1—O3	2.693 (2)	C7—H7A	0.9300
N2—C1	1.317 (3)	S1—O2	1.429 (2)
N2—C4	1.351 (3)	S1—O3	1.438 (2)
N3—C9	1.340 (3)	S1—O1	1.439 (2)
N3—C5	1.342 (3)	S1—C1	1.803 (2)
C3—C2	1.368 (4)	N1—C1	1.333 (3)
C3—C4	1.384 (3)	N1—C2	1.344 (3)
C3—H3A	0.9300	N1—Ag1^{ii}	2.279 (2)
C4—C5	1.487 (3)	C2—H2B	0.9300
C6—C7	1.388 (4)	O4—H2	0.8500
C6—C5	1.389 (4)	O4—H1	0.8500
C6—H6A	0.9300		
N1^{i}—Ag1—N3	145.30 (7)	C8—C9—H9A	118.5
N1^{i}—Ag1—N2	139.26 (7)	C7—C8—C9	119.0 (3)
N3—Ag1—N2	69.52 (7)	C7—C8—H8A	120.5
O1^{i}—Ag1—N2	146.68 (7)	C9—C8—H8A	120.5
O1^{i}—Ag1—N3	89.82 (7)	C8—C7—C6	119.0 (3)
O1^{i}—Ag1—N1^{i}	71.05 (8)	C8—C7—H7A	120.5
O3—Ag1—N1^{i}	79.63 (7)	C6—C7—H7A	120.5
O3—Ag1—N2	67.83 (7)	N3—C5—C6	121.6 (2)
O3—Ag1—N3	134.83 (6)	N3—C5—C4	116.7 (2)
C1—N2—C4	117.7 (2)	C6—C5—C4	121.7 (2)
C1—N2—Ag1	124.89 (16)	O2—S1—O3	113.36 (16)
C4—N2—Ag1	117.21 (15)	O2—S1—O1	115.00 (18)
C9—N3—C5	118.4 (2)	O3—S1—O1	113.20 (14)
C9—N3—Ag1	121.87 (19)	O2—S1—C1	103.76 (13)

C5—N3—Ag1	119.59 (16)	O3—S1—C1	105.92 (11)
C2—C3—C4	118.3 (2)	O1—S1—C1	104.21 (12)
C2—C3—H3A	120.9	C1—N1—C2	115.2 (2)
C4—C3—H3A	120.9	C1—N1—Ag1^{ii}	121.18 (17)
N2—C4—C3	119.6 (2)	C2—N1—Ag1^{ii}	123.49 (17)
N2—C4—C5	116.7 (2)	N2—C1—N1	126.8 (2)
C3—C4—C5	123.7 (2)	N2—C1—S1	117.60 (18)
C7—C6—C5	119.0 (3)	N1—C1—S1	115.62 (18)
C7—C6—H6A	120.5	N1—C2—C3	122.4 (2)
C5—C6—H6A	120.5	N1—C2—H2B	118.8
N3—C9—C8	122.9 (3)	C3—C2—H2B	118.8
N3—C9—H9A	118.5	H2—O4—H1	126.2

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) x, $-y+1/2$, $z-1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H2···O3	0.85	1.95	2.793 (4)	173
O4—H1···O2^{iii}	0.85	2.07	2.913 (4)	173

Symmetry code: (iii) $-x+2$, $-y+1$, $-z$.