

Poly[μ_2 -chlorido-(μ_2 -3*H*⁺-1,3,4-thiadiazolium-2-thiolato- κ^2 S:S)silver(I)]

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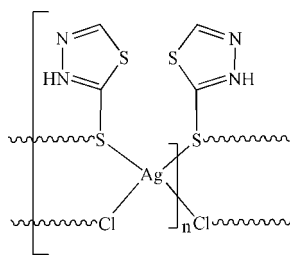
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 Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{N}-\text{C}) = 0.007$ Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 15.9.

In the title compound, $[\text{AgCl}(\text{C}_2\text{H}_2\text{N}_2\text{S}_2)]_n$, the Ag^{I} ion has a distorted tetrahedral geometry, defined by two S atoms of two symmetry-related 1,3,4-thiadiazolium-2-thiolate ligands and two chloride ions. The Ag^{I} ions are bridged into a two-dimensional network parallel to the ab plane by chloride ions and thiadiazole ligands. In the network, the Ag^{I} ions are separated by 4.0316 (12) Å along the a axis and by 4.8822 (13) Å along the b axis. $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds are observed within the network.

Related literature

For bond-length data, see: Dinger *et al.* (1998); Wei *et al.* (2008).



Experimental

Crystal data

 $[\text{AgCl}(\text{C}_2\text{H}_2\text{N}_2\text{S}_2)]$
 $M_r = 261.50$

 Orthorhombic, $P2_12_12_1$
 $a = 4.0316$ (9) Å

 $b = 8.473$ (2) Å

 $c = 18.368$ (4) Å

 $V = 627.4$ (2) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 4.19$ mm⁻¹
 $T = 294$ K
 $0.23 \times 0.13 \times 0.06$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

 Absorption correction: multi-scan (SADABS; Bruker, 1997)
 $T_{\text{min}} = 0.446$, $T_{\text{max}} = 0.786$

 4169 measured reflections
 1161 independent reflections
 1085 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.083$
 $S = 1.09$

1161 reflections

73 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.65$ e Å⁻³

Absolute structure: Flack (1983),

438 Friedel pairs

Flack parameter: 0.05 (6)

Table 1

Selected bond lengths (Å).

Ag1–S2 ⁱ	2.5454 (14)	Ag1–Cl1 ⁱⁱ	2.5897 (15)
Ag1–S2	2.5695 (15)	Ag1–Cl1	2.6514 (15)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{Cl1}^{\text{ii}}$	0.86	2.38	3.197 (4)	158

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; 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: CI2771).

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supporting information

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Poly[μ_2 -chlorido-(μ_2 -3*H*⁺-1,3,4-thiadiazolium-2-thiolato- κ^2 S:S)silver(I)]

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S1. Comment

The asymmetric unit of the title compound consists of one Ag^I ion, one 1,3,4-thiadiazolium-2-thiolate ligand, and one Cl atom. As depicted in Fig. 1, the Ag^I ion is coordinated by two S atoms from two thiadiazole ligands and two Cl atoms in a distorted tetrahedral geometry. The Ag—S and Ag—Cl bond distances (Table 1) are within the range expected for such coordination bonds (Dinger *et al.*, 1998; Wei *et al.*, 2008). The thiadiazole ligand shows a monodentate bridging mode. The adjacent Ag^I atoms are bridged by Cl atoms to form chains, which are cross-linked by thiadiazole ligands to form a two-dimensional network parallel to the *ab* plane (Fig. 2). In the network, the Ag atoms are separated by 4.0316 (12) Å along the *a* axis and 4.8822 (13) Å along the *b* axis. Intramolecular N—H···Cl hydrogen bonds are observed in the network (Table 2).

S2. Experimental

1,3,4-Thiadiazolium-2-thiolate (0.5 mmol) was added at room temperature to a ammonia solution (10 ml) of AgCl (0.5 mmol). After the addition, a colourless precipitate immediately formed and the suspension was stirred for 2 h. The precipitate was filtered off and washed with MeCN. Single crystals suitable for X-ray analysis were obtained by slow diffusion of Et₂O into a water solution of the solid.

S3. Refinement

H atoms were positioned geometrically and treated as riding, with N—H = 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$, and C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

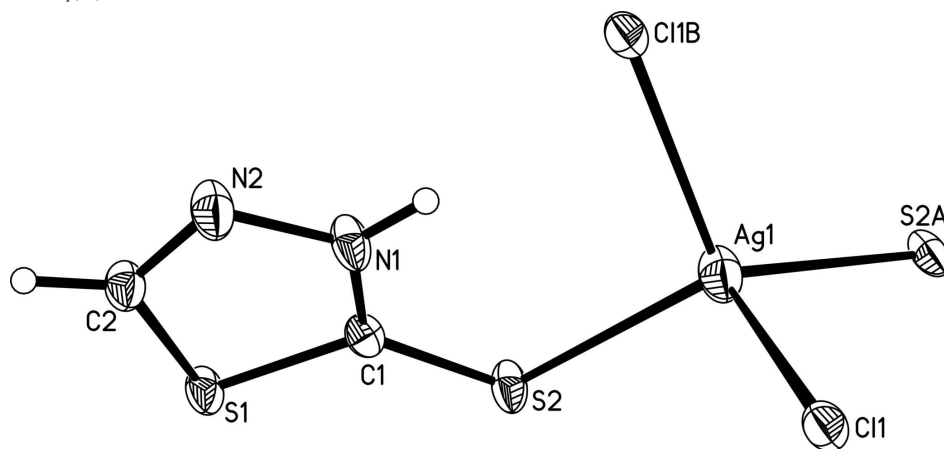


Figure 1

A view of the local coordination of the Ag^I atom in the title compound. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (A) 2 -*x*, *y* - 1/2, 1/2 - *z*; (B) *x* - 1, *y*, *z*.

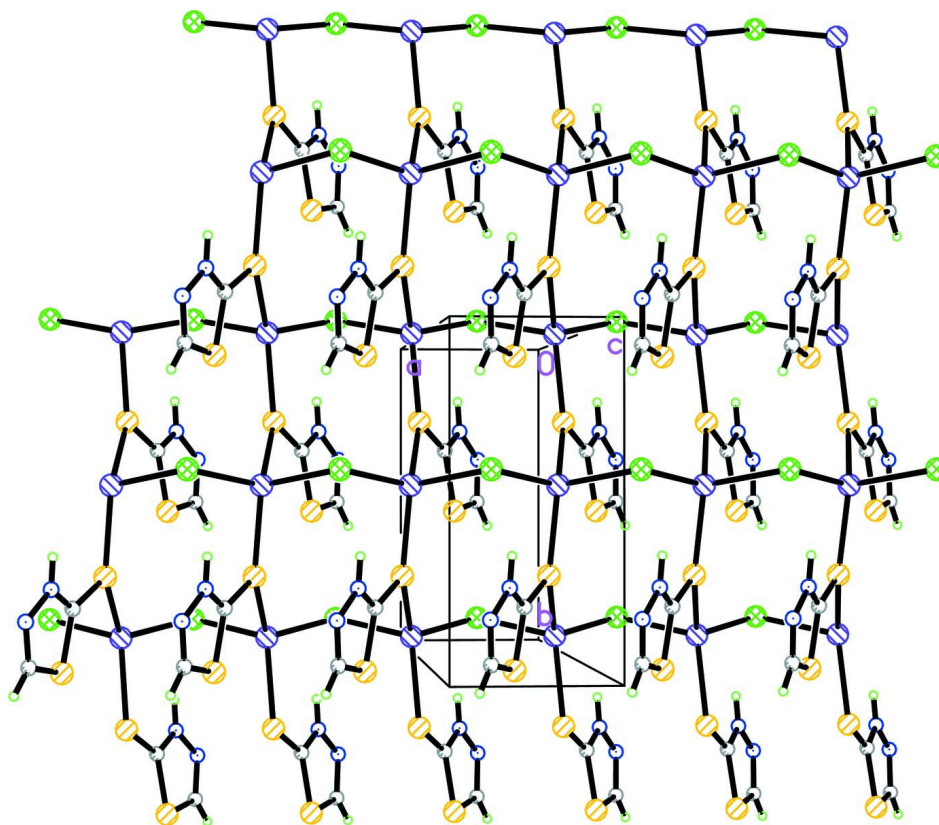


Figure 2

A view of the two-dimensional network parallel to the *ab* plane.

Poly[μ_2 -chlorido-(μ_2 -3*H*⁺-1,3,4-thiadiazolium-2-thiolato- κ^2 S:S)silver(I)]

Crystal data

[AgCl(C₂H₂N₂S₂)]

$M_r = 261.50$

Orthorhombic, *P*2₁2₁2₁

Hall symbol: P 2ac 2ab

$a = 4.0316$ (9) Å

$b = 8.473$ (2) Å

$c = 18.368$ (4) Å

$V = 627.4$ (2) Å³

$Z = 4$

$F(000) = 496$

$D_x = 2.768$ Mg m⁻³

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 1870 reflections

$\theta = 3.3$ – 27.2°

$\mu = 4.19$ mm⁻¹

$T = 294$ K

Block, colourless

$0.23 \times 0.13 \times 0.06$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 1997)

$T_{\min} = 0.446$, $T_{\max} = 0.786$

4169 measured reflections

1161 independent reflections

1085 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -4 \rightarrow 4$

$k = -10 \rightarrow 10$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.083$
 $S = 1.09$
 1161 reflections
 73 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
 $w = 1/[\sigma^2(F_o^2) + (0.0526P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.22 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.65 \text{ e } \text{Å}^{-3}$
 Absolute structure: Flack (1983), 438 Friedel
 pairs
 Absolute structure parameter: 0.05 (6)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.97702 (12)	-0.03604 (5)	0.18414 (2)	0.04254 (19)
Cl1	1.4870 (4)	-0.08711 (14)	0.09609 (6)	0.0323 (3)
S1	0.6628 (4)	0.55205 (15)	0.14333 (7)	0.0346 (3)
S2	0.9323 (4)	0.25800 (16)	0.21696 (7)	0.0356 (4)
N1	0.6067 (12)	0.2855 (5)	0.0889 (2)	0.0350 (12)
H1	0.6188	0.1852	0.0823	0.042*
N2	0.4580 (15)	0.3800 (5)	0.0387 (2)	0.0420 (13)
C1	0.7324 (12)	0.3512 (6)	0.1482 (2)	0.0266 (11)
C2	0.4723 (15)	0.5228 (6)	0.0601 (3)	0.0329 (12)
H2	0.3863	0.6056	0.0327	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0574 (3)	0.0311 (3)	0.0391 (3)	0.0042 (2)	-0.0090 (2)	0.00192 (16)
Cl1	0.0369 (7)	0.0237 (6)	0.0365 (6)	-0.0013 (6)	-0.0016 (6)	-0.0009 (5)
S1	0.0485 (8)	0.0187 (6)	0.0364 (7)	0.0010 (6)	-0.0108 (6)	-0.0037 (6)
S2	0.0546 (9)	0.0215 (6)	0.0307 (7)	0.0065 (6)	-0.0107 (6)	-0.0034 (5)
N1	0.059 (3)	0.019 (2)	0.026 (2)	0.003 (2)	-0.007 (2)	-0.0031 (18)
N2	0.065 (4)	0.027 (3)	0.034 (2)	0.003 (3)	-0.015 (3)	0.0008 (19)
C1	0.032 (3)	0.023 (3)	0.025 (2)	0.000 (2)	0.004 (2)	-0.001 (2)
C2	0.044 (3)	0.026 (3)	0.028 (2)	0.002 (3)	-0.008 (2)	0.001 (2)

Geometric parameters (Å , $^\circ$)

Ag1—S2 ⁱ	2.5454 (14)	S2—C1	1.694 (5)
Ag1—S2	2.5695 (15)	S2—Ag1 ^{iv}	2.5453 (14)
Ag1—Cl1 ⁱⁱ	2.5897 (15)	N1—C1	1.323 (6)
Ag1—Cl1	2.6514 (15)	N1—N2	1.361 (6)
Cl1—Ag1 ⁱⁱⁱ	2.5897 (15)	N1—H1	0.86
S1—C1	1.727 (5)	N2—C2	1.273 (7)
S1—C2	1.729 (5)	C2—H2	0.93

S2 ⁱ —Ag1—S2	120.49 (3)	C1—N1—N2	118.6 (4)
S2 ⁱ —Ag1—Cl1 ⁱⁱ	116.15 (5)	C1—N1—H1	120.7
S2—Ag1—Cl1 ⁱⁱⁱ	104.77 (4)	N2—N1—H1	120.7
S2 ⁱ —Ag1—Cl1	102.24 (5)	C2—N2—N1	109.3 (4)
S2—Ag1—Cl1	110.84 (5)	N1—C1—S2	126.8 (4)
Cl1 ⁱⁱ —Ag1—Cl1	100.56 (5)	N1—C1—S1	108.1 (4)
Ag1 ⁱⁱⁱ —Cl1—Ag1	100.56 (5)	S2—C1—S1	125.1 (3)
C1—S1—C2	88.6 (2)	N2—C2—S1	115.4 (4)
C1—S2—Ag1 ^{iv}	106.32 (18)	N2—C2—H2	122.3
C1—S2—Ag1	108.09 (18)	S1—C2—H2	122.3
Ag1 ^{iv} —S2—Ag1	145.29 (5)		
S2 ⁱ —Ag1—Cl1—Ag1 ⁱⁱⁱ	-60.05 (5)	N2—N1—C1—S2	-179.1 (4)
S2—Ag1—Cl1—Ag1 ⁱⁱⁱ	69.61 (5)	N2—N1—C1—S1	0.2 (6)
Cl1 ⁱⁱⁱ —Ag1—Cl1—Ag1 ⁱⁱⁱ	180.0	Ag1 ^{iv} —S2—C1—N1	-172.7 (5)
S2 ⁱ —Ag1—S2—C1	-158.63 (19)	Ag1—S2—C1—N1	2.7 (5)
Cl1 ⁱⁱ —Ag1—S2—C1	-25.46 (19)	Ag1 ^{iv} —S2—C1—S1	8.2 (4)
Cl1—Ag1—S2—C1	82.19 (19)	Ag1—S2—C1—S1	-176.5 (3)
S2 ⁱ —Ag1—S2—Ag1 ^{iv}	13.55 (10)	C2—S1—C1—N1	-0.5 (4)
Cl1 ⁱⁱⁱ —Ag1—S2—Ag1 ^{iv}	146.72 (12)	C2—S1—C1—S2	178.8 (4)
Cl1—Ag1—S2—Ag1 ^{iv}	-105.63 (12)	N1—N2—C2—S1	-0.9 (7)
C1—N1—N2—C2	0.4 (8)	C1—S1—C2—N2	0.8 (5)

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

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>
N1—H1...Cl1 ⁱⁱ	0.86	2.38	3.197 (4)	158

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