

# Poly[ $\mu_2$ -chlorido-( $\mu_2$ -3*H*<sup>+</sup>-1,3,4-thiadiazolium-2-thiolato- $\kappa^2$ S:S)silver(I)]

Jian-Ge Wang, Jian-Hua Qin\* and Pu-Zhou Hu

College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, People's Republic of China  
Correspondence e-mail: jh\_q128105@126.com

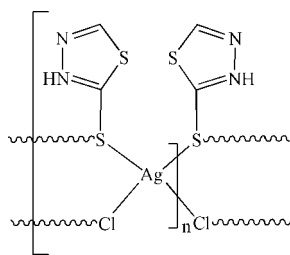
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Key indicators: single-crystal X-ray study;  $T = 294$  K; mean  $\sigma(\text{N}-\text{C}) = 0.007$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.083; data-to-parameter ratio = 15.9.

In the title compound,  $[\text{AgCl}(\text{C}_2\text{H}_2\text{N}_2\text{S}_2)]_n$ , the  $\text{Ag}^{\text{I}}$  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  $\text{Ag}^{\text{I}}$  ions are bridged into a two-dimensional network parallel to the  $ab$  plane by chloride ions and thiadiazole ligands. In the network, the  $\text{Ag}^{\text{I}}$  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) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 4.19$  mm<sup>-1</sup>

$T = 294$  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<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.65$  e Å<sup>-3</sup>

Absolute structure: Flack (1983),

438 Friedel pairs

Flack parameter: 0.05 (6)

**Table 1**

Selected bond lengths (Å).

Ag1–S2 <sup>i</sup>	2.5454 (14)	Ag1–Cl1 <sup>ii</sup>	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.

The authors thank Luoyang Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2771).

## References

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**supplementary materials**

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### Comment

The asymmetric unit of the title compound consists of one Ag<sup>I</sup> ion, one 1,3,4-thiadiazolium-2-thiolate ligand, and one Cl atom. As depicted in Fig. 1, the Ag<sup>I</sup> 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<sup>I</sup> 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).

### 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 Et<sub>2</sub>O into a water solution of the solid.

### 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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

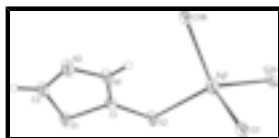


Fig. 1. A view of the local coordination of the Ag<sup>I</sup> atom in the title compound. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (A) 2 - *x*, *y* - 1/2, 1/2 - *z*; (B) *x* - 1, *y*, *z*.

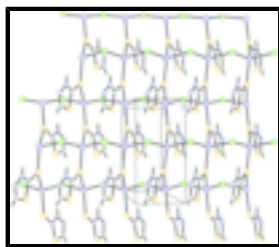


Fig. 2. A view of the two-dimensional network parallel to the *ab* plane.

## Poly[ $\mu_2$ -chlorido-( $\mu_2$ -3H<sup>+</sup>-1,3,4-thiadiazolium-2-thiolato- $\kappa^2$ S:S)silver(I)]

### Crystal data

[AgCl(C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> S <sub>2</sub> )]	$F_{000} = 496$
$M_r = 261.50$	$D_x = 2.768 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
Hall symbol: P 2ac 2ab	$\lambda = 0.71073 \text{ \AA}$
$a = 4.0316 (9) \text{ \AA}$	Cell parameters from 1870 reflections
$b = 8.473 (2) \text{ \AA}$	$\theta = 3.3\text{--}27.2^\circ$
$c = 18.368 (4) \text{ \AA}$	$\mu = 4.19 \text{ mm}^{-1}$
$V = 627.4 (2) \text{ \AA}^3$	$T = 294 \text{ K}$
$Z = 4$	Block, colourless
	$0.23 \times 0.13 \times 0.06 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer	1161 independent reflections
Radiation source: fine-focus sealed tube	1085 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.035$
$T = 294 \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 2.7^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -4 \rightarrow 4$
$T_{\text{min}} = 0.446$ , $T_{\text{max}} = 0.786$	$k = -10 \rightarrow 10$
4169 measured reflections	$l = -22 \rightarrow 22$

### Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.031$	$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2]$
$wR(F^2) = 0.083$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1161 reflections	$\Delta\rho_{\text{max}} = 1.22 \text{ e \AA}^{-3}$
73 parameters	$\Delta\rho_{\text{min}} = -0.65 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 438 Friedel pairs
	Flack parameter: 0.05 (6)

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 ( $\text{\AA}$ ,  $^\circ$ )

Ag1—S2 <sup>i</sup>	2.5454 (14)	S2—C1	1.694 (5)
Ag1—S2	2.5695 (15)	S2—Ag1 <sup>iv</sup>	2.5453 (14)
Ag1—Cl1 <sup>ii</sup>	2.5897 (15)	N1—C1	1.323 (6)
Ag1—Cl1	2.6514 (15)	N1—N2	1.361 (6)
Cl1—Ag1 <sup>iii</sup>	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 <sup>i</sup> —Ag1—S2	120.49 (3)	C1—N1—N2	118.6 (4)
S2 <sup>i</sup> —Ag1—Cl1 <sup>ii</sup>	116.15 (5)	C1—N1—H1	120.7
S2—Ag1—Cl1 <sup>ii</sup>	104.77 (4)	N2—N1—H1	120.7
S2 <sup>i</sup> —Ag1—Cl1	102.24 (5)	C2—N2—N1	109.3 (4)
S2—Ag1—Cl1	110.84 (5)	N1—C1—S2	126.8 (4)
Cl1 <sup>ii</sup> —Ag1—Cl1	100.56 (5)	N1—C1—S1	108.1 (4)
Ag1 <sup>iii</sup> —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 <sup>iv</sup>	106.32 (18)	N2—C2—H2	122.3
C1—S2—Ag1	108.09 (18)	S1—C2—H2	122.3
Ag1 <sup>iv</sup> —S2—Ag1	145.29 (5)		
S2 <sup>i</sup> —Ag1—Cl1—Ag1 <sup>iii</sup>	-60.05 (5)	N2—N1—C1—S2	-179.1 (4)
S2—Ag1—Cl1—Ag1 <sup>iii</sup>	69.61 (5)	N2—N1—C1—S1	0.2 (6)

## supplementary materials

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Cl1 <sup>ii</sup> —Ag1—Cl1—Ag1 <sup>iii</sup>	180.0	Ag1 <sup>iv</sup> —S2—C1—N1	-172.7 (5)
S2 <sup>i</sup> —Ag1—S2—C1	-158.63 (19)	Ag1—S2—C1—N1	2.7 (5)
Cl1 <sup>ii</sup> —Ag1—S2—C1	-25.46 (19)	Ag1 <sup>iv</sup> —S2—C1—S1	8.2 (4)
Cl1—Ag1—S2—C1	82.19 (19)	Ag1—S2—C1—S1	-176.5 (3)
S2 <sup>i</sup> —Ag1—S2—Ag1 <sup>iv</sup>	13.55 (10)	C2—S1—C1—N1	-0.5 (4)
Cl1 <sup>ii</sup> —Ag1—S2—Ag1 <sup>iv</sup>	146.72 (12)	C2—S1—C1—S2	178.8 (4)
Cl1—Ag1—S2—Ag1 <sup>iv</sup>	-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 ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ Cl1 <sup>ii</sup>	0.86	2.38	3.197 (4)	158

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

Fig. 1

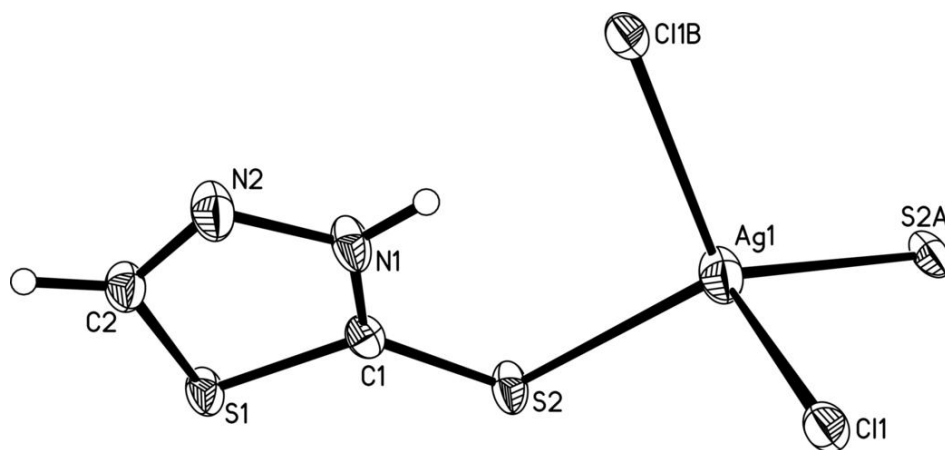


Fig. 2

