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Poly[[μ_3 -chlorido-bis(μ_2 -thiourea- κ S)-disilver(I)] nitrate]

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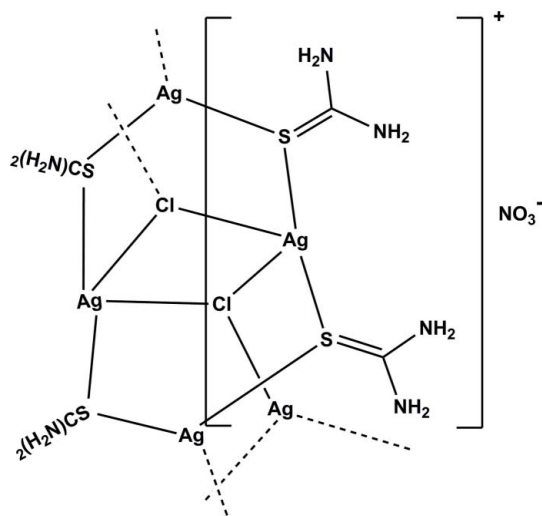
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{N}-\text{C}) = 0.008$ Å; R factor = 0.044; wR factor = 0.114; data-to-parameter ratio = 15.1.

The molecular structure of the title polymeric complex, $\{[\text{Ag}_2\text{Cl}(\text{CH}_4\text{N}_2\text{S})_2]\text{NO}_3\}_n$, consists of a binuclear cationic complex and a nitrate counter-ion. The cationic complex contains two bridging thiourea (Tu) ligands and a triply bridging μ_3 -Cl anion. The latter is probably released from 2-aminoethanethiol hydrochloride during the synthesis. The coordination environment around the two Ag^{I} atoms is different; one is trigonal planar, being coordinated by two thiourea ligands through the S atoms and to one Cl^- ion, while in the other the Ag^{I} atom is tetrahedrally coordinated by two thiourea ligands through the S atoms and to two Cl^- ions. These units aggregate through the Cl^- anion and the Tu S atoms, forming a chain propagating in $[100]$. In the crystal structure, the polymeric chains are linked *via* $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming a double layer two-dimensional network propagating in (011) .

Related literature

For silver(I) complexes with sulfur-containing ligands with applications in medicine and analytical chemistry, see: Raper (1996); Akrivos (2001). For silver(I) complexes containing thiones, see: Stocker *et al.* (2000); Pakawatchai *et al.* (1996); Casas *et al.* (1996); Aslandis *et al.* (2005); Ashraf *et al.* (2004); Isab *et al.* (2002). For silver(I) complexes containing thiolates, see: Nomiya *et al.* (2000); Zachariadis *et al.* (2003); Tsyba *et al.* (2003). For argentophilic interactions, see: Nomiya *et al.* (2000); Zachariadis *et al.* (2003); Tsyba *et al.* (2003). For the structures of some silver(I) complexes of thiourea, see: Udupa *et al.* (1976); Hanif *et al.* (2007).



Experimental

Crystal data

$[\text{Ag}_2\text{Cl}(\text{CH}_4\text{N}_2\text{S})_2]\text{NO}_3$
 $M_r = 465.44$
 Triclinic, $P\bar{1}$
 $a = 6.3981$ (8) Å
 $b = 7.7060$ (9) Å
 $c = 11.8478$ (14) Å
 $\alpha = 83.041$ (14)°
 $\beta = 82.868$ (14)°

$\gamma = 77.312$ (14)°
 $V = 562.80$ (12) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 4.08$ mm⁻¹
 $T = 173$ K
 $0.34 \times 0.23 \times 0.12$ mm

Data collection

Stoe IPDS diffractometer
 Absorption correction: multi-scan
 (*MULScanABS* in *PLATON*;
 Spek, 2009)
 $T_{\text{min}} = 0.771$, $T_{\text{max}} = 1.353$

4473 measured reflections
 2055 independent reflections
 1682 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.114$
 $S = 0.98$
 2055 reflections

136 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O3}^{\text{i}}$	0.88	2.28	3.153 (8)	170
$\text{N2}-\text{H2A}\cdots\text{O1}^{\text{i}}$	0.88	1.95	2.831 (7)	177
$\text{N2}-\text{H2B}\cdots\text{O3}$	0.88	2.11	2.932 (7)	155
$\text{N3}-\text{H3A}\cdots\text{O1}^{\text{ii}}$	0.88	2.00	2.881 (7)	174
$\text{N3}-\text{H3B}\cdots\text{O2}^{\text{iii}}$	0.88	2.08	2.930 (7)	163
$\text{N4}-\text{H4A}\cdots\text{O2}^{\text{ii}}$	0.88	2.22	3.095 (8)	173
$\text{N1}-\text{H1B}\cdots\text{Cl1}^{\text{iv}}$	0.88	2.56	3.372 (6)	155
$\text{N4}-\text{H4B}\cdots\text{Cl1}^{\text{v}}$	0.88	2.62	3.396 (6)	147

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

Data collection: *EXPOSE* (Stoe & Cie, 2004); cell refinement: *CELL* (Stoe & Cie, 2004); data reduction: *INTEGRATE* (Stoe & Cie, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury*

(Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* and *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5309).

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Poly[[μ_3 -chlorido-bis(μ_2 -thiourea- κ S)]disilver(I)] nitrate]

Saeed Ahmad, Aisha Saddiqa, Muhammad Monim-ul-Mehboob, Muhammad Altaf and Helen Stoeckli-Evans

S1. Comment

The study of the coordination and structural chemistry of silver(I) complexes with sulfur containing ligands has been a matter of interest over the last decades due to their wide range of applications in medicine and in analytical chemistry (Raper, 1996; Akrivos, 2001), and also due to their ability to adopt geometries with variable nuclearities and structural diversity. Consequently, several silver(I) complexes containing thiones (Stocker *et al.*, 2000; Pakawatchai *et al.*, 1996; Casas *et al.*, 1996; Aslandis *et al.*, 2005; Ashraf *et al.*, 2004; Isab *et al.*, 2002) and thiolates (Nomiya *et al.*, 2000; Zachariadis *et al.*, 2003; Tsyba *et al.*, 2003) have been prepared and structurally characterized. Silver(I) complexes with thiolates like thiomalic acid, thiosalisalic acid and 2-mercaptonicotinic acid [Nomiya *et al.*, 2000; Zachariadis *et al.*, 2003] also have remarkable antimicrobial activities for bacteria, yeast, and mold. The present report describes the structure of the new title silver(I) cluster of thiourea (Tu).

The molecular structure of the title complex is shown in Fig. 1. The asymmetric unit consists of a binuclear cationic complex and a nitrate counter ion. The cationic complex contains two silver(I) atoms, Ag1 and Ag2, two Tu ligands which bridge the silver(I) atoms *via* the S-atoms, and a triply bridging (μ_3)Cl⁻ anion. The latter is probably released from 2-aminoethanethiol hydrochloride during the synthesis. The coordination environments around the two silver atoms are different. Atom Ag1 possesses a tetrahedral geometry, being coordinated to two thiourea ligands through the S-atoms, and two Cl⁻ anions. Atom Ag2 has a trigonal planar geometry, being coordinated to two thiourea ligands through S-atoms and to one Cl⁻ anion. These units aggregate through the Cl⁻ anion, and the Tu sulfur atoms, to form a one-dimensional chain which propagates in [100], as shown in Fig. 1.

The Ag—S distances around the trigonally coordinated Ag2 center [Ag2—S1 = 2.4827 (15) Å, Ag2—S2 = 2.4913 (16) Å] are somewhat longer than those around tetrahedrally coordinated Ag1 center [Ag1—S1 = 2.4305 (15) Å, Ag1—S2 = 2.4278 (15) Å]. In contrast the Ag—Cl bond distances are lengthened. The Ag1—Cl1 and Ag1—Cl1^c [symmetry code: (c) 1 - x, 2 - y, 1 - z] distances are 2.8393 (15) and 2.9280 (16) Å, respectively, compared to distance Ag2—Cl1 which is 2.5477 (14) Å. The individual distances and angles within the Tu ligand are comparable to those reported for other Ag-thiourea complexes [Udupa *et al.*, 1976; Hanif *et al.*, 2007].

The shortest silver(I)⋯silver(I) distance of 3.2889 (8) Å [Ag1—Ag2^a; symmetry code: (a) -1 + x, y, z] indicates that the complex is stabilized by significant argentophilic interactions. This distance is comparable to values reported previously [Nomiya *et al.*, 2000; Zachariadis *et al.*, 2003; Tsyba *et al.*, 2003]. The other short Ag⋯Ag distances include Ag2⋯Ag2^d and Ag1⋯Ag2^d of 3.5169 (8) and 3.5753 (8) Å, respectively [symmetry code: (d) 2 - x, 2 - y, -z], see Fig. 1.

In the crystal the polymeric chains are linked *via* N—H⋯O hydrogen bonds, involving the thiourea NH₂ H-atoms and the nitrate O-atoms, and N—H⋯Cl contacts (Fig. 2, Table 1), to form a double layer two-dimensional network propagating in plane (011).

S2. Experimental

The title complex was prepared by adding 1 mmol (0.113 g) of 2-aminoethanethiol hydrochloride, dissolved in 10 ml of distilled water, to 1 mmol (0.170 g) of AgNO₃, dissolved in 30 ml of distilled water. The mixture was stirred for 15–20 min giving a clear solution. 1 mmol (0.076 g) of thiourea, dissolved in 10 ml of methanol, was then added and the mixture was stirred for a further 15 min. The solution was then filtered and the filtrate kept at RT for slow evaporation of the solvent. After 2–3 days colourless crystals, suitable for X-ray diffraction analysis, were obtained.

S3. Refinement

The NH₂ H-atoms could be located in difference electron-density maps. In the final cycles of least-squares refinement they were included in calculated positions and treated as riding atoms: N—H = 0.88 Å, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

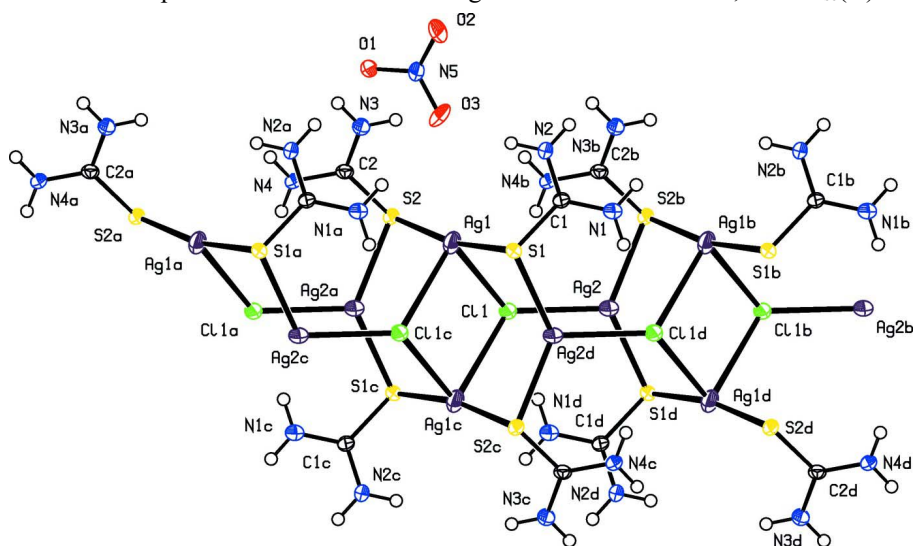


Figure 1

A view of the molecular structure of the title complex with displacement ellipsoids drawn at the 50% probability level [Symmetry codes: (a) = $-1 + x, y, z$; (b) = $1 + x, y, z$; (c) = $1 - x, 2 - y, 1 - z$; (d) = $2 - x, 2 - y, -z$].

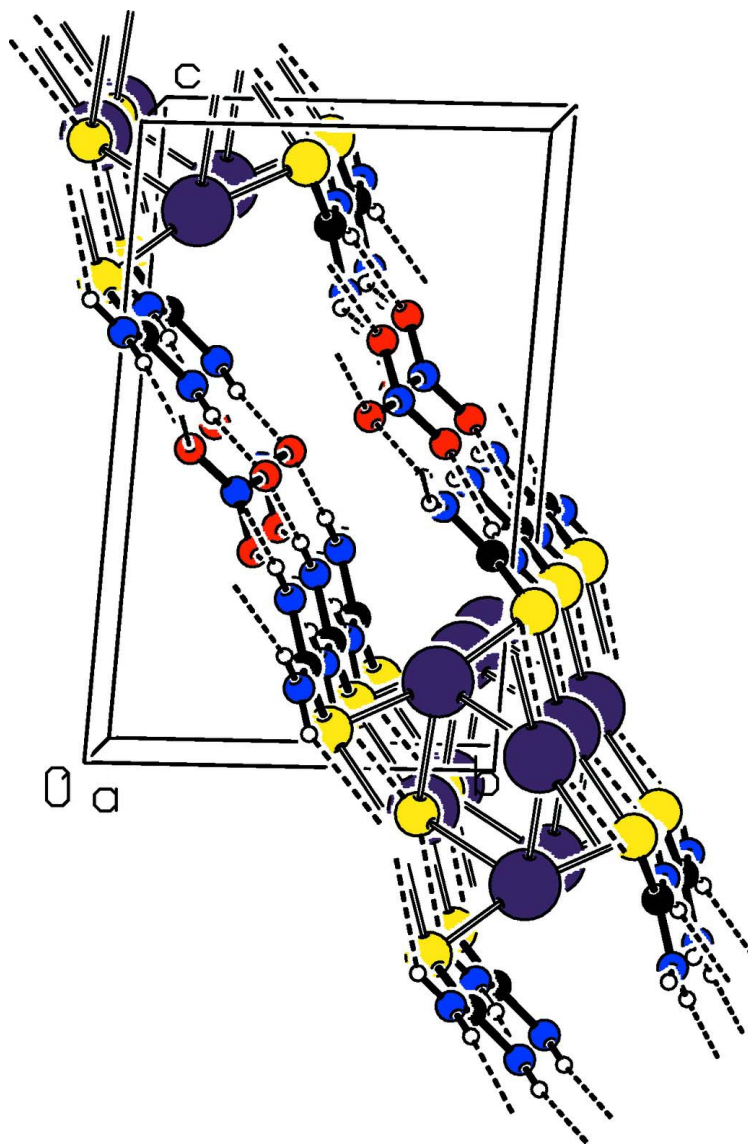


Figure 2

A view along the *a*-axis of the crystal packing of the title complex showing the N—H...O and N—H...Cl hydrogen bonds [dotted lines; see Table 1 for details].

Poly[[μ_3 -chlorido-bis(μ_2 -thiourea- κ S)]disilver(I)] nitrate]

Crystal data

[Ag₂Cl(CH₄N₂S)₂]NO₃

M_r = 465.44

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

a = 6.3981 (8) Å

b = 7.7060 (9) Å

c = 11.8478 (14) Å

α = 83.041 (14)°

β = 82.868 (14)°

γ = 77.312 (14)°

V = 562.80 (12) Å³

Z = 2

F(000) = 444

D_x = 2.747 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 5310 reflections

θ = 2.7–26.0°

μ = 4.08 mm⁻¹

$T = 173$ K $0.34 \times 0.23 \times 0.12$ mm
 Plate, colourless

Data collection

Stoe IPDS diffractometer	4473 measured reflections 2055 independent reflections
Radiation source: fine-focus sealed tube	1682 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.056$
φ scans	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.7^\circ$
Absorption correction: multi-scan (MULscanABS in PLATON; Spek, 2009)	$h = -7 \rightarrow 7$ $k = -9 \rightarrow 8$ $l = -14 \rightarrow 13$
$T_{\text{min}} = 0.771$, $T_{\text{max}} = 1.353$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.114$	$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2]$
$S = 0.98$	where $P = (F_o^2 + 2F_c^2)/3$
2055 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
136 parameters	$\Delta\rho_{\text{max}} = 1.49 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -1.27 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. The NH_2H -atoms were included in calculated positions and treated as riding atoms: N—H 0.88 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent N-atom})$.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.48799 (7)	0.87109 (6)	0.15613 (4)	0.0303 (2)
Ag2	1.07497 (7)	1.16730 (7)	0.06513 (4)	0.0327 (2)
Cl1	0.6808 (2)	1.16001 (19)	0.05756 (13)	0.0245 (4)
S1	0.7764 (2)	0.63258 (18)	0.08944 (12)	0.0197 (4)
S2	0.2032 (2)	1.07487 (18)	0.25782 (13)	0.0201 (4)
N1	1.1617 (8)	0.5710 (7)	0.1682 (5)	0.0264 (16)
N2	0.8858 (7)	0.5149 (7)	0.2959 (5)	0.0271 (16)
N3	0.0979 (8)	0.8245 (7)	0.4138 (5)	0.0319 (16)
N4	-0.1790 (8)	0.9882 (7)	0.3218 (5)	0.0276 (16)
C1	0.9560 (8)	0.5703 (7)	0.1930 (5)	0.0179 (14)
C2	0.0266 (8)	0.9512 (7)	0.3359 (5)	0.0183 (17)
O1	0.1853 (6)	0.3896 (6)	0.4594 (4)	0.0303 (15)
O2	0.4735 (7)	0.2157 (7)	0.5106 (5)	0.0440 (16)
O3	0.4800 (8)	0.3913 (8)	0.3521 (5)	0.0481 (18)
N5	0.3826 (7)	0.3331 (7)	0.4412 (5)	0.0268 (16)
H1A	1.25110	0.53410	0.22110	0.0320*
H1B	1.21010	0.60840	0.09880	0.0320*

H2A	0.97600	0.47810	0.34840	0.0330*
H2B	0.74820	0.51410	0.31310	0.0330*
H3A	0.00830	0.76530	0.45590	0.0380*
H3B	0.23560	0.79830	0.42420	0.0380*
H4A	-0.26680	0.92790	0.36460	0.0330*
H4B	-0.22930	1.07330	0.26960	0.0330*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0177 (3)	0.0356 (3)	0.0341 (3)	-0.0027 (2)	0.0032 (2)	-0.0001 (2)
Ag2	0.0266 (3)	0.0465 (3)	0.0235 (3)	-0.0128 (2)	-0.0058 (2)	0.0155 (2)
Cl1	0.0214 (6)	0.0313 (7)	0.0219 (8)	-0.0123 (5)	-0.0056 (5)	0.0089 (6)
S1	0.0155 (6)	0.0263 (7)	0.0163 (8)	-0.0040 (5)	-0.0036 (5)	0.0038 (6)
S2	0.0160 (6)	0.0234 (7)	0.0198 (8)	-0.0062 (5)	-0.0013 (5)	0.0057 (6)
N1	0.024 (2)	0.036 (3)	0.019 (3)	-0.010 (2)	-0.0043 (19)	0.007 (2)
N2	0.014 (2)	0.043 (3)	0.022 (3)	-0.007 (2)	-0.0018 (19)	0.008 (2)
N3	0.019 (2)	0.042 (3)	0.029 (3)	-0.005 (2)	-0.005 (2)	0.019 (3)
N4	0.018 (2)	0.041 (3)	0.022 (3)	-0.011 (2)	-0.0029 (19)	0.014 (2)
C1	0.018 (2)	0.016 (2)	0.019 (3)	-0.0056 (19)	-0.002 (2)	0.005 (2)
C2	0.019 (3)	0.022 (3)	0.012 (3)	-0.001 (2)	-0.001 (2)	-0.001 (2)
O1	0.0158 (18)	0.044 (3)	0.024 (3)	0.0012 (17)	-0.0020 (16)	0.011 (2)
O2	0.022 (2)	0.056 (3)	0.047 (3)	-0.001 (2)	-0.013 (2)	0.019 (3)
O3	0.028 (2)	0.071 (4)	0.041 (3)	-0.020 (2)	0.010 (2)	0.016 (3)
N5	0.016 (2)	0.035 (3)	0.028 (3)	-0.008 (2)	-0.002 (2)	0.007 (2)

Geometric parameters (Å, °)

Ag1—C11	2.8393 (15)	N1—C1	1.314 (8)
Ag1—S1	2.4305 (15)	N2—C1	1.301 (8)
Ag1—S2	2.4278 (15)	N3—C2	1.305 (8)
Ag1—C11 ⁱ	2.9280 (16)	N4—C2	1.311 (8)
Ag2—C11	2.5477 (14)	N1—H1A	0.8800
Ag2—S2 ⁱⁱ	2.4913 (16)	N1—H1B	0.8800
Ag2—S1 ⁱⁱⁱ	2.4827 (15)	N2—H2B	0.8800
S1—C1	1.738 (6)	N2—H2A	0.8800
S2—C2	1.744 (6)	N3—H3A	0.8800
O1—N5	1.242 (6)	N3—H3B	0.8800
O2—N5	1.241 (8)	N4—H4A	0.8800
O3—N5	1.244 (8)	N4—H4B	0.8800
Cl1—Ag1—S1	96.91 (5)	C1—N1—H1A	120.00
Cl1—Ag1—S2	90.60 (5)	C1—N2—H2A	120.00
Cl1—Ag1—C11 ⁱ	92.64 (5)	H2A—N2—H2B	120.00
S1—Ag1—S2	169.00 (5)	C1—N2—H2B	120.00
Cl1 ⁱ —Ag1—S1	82.74 (5)	C2—N3—H3A	120.00
Cl1 ⁱ —Ag1—S2	105.01 (5)	H3A—N3—H3B	120.00
Cl1—Ag2—S2 ⁱⁱ	114.00 (5)	C2—N3—H3B	120.00

Cl1—Ag2—S1 ⁱⁱⁱ	114.55 (5)	C2—N4—H4B	120.00
S1 ⁱⁱⁱ —Ag2—S2 ⁱⁱ	126.77 (5)	H4A—N4—H4B	120.00
Ag1—Cl1—Ag2	123.99 (6)	C2—N4—H4A	120.00
Ag1—Cl1—Ag1 ⁱ	87.36 (4)	O2—N5—O3	122.5 (5)
Ag1 ⁱ —Cl1—Ag2	121.83 (6)	O1—N5—O2	118.6 (5)
Ag1—S1—C1	108.15 (19)	O1—N5—O3	118.8 (5)
Ag1—S1—Ag2 ⁱⁱⁱ	93.38 (5)	S1—C1—N1	121.4 (5)
Ag2 ⁱⁱⁱ —S1—C1	108.74 (19)	S1—C1—N2	119.0 (4)
Ag1—S2—C2	108.27 (19)	N1—C1—N2	119.6 (5)
Ag1—S2—Ag2 ^{iv}	83.91 (5)	S2—C2—N3	119.6 (4)
Ag2 ^{iv} —S2—C2	107.4 (2)	S2—C2—N4	121.3 (4)
C1—N1—H1B	120.00	N3—C2—N4	119.0 (5)
H1A—N1—H1B	120.00		
S1—Ag1—Cl1—Ag2	-44.29 (8)	S2—Ag1—Cl1 ⁱ —Ag1 ⁱ	91.33 (5)
S1—Ag1—Cl1—Ag1 ⁱ	83.00 (5)	S2—Ag1—Cl1 ⁱ —Ag2 ⁱ	-37.73 (8)
S2—Ag1—Cl1—Ag2	127.66 (7)	S2 ⁱⁱ —Ag2—Cl1—Ag1	-46.44 (8)
S2—Ag1—Cl1—Ag1 ⁱ	-105.06 (5)	S2 ⁱⁱ —Ag2—Cl1—Ag1 ⁱ	-157.13 (6)
Cl1 ⁱ —Ag1—Cl1—Ag2	-127.29 (7)	S1 ⁱⁱⁱ —Ag2—Cl1—Ag1	156.10 (6)
Cl1 ⁱ —Ag1—Cl1—Ag1 ⁱ	-0.02 (9)	S1 ⁱⁱⁱ —Ag2—Cl1—Ag1 ⁱ	45.41 (8)
Cl1—Ag1—S1—C1	90.6 (2)	Cl1—Ag2—S2 ⁱⁱ —Ag1 ⁱⁱ	127.70 (5)
Cl1—Ag1—S1—Ag2 ⁱⁱⁱ	-20.40 (5)	Cl1—Ag2—S2 ⁱⁱ —C2 ⁱⁱ	20.4 (2)
Cl1 ⁱ —Ag1—S1—C1	-177.6 (2)	Cl1—Ag2—S1 ⁱⁱⁱ —Ag1 ⁱⁱⁱ	-123.22 (5)
Cl1 ⁱ —Ag1—S1—Ag2 ⁱⁱⁱ	71.40 (5)	Cl1—Ag2—S1 ⁱⁱⁱ —C1 ⁱⁱⁱ	-12.8 (2)
Cl1—Ag1—S2—C2	179.2 (2)	Ag1—S1—C1—N1	-124.7 (4)
Cl1—Ag1—S2—Ag2 ^{iv}	72.83 (5)	Ag1—S1—C1—N2	58.3 (5)
Cl1 ⁱ —Ag1—S2—C2	86.3 (2)	Ag2 ⁱⁱⁱ —S1—C1—N1	-24.5 (5)
Cl1 ⁱ —Ag1—S2—Ag2 ^{iv}	-20.06 (5)	Ag2 ⁱⁱⁱ —S1—C1—N2	158.4 (4)
Cl1—Ag1—Cl1 ⁱ —Ag1 ⁱ	0.02 (10)	Ag1—S2—C2—N3	60.2 (5)
Cl1—Ag1—Cl1 ⁱ —Ag2 ⁱ	-129.06 (7)	Ag1—S2—C2—N4	-123.1 (5)
S1—Ag1—Cl1 ⁱ —Ag1 ⁱ	-96.64 (5)	Ag2 ^{iv} —S2—C2—N3	149.4 (4)
S1—Ag1—Cl1 ⁱ —Ag2 ⁱ	134.30 (7)	Ag2 ^{iv} —S2—C2—N4	-33.8 (5)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1A \cdots O3 ⁱⁱ	0.88	2.28	3.153 (8)	170
N2—H2A \cdots O1 ⁱⁱ	0.88	1.95	2.831 (7)	177
N2—H2B \cdots O3	0.88	2.11	2.932 (7)	155
N3—H3A \cdots O1 ^v	0.88	2.00	2.881 (7)	174
N3—H3B \cdots O2 ^{vi}	0.88	2.08	2.930 (7)	163
N4—H4A \cdots O2 ^v	0.88	2.22	3.095 (8)	173
N1—H1B \cdots Cl1 ⁱⁱⁱ	0.88	2.56	3.372 (6)	155
N4—H4B \cdots Cl1 ^{iv}	0.88	2.62	3.396 (6)	147

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