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Crystal structure of a twisted-ribbon type double-stranded Ag^{I} coordination polymer: *catena*-poly-[[silver(I)-μ_3-bis(pyridin-3-ylmethyl)sulfane-$\kappa^3 N:N':S$] nitrate]

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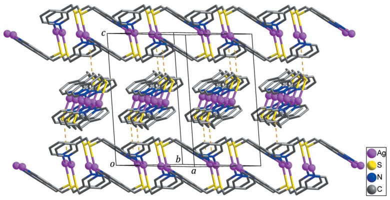
The asymmetric unit in the title compound, $\{[Ag(C_{12}H_{12}N_2S)]\cdot NO_3\}_n$ or $\{[AgL]\cdot NO_3\}_n$, L = bis(pyridin-3-ylmethyl)sulfane, consists of an Ag^{I} cation bound to a pyridine N atom of an L ligand and an NO_3^- anion that is disordered over two orientations in an 0.570 (17):0.430 (17) occupancy ratio. Each Ag^{I} cation is coordinated by two pyridine N atoms from adjacent L ligands to form an infinite zigzag chain along [110]. In addition, each Ag^{I} ion binds to an S donor from a third L ligand in an adjacent parallel chain, resulting in the formation of a twisted-ribbon type of double-stranded chain propagating along the [110] or [1$\overline{1}$0] directions. The Ag^{I} atom is displaced out of the trigonal N_2S coordination plane by 0.371 (3) Å because of interactions between the Ag^{I} cation and O atoms of the disordered nitrate anions. Intermolecular π–π stacking interactions [centroid-to-centroid distance = 3.824 (3) Å] occur between one pair of corresponding pyridine rings in the double-stranded chain. In the crystal, the double-stranded chains are alternately stacked along the c axis with alternate stacks linked by intermolecular π–π stacking interactions [centroid-to-centroid distance = 3.849 (3) Å], generating a three-dimensional supramolecular architecture. Weak intermolecular C—H$\cdots$O hydrogen bonds between the polymer chains and the O atoms of the nitrate anions also occur.



1. Chemical context

Among the diverse key factors in the development of Ag^{I} coordination polymers, the structures of the spacer ligands play important roles in determining the structural topology of the self-assembled polymer units (Zheng *et al.*, 2009; Liu *et al.*, 2011). For this reason, continuous efforts have focused on the design and development of such suitable ligands. In particular, dipyridyl-type molecules functioning as bridging ligands have been widely used to construct diverse Ag^{I} coordination polymers with fascinating structures and attractive functional properties (Leong & Vittal, 2011; Moulton & Zaworotko, 2001; Wang *et al.*, 2012). We have also reported several Ag^{I} coordination polymers with interesting structures using dipyridyl-type ligands (Lee *et al.*, 2012, 2015; Moon *et al.*, 2015, 2016; Park *et al.*, 2010). The continuing interest in dipyridyl-type-ligand-based Ag^{I} coordination polymers prompted us to investigate the use of the ligand bis(pyridin-3-ylmethyl)sulfane (L), which can coordinate to three Ag^{I} cations in a T-shape *via* the two pyridine nitrogen donors as a bridgehead

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and the sulfur donor atoms, binding to the Ag^{I} cations at both ends of the dipyridyl bridge as well as at its centre. A reaction of silver(I) nitrate with *L* (synthesized using a literature procedure; Park *et al.*, 2010; Lee *et al.*, 2012) afforded the title compound. Herein, we report its one-dimensional twisted-ribbon type double-stranded chain structure in the crystal.

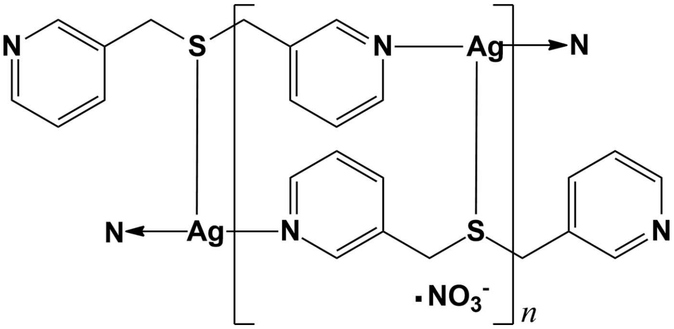

Table 1
Selected geometric parameters (Å, °).

Ag1—N2^{i}	2.276 (5)	Ag1—S1^{ii}	2.5305 (14)
Ag1—N1	2.333 (4)		
N2^{i}—Ag1—N1	113.22 (16)	N1—Ag1—S1^{ii}	106.03 (12)
N2^{i}—Ag1—S1^{ii}	133.18 (12)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2	0.93	2.59	2.924 (12)	102
C5—H5···O2^{iii}	0.93	2.60	3.318 (14)	135
C6—H6*A*···O2^{iv}	0.97	2.52	3.464 (14)	163
C6—H6*B*···O2$'^{v}$	0.97	2.60	3.44 (2)	145
C7—H7*B*···O3$'^{iv}$	0.97	2.38	3.233 (15)	147
C9—H9···O1^{vi}	0.93	2.49	3.221 (18)	136
C12—H12···O3^{vii}	0.93	2.45	3.256 (12)	145

Symmetry codes: (iii) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (iv) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $x, y - 1, z$; (vi) $x + \frac{1}{2}, y - \frac{1}{2}, z$; (vii) $-x + \frac{1}{2}, y - \frac{3}{2}, -z + \frac{1}{2}$.

2. Structural commentary

As shown in Fig. 1, the asymmetric unit of the title compound comprises one Ag^{I} cation, bound to the N1 pyridine atom of a bis(pyridin-3-ylmethyl)sulfane ligand, *L*, and an NO_3^- anion that is disordered over two orientations in an 0.570 (17):0.430 (17) occupancy ratio. Pyridine N atoms N1 and N2 from two symmetry-related *L* ligands bind to the Ag^{I} cations to form an infinite zigzag chain. In addition, each Ag^{I} ion binds to an S1 donor from a third *L* ligand in an adjacent parallel chain, resulting in the formation of a twisted-ribbon type of double-stranded chain propagating along the [110] or [$1\bar{1}0$] directions (Figs. 2 and 3). The Ag^{I} atom is therefore three-coordinated and the coordination geometry around the Ag^{I} cation can be considered as a highly distorted trigonal plane. Selected bond lengths and angles around the Ag1 atom are given in Table 1. N—Ag—N and N—Ag—S angles fall in the range 106.03 (12)–133.18 (12)°, deviating significantly from ideal trigonal–planar geometry. This may reflect the influence of additional Ag···O–NO_2^- interactions between the Ag^{I} ion and O atoms of the disordered nitrate anion [Ag1···O1 = 2.730 (18), Ag1···O1′ = 2.55 (2) Å; indicated by a dashed line in Fig. 1]. The Ag^{I} atom is displaced out of the trigonal N1, S1, N2 coordination plane by 0.372 (2) Å. The two pyridine rings coordinated to the Ag^{I} centre are tilted by 53.20 (15)° with respect to each other. In the double-stranded chain, intermolecular π–π stacking interactions between the N1-pyridine rings [*Cg*1···*Cg*1^{i} = 3.824 (3) Å; yellow dashed lines in Fig. 2; *Cg*1 is the centroid of the N1/C1–C5 ring; symmetry code: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$] contribute to the stabilization of the double-stranded chain.

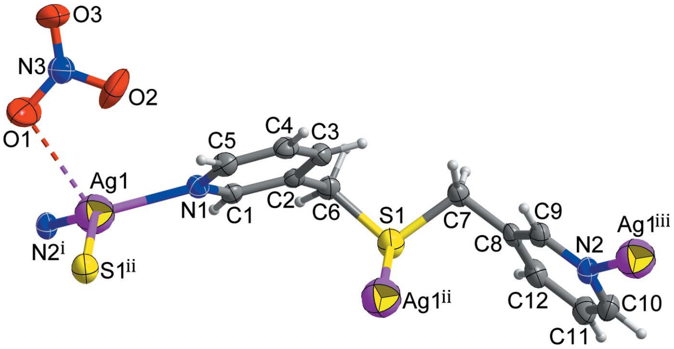

Figure 1
View of the molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Disordered O atoms of the NO_3^- anion have been omitted for clarity. The dashed line represents the Ag···O interaction. [Symmetry codes: (i) $x - \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (iii) $x + \frac{1}{2}, y - \frac{1}{2}, z$.]

3. Supramolecular features

As shown in Fig. 3, the double-stranded chains propagate along the [110] and [$1\bar{1}0$] directions in the crystal and are alternately stacked along the *c* axis. Adjacent chains are linked by intermolecular π–π stacking interactions between N2-

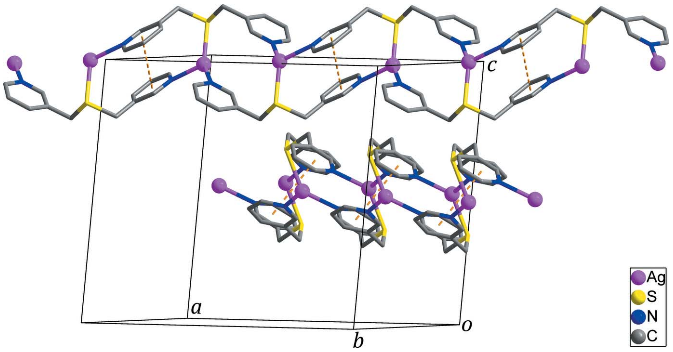

Figure 2
The double-stranded polymeric chains propagating along the [110] (upper chain) and [$1\bar{1}0$] (lower chain) directions. Yellow dashed lines represent intermolecular π–π stacking interactions [centroid-to-centroid distance = 3.824 (3) Å] between the N1-containing pyridine rings in the chain. NO_3^- anions and H atoms have been omitted for clarity.

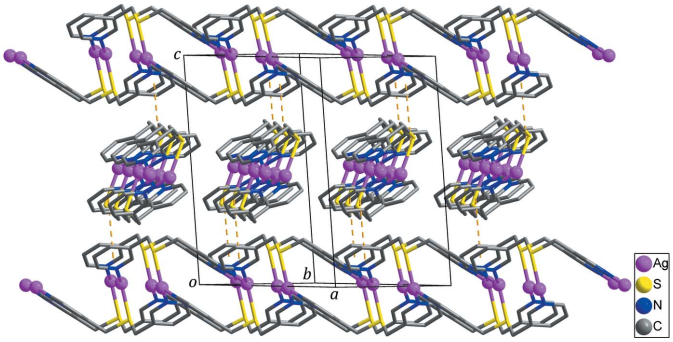

Figure 3
Three-dimensional supramolecular network *via* intermolecular π–π stacking interactions (yellow dashed lines) between the N2-containing pyridine rings. NO_3^- anions and H atoms have been omitted for clarity.

pyridine rings [$Cg2\cdots Cg2^{ii}$ = 3.849 (3) Å; yellow dashed lines in Fig. 3; *Cg*2 is the centroid of the N2/C8–C12 ring; symmetry code: (ii) $-x + 1, y, -z + \frac{1}{2}$], resulting in the formation of a three-dimensional supramolecular architecture (Fig. 3). Weak intermolecular C—H⋯O hydrogen bonds (Table 2) between the double-stranded chains and the NO_3^- anions are also observed in the crystal.

4. Synthesis and crystallization

The *L* ligand was synthesized according to a literature method (Park *et al.*, 2010; Lee *et al.*, 2012). Colourless plate-like X-ray quality single crystals of the title compound were obtained by vapor diffusion of diethyl ether into a DMSO solution of the *L* ligand with $AgNO_3$ in a 1:1 molar ratio.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The NO_3^- anion is disordered over two orientations and the occupancies of the disorder components refined to a 0.570 (17):0.430 (17) ratio. The anisotropic displacement ellipsoids of four oxygen atoms (O3, O1′, O2′ and O3′) in the disordered NO_3^- anion were very elongated and therefore ISOR restraints were applied for these atoms (McArdle, 1995; Sheldrick, 2008). All H atoms were positioned geometrically and refined as riding: C—H = 0.93 Å for Csp^2—H and 0.97 Å for methylene C—H, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ag(C_{12}H_{12}N_2S)]NO_3$
M_r	386.18
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	298
a, *b*, *c* (Å)	22.432 (3), 8.1656 (12), 15.036 (2)
β (°)	98.636 (3)
V (Å^3)	2722.9 (7)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	1.64
Crystal size (mm)	0.25 × 0.20 × 0.05
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.658, 0.896
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7550, 2676, 1763
R_{int}	0.079
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.109, 0.97
No. of reflections	2676
No. of parameters	209
No. of restraints	24
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.66, −0.66

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010) and *publCIF* (Westrip, 2010).

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Crystal structure of a twisted-ribbon type double-stranded Ag^I coordination polymer: *catena*-poly[[silver(I)-μ_3-bis(pyridin-3-ylmethyl)sulfane-κ^3N:N':S] nitrate]

Suk-Hee Moon, Youngjin Kang and Ki-Min Park

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

catena-Poly[[silver(I)-μ_3-bis(pyridin-3-ylmethyl)sulfane-κ^3N:N':S] nitrate]

Crystal data

$[Ag(C_{12}H_{12}N_2S)]NO_3$	$F(000) = 1536$
$M_r = 386.18$	$D_x = 1.884$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 22.432$ (3) Å	Cell parameters from 3272 reflections
$b = 8.1656$ (12) Å	$\theta = 1.8$–$28.3°$
$c = 15.036$ (2) Å	$\mu = 1.64$ mm^{-1}
$\beta = 98.636$ (3)°	$T = 298$ K
$V = 2722.9$ (7) Å^3	Plate, colourless
$Z = 8$	0.25 × 0.20 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer	2676 independent reflections
φ and ω scans	1763 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$R_{\rm int} = 0.079$
$T_{\rm min} = 0.658$, $T_{\rm max} = 0.896$	$\theta_{\rm max} = 26.0°$, $\theta_{\rm min} = 2.7°$
7550 measured reflections	$h = -27 \rightarrow 26$
	$k = -10 \rightarrow 8$
	$l = -18 \rightarrow 9$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.109$	$(\Delta/\sigma)_{\rm max} < 0.001$
$S = 0.97$	$\Delta\rho_{\rm max} = 0.66$ e Å^{-3}
2676 reflections	$\Delta\rho_{\rm min} = -0.66$ e Å^{-3}
209 parameters	
24 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
Ag1	0.13008 (2)	0.47824 (6)	0.49130 (3)	0.05552 (19)	
S1	0.33342 (6)	−0.07112 (16)	0.34926 (9)	0.0417 (3)	
N1	0.2163 (2)	0.4068 (5)	0.4306 (3)	0.0460 (11)	
N2	0.5458 (2)	−0.1552 (6)	0.4256 (3)	0.0501 (11)	
N3	0.1183 (3)	0.8084 (7)	0.3663 (4)	0.0662 (15)	
O1	0.0800 (7)	0.756 (2)	0.4114 (15)	0.106 (6)	0.570 (17)
O2	0.1701 (6)	0.7472 (18)	0.3893 (9)	0.117 (5)	0.570 (17)
O3	0.1169 (6)	0.9256 (15)	0.3181 (8)	0.105 (5)	0.570 (17)
O1′	0.1009 (9)	0.764 (3)	0.4311 (15)	0.072 (5)	0.430 (17)
O2′	0.1641 (12)	0.845 (3)	0.3590 (16)	0.133 (8)	0.430 (17)
O3′	0.0762 (7)	0.815 (2)	0.2930 (9)	0.096 (6)	0.430 (17)
C1	0.2231 (2)	0.2722 (6)	0.3824 (3)	0.0391 (12)	
H1	0.1905	0.2011	0.3699	0.047*	
C2	0.2760 (2)	0.2324 (6)	0.3498 (3)	0.0386 (12)	
C3	0.3244 (2)	0.3392 (6)	0.3697 (4)	0.0464 (13)	
H3	0.3606	0.3175	0.3487	0.056*	
C4	0.3188 (2)	0.4778 (6)	0.4206 (4)	0.0483 (13)	
H4	0.3510	0.5498	0.4349	0.058*	
C5	0.2640 (3)	0.5066 (6)	0.4498 (4)	0.0503 (13)	
H5	0.2601	0.5995	0.4842	0.060*	
C6	0.2786 (2)	0.0785 (7)	0.2966 (4)	0.0466 (13)	
H6A	0.2884	0.1065	0.2378	0.056*	
H6B	0.2389	0.0284	0.2877	0.056*	
C7	0.3975 (2)	−0.0395 (7)	0.2890 (4)	0.0478 (13)	
H7A	0.3870	−0.0722	0.2266	0.057*	
H7B	0.4089	0.0752	0.2908	0.057*	
C8	0.4488 (2)	−0.1419 (6)	0.3345 (3)	0.0426 (12)	
C9	0.4985 (2)	−0.0697 (7)	0.3829 (4)	0.0451 (12)	
H9	0.4997	0.0440	0.3866	0.054*	
C10	0.5422 (3)	−0.3178 (8)	0.4195 (4)	0.0591 (16)	
H10	0.5739	−0.3792	0.4496	0.071*	
C11	0.4946 (3)	−0.4000 (7)	0.3715 (5)	0.0631 (17)	
H11	0.4944	−0.5137	0.3684	0.076*	
C12	0.4474 (3)	−0.3106 (7)	0.3282 (4)	0.0538 (15)	
H12	0.4147	−0.3631	0.2947	0.065*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0456 (3)	0.0747 (3)	0.0449 (3)	0.0096 (2)	0.00258 (18)	−0.0054 (2)
S1	0.0366 (6)	0.0477 (7)	0.0410 (7)	0.0028 (5)	0.0063 (5)	−0.0036 (6)
N1	0.046 (3)	0.051 (3)	0.042 (3)	0.003 (2)	0.010 (2)	−0.001 (2)
N2	0.043 (3)	0.062 (3)	0.045 (3)	0.007 (2)	0.006 (2)	−0.008 (2)
N3	0.076 (4)	0.060 (4)	0.066 (4)	0.007 (3)	0.020 (4)	−0.003 (3)
O1	0.071 (9)	0.100 (9)	0.147 (15)	−0.021 (7)	0.014 (9)	0.046 (9)
O2	0.102 (8)	0.110 (9)	0.127 (10)	0.063 (7)	−0.016 (7)	0.004 (8)
O3	0.132 (8)	0.088 (7)	0.102 (7)	0.033 (6)	0.045 (6)	0.049 (6)
O1′	0.081 (7)	0.069 (6)	0.068 (6)	−0.005 (5)	0.013 (5)	0.003 (4)
O2′	0.125 (11)	0.145 (11)	0.131 (11)	−0.033 (9)	0.027 (8)	−0.006 (8)
O3′	0.100 (9)	0.110 (9)	0.074 (8)	0.040 (7)	−0.001 (6)	−0.019 (6)
C1	0.037 (3)	0.045 (3)	0.033 (3)	0.003 (2)	0.000 (2)	0.003 (2)
C2	0.041 (3)	0.041 (3)	0.033 (3)	0.006 (2)	0.002 (2)	0.007 (2)
C3	0.042 (3)	0.050 (3)	0.048 (3)	0.001 (2)	0.010 (2)	0.006 (3)
C4	0.046 (3)	0.043 (3)	0.054 (3)	−0.006 (2)	0.003 (3)	0.008 (3)
C5	0.059 (3)	0.047 (3)	0.043 (3)	0.003 (3)	0.004 (3)	−0.004 (3)
C6	0.045 (3)	0.056 (3)	0.037 (3)	0.006 (2)	0.002 (2)	0.000 (3)
C7	0.039 (3)	0.064 (3)	0.040 (3)	0.002 (2)	0.006 (2)	−0.003 (3)
C8	0.037 (3)	0.055 (3)	0.039 (3)	0.001 (2)	0.015 (2)	−0.004 (3)
C9	0.042 (3)	0.051 (3)	0.043 (3)	0.006 (2)	0.009 (2)	−0.005 (3)
C10	0.051 (4)	0.064 (4)	0.063 (4)	0.019 (3)	0.010 (3)	0.005 (3)
C11	0.060 (4)	0.048 (3)	0.085 (5)	0.003 (3)	0.023 (4)	−0.002 (3)
C12	0.045 (3)	0.061 (4)	0.059 (4)	−0.004 (3)	0.018 (3)	−0.012 (3)

Geometric parameters (Å, º)

Ag1—N2^{i}	2.276 (5)	C2—C3	1.389 (7)
Ag1—N1	2.333 (4)	C2—C6	1.495 (7)
Ag1—S1^{ii}	2.5305 (14)	C3—C4	1.383 (7)
Ag1—O1′	2.55 (2)	C3—H3	0.9300
S1—C6	1.828 (5)	C4—C5	1.385 (8)
S1—C7	1.829 (5)	C4—H4	0.9300
S1—Ag1^{ii}	2.5305 (14)	C5—H5	0.9300
N1—C1	1.338 (6)	C6—H6A	0.9700
N1—C5	1.342 (7)	C6—H6B	0.9700
N2—C10	1.333 (7)	C7—C8	1.500 (7)
N2—C9	1.348 (7)	C7—H7A	0.9700
N2—Ag1^{iii}	2.276 (5)	C7—H7B	0.9700
N3—O2′	1.09 (2)	C8—C9	1.371 (7)
N3—O1′	1.16 (2)	C8—C12	1.381 (7)
N3—O3	1.199 (11)	C9—H9	0.9300
N3—O1	1.246 (17)	C10—C11	1.371 (9)
N3—O2	1.265 (12)	C10—H10	0.9300
N3—O3′	1.340 (14)	C11—C12	1.367 (8)
C1—C2	1.389 (7)	C11—H11	0.9300

C1—H1	0.9300	C12—H12	0.9300

N2^{i}—Ag1—N1	113.22 (16)	C3—C4—H4	120.9
N2^{i}—Ag1—S1^{ii}	133.18 (12)	C5—C4—H4	120.9
N1—Ag1—S1^{ii}	106.03 (12)	N1—C5—C4	123.1 (5)
N2^{i}—Ag1—O1′	97.5 (4)	N1—C5—H5	118.4
N1—Ag1—O1′	105.9 (5)	C4—C5—H5	118.4
S1^{ii}—Ag1—O1′	95.2 (5)	C2—C6—S1	114.0 (4)
C6—S1—C7	102.7 (3)	C2—C6—H6A	108.7
C6—S1—Ag1^{ii}	108.12 (18)	S1—C6—H6A	108.7
C7—S1—Ag1^{ii}	105.08 (18)	C2—C6—H6B	108.7
C1—N1—C5	117.6 (5)	S1—C6—H6B	108.7
C1—N1—Ag1	125.9 (3)	H6A—C6—H6B	107.6
C5—N1—Ag1	116.5 (3)	C8—C7—S1	107.6 (4)
C10—N2—C9	116.7 (5)	C8—C7—H7A	110.2
C10—N2—Ag1^{iii}	122.9 (4)	S1—C7—H7A	110.2
C9—N2—Ag1^{iii}	120.1 (4)	C8—C7—H7B	110.2
O2′—N3—O1′	127.6 (17)	S1—C7—H7B	110.2
O3—N3—O1	130.1 (11)	H7A—C7—H7B	108.5
O3—N3—O2	114.9 (11)	C9—C8—C12	118.2 (5)
O1—N3—O2	113.4 (12)	C9—C8—C7	120.6 (5)
O2′—N3—O3′	117.6 (16)	C12—C8—C7	121.1 (5)
O1′—N3—O3′	114.7 (13)	N2—C9—C8	123.3 (5)
N3—O1′—Ag1	118.8 (14)	N2—C9—H9	118.3
N1—C1—C2	123.8 (5)	C8—C9—H9	118.3
N1—C1—H1	118.1	N2—C10—C11	123.9 (6)
C2—C1—H1	118.1	N2—C10—H10	118.1
C3—C2—C1	117.3 (5)	C11—C10—H10	118.1
C3—C2—C6	123.5 (5)	C12—C11—C10	118.4 (6)
C1—C2—C6	119.2 (5)	C12—C11—H11	120.8
C4—C3—C2	120.0 (5)	C10—C11—H11	120.8
C4—C3—H3	120.0	C11—C12—C8	119.5 (6)
C2—C3—H3	120.0	C11—C12—H12	120.3
C3—C4—C5	118.2 (5)	C8—C12—H12	120.3

O2′—N3—O1′—Ag1	−73 (3)	Ag1^{ii}—S1—C6—C2	10.9 (4)
O3′—N3—O1′—Ag1	107.3 (14)	C6—S1—C7—C8	173.0 (4)
C5—N1—C1—C2	−1.3 (7)	Ag1^{ii}—S1—C7—C8	60.0 (4)
Ag1—N1—C1—C2	−178.0 (4)	S1—C7—C8—C9	−110.0 (5)
N1—C1—C2—C3	0.5 (7)	S1—C7—C8—C12	70.4 (6)
N1—C1—C2—C6	180.0 (5)	C10—N2—C9—C8	−0.5 (8)
C1—C2—C3—C4	0.5 (7)	Ag1^{iii}—N2—C9—C8	173.4 (4)
C6—C2—C3—C4	−178.9 (5)	C12—C8—C9—N2	−0.8 (8)
C2—C3—C4—C5	−0.7 (8)	C7—C8—C9—N2	179.6 (5)
C1—N1—C5—C4	1.2 (8)	C9—N2—C10—C11	1.5 (9)
Ag1—N1—C5—C4	178.2 (4)	Ag1^{iii}—N2—C10—C11	−172.3 (5)
C3—C4—C5—N1	−0.2 (8)	N2—C10—C11—C12	−1.0 (10)
C3—C2—C6—S1	62.6 (6)	C10—C11—C12—C8	−0.5 (9)

C1—C2—C6—S1	−116.9 (4)	C9—C8—C12—C11	1.3 (8)
C7—S1—C6—C2	−99.9 (4)	C7—C8—C12—C11	−179.1 (5)

Symmetry codes: (i) *x*−1/2, *y*+1/2, *z*; (ii) −*x*+1/2, −*y*+1/2, −*z*+1; (iii) *x*+1/2, *y*−1/2, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2	0.93	2.59	2.924 (12)	102
C5—H5···O2^{iv}	0.93	2.60	3.318 (14)	135
C6—H6*A*···O2^{v}	0.97	2.52	3.464 (14)	163
C6—H6*B*···O2′^{vi}	0.97	2.60	3.44 (2)	145
C7—H7*B*···O3′^{v}	0.97	2.38	3.233 (15)	147
C9—H9···O1^{iii}	0.93	2.49	3.221 (18)	136
C12—H12···O3^{vii}	0.93	2.45	3.256 (12)	145

Symmetry codes: (iii) *x*+1/2, *y*−1/2, *z*; (iv) −*x*+1/2, −*y*+3/2, −*z*+1; (v) −*x*+1/2, *y*−1/2, −*z*+1/2; (vi) *x*, *y*−1, *z*; (vii) −*x*+1/2, *y*−3/2, −*z*+1/2.