

Bis[μ -N-(pyridin-2-ylmethyl)pyridin-2-amine- κ^2 N:N']disilver(I) bis(trifluoromethanesulfonate)

Suk-Hee Moon,^a Tae Ho Kim^{b*} and Ki-Min Park^{b*}

^aDepartment of Food & Nutrition, Kyungnam College of Information and Technology, Busan 617-701, Republic of Korea, and ^bDepartment of Chemistry and Research Institute of Natural Sciences, Gyeongsang, National University, Jinju 660-701, Republic of Korea

Correspondence e-mail: thkim@gnu.ac.kr, kmpark@gnu.ac.kr

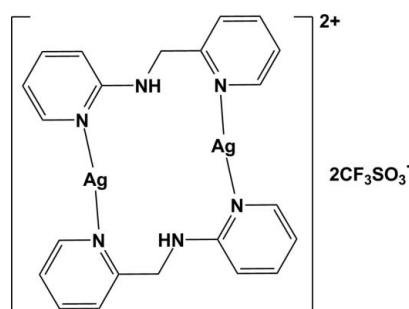
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 13.4.

In the binuclear title compound, $[Ag_2(C_{11}H_{11}N_3)_2](CF_3O_3S)_2$, the complex cation is centrosymmetric, with the unique Ag^+ cation coordinated by two pyridine N atoms from two symmetry-related N-(pyridin-2-ylmethyl)pyridin-2-amine ligands in a geometry slightly distorted from linear [N—Ag—N 161.02 (7)°]. This set-up leads to the formation of a 14-membered cyclic dimer. The two pyridine rings coordinated to the Ag^+ cation are tilted by 80.19 (7)° with respect to each other. Intermolecular N—H···O hydrogen-bonding interactions between the cyclic dimer and the anion exist. A two-dimensional network parallel to the *ac* plane is constructed by three weak Ag···(O,N) interactions as well as an F···F contact of 2.890 (4) Å.

Related literature

For the synthesis of the ligand, see: Foxon *et al.* (2002). For the crystal structure of the free ligand, see: Moon *et al.* (2011). For the structures of related copper complexes, see: Lee *et al.* (2008).



Experimental

Crystal data

$[Ag_2(C_{11}H_{11}N_3)_2](CF_3O_3S)_2$	$\gamma = 116.606 (1)^\circ$
$M_r = 884.34$	$V = 725.58 (8) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 1$
$a = 8.4105 (5) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.3500 (6) \text{ \AA}$	$\mu = 1.58 \text{ mm}^{-1}$
$c = 11.1693 (7) \text{ \AA}$	$T = 173 \text{ K}$
$\alpha = 108.489 (1)^\circ$	$0.35 \times 0.35 \times 0.25 \text{ mm}$
$\beta = 92.826 (1)^\circ$	

Data collection

Bruker APEXII CCD diffractometer	4132 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	2791 independent reflections
$T_{\min} = 0.607$, $T_{\max} = 0.693$	2665 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.012$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$	208 parameters
$wR(F^2) = 0.058$	H-atom parameters constrained
$S = 1.07$	$\Delta\rho_{\max} = 0.52 \text{ e \AA}^{-3}$
2791 reflections	$\Delta\rho_{\min} = -0.58 \text{ e \AA}^{-3}$

Table 1
Selected bond lengths (Å).

$Ag1—N2^i$	2.1500 (19)	$Ag1—O2$	2.890 (2)
$Ag1—N1$	2.1673 (19)	$Ag1—O1^{ii}$	3.0402 (18)
$Ag1—N3$	2.8573 (19)		

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

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

$D—H···A$	$D—H$	$H···A$	$D···A$	$D—H···A$
$N3—H3N···O2^i$	0.88	2.16	2.925 (3)	145

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1998); 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: WM2556).

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supporting information

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Bis[μ -N-(pyridin-2-ylmethyl)pyridin-2-amine- κ^2 N:N']disilver(I) bis(trifluoromethanesulfonate)

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S1. Comment

The dipyridyl ligand *N*-(pyridin-2-ylmethyl)pyridin-2-amine has been synthesized by the reaction of 2-aminopyridine and 2-pyridinecarboxaldehyde according to literature (Foxon *et al.*, 2002) and its crystal structure was already reported by our group (Moon *et al.*, 2011). In the reaction of the ligand and Cu X (X = I and Br), two-dimensional brick-wall type coordination polymers, in which rhomboid Cu $_2$ X $_2$ nodes interconnect the dipyridyl ligands, were obtained (Lee *et al.*, 2008). Herein, we report the crystal structure of the title compound prepared by the reaction of silver trifluoromethanesulfonate with the dipyridyl ligand.

The binuclear cation of the title compound, [Ag $_2$ (C $_{11}$ H $_{11}$ N $_3$) $_2$](CF $_3$ SO $_3$) $_2$, is located on an inversion centre. The asymmetric unit of the compound therefore consists of a Ag $^+$ cation, an *N*-(pyridin-2-ylmethyl)pyridin-2-amine ligand and a trifluoromethanesulfonate anion. The two Ag $^+$ cations, each in a geometry slightly distorted from linear (N—Ag—N 161.02 (7) $^\circ$), are coordinated by two pyridine N atoms from two symmetry-related *N*-(pyridine-2-ylmethyl)pyridine-2-amine ligands, leading to the formation of a centrosymmetric 14-membered cyclic dimer (Fig. 1). Two pyridine rings coordinated to the Ag $^+$ cations are tilted by 80.19 (7) $^\circ$ with respect to each other.

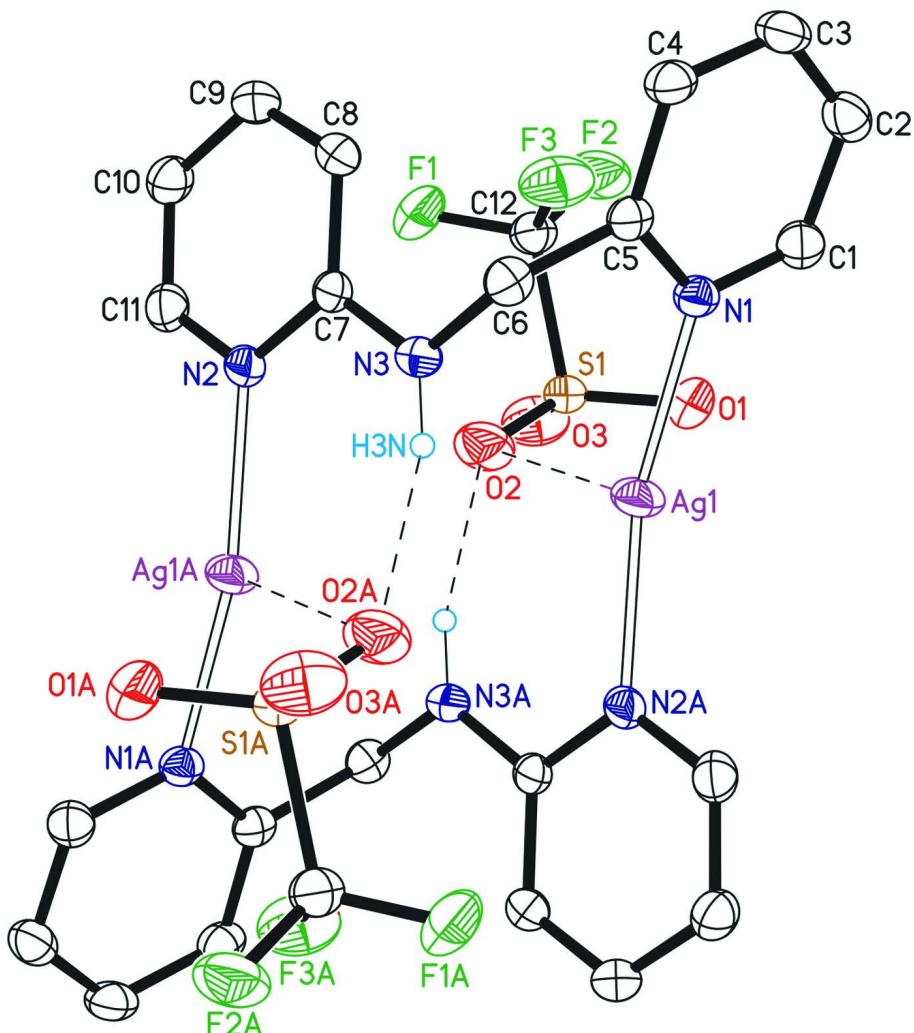
The non-coordinated CF $_3$ SO $_3^-$ anions participate in N—H \cdots O hydrogen-bonding (Table 1, Fig. 1) and weak Ag \cdots O interactions, as well as an F \cdots F contact of 2.890 (4) Å. Together with another weak Ag—N contact, this leads to the construction of a two-dimensional network extending parallel to the *ac* plane (Fig. 2).

S2. Experimental

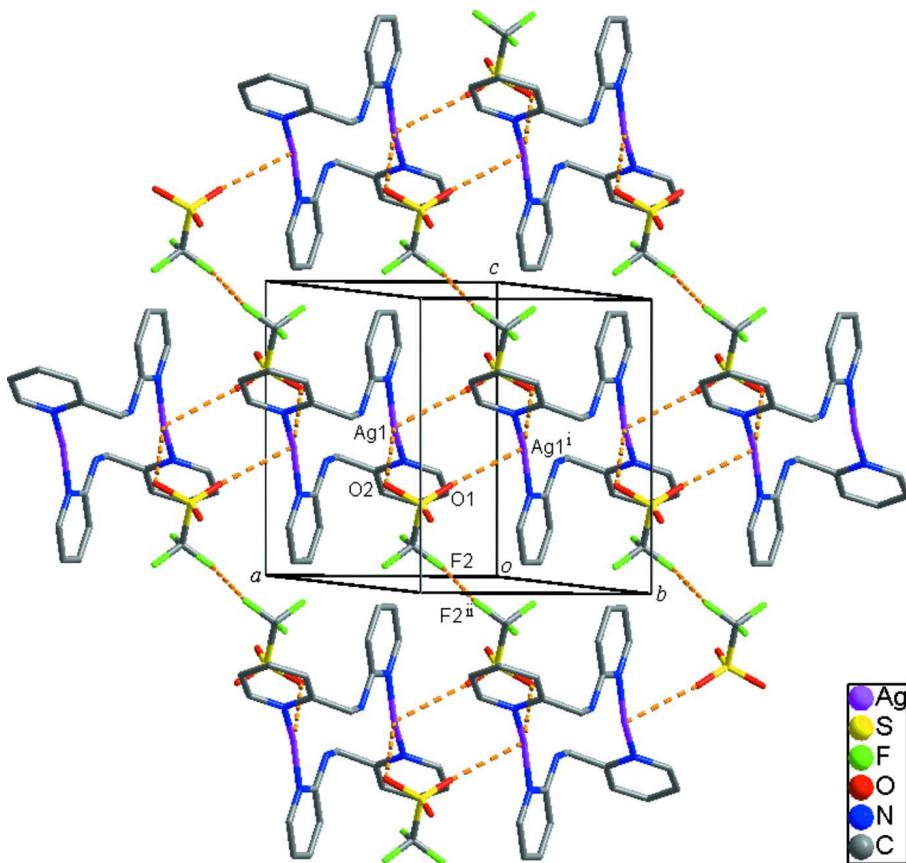
The ligand (*N*-(pyridine-2-ylmethyl)pyridine-2-amine) was synthesized according to a procedure described by Foxon *et al.* (2002). Crystals of the title compound suitable for X-ray analysis were obtained by vapor diffusion of diethyl ether into a DMSO solution of the white precipitate afforded by the reaction of the ligand with silver(I) trifluoromethanesulfonate in the molar ratio 1:1 in methanol.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with d(C—H) = 0.95 Å for Csp 2 —H, 0.88 Å for amine N—H and 0.99 Å for methylene C—H. For all H atoms $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

**Figure 1**

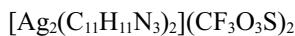
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms not involved in intermolecular interactions have been omitted for clarity. H atoms are depicted as spheres with arbitrary radii; N–H···O hydrogen bonds and Ag···O interactions are shown as dashed lines. (Symmetry code: (A) $-x + 2, -y + 1, -z + 1$)

**Figure 2**

Two-dimensional network constructed by intermolecular $\text{Ag}\cdots\text{O}$ and $\text{F}\cdots\text{F}$ interactions shown as dashed lines. H atoms have been omitted for clarity. (Symmetry codes: i) $-x + 1, -y + 1, -z + 1$; ii) $-x + 1, -y + 1, -z$)

Bis[μ -N-(pyridin-2-ylmethyl)pyridin-2-amine- $\kappa^2\text{N}:\text{N}'$]disilver(I) bis(trifluoromethanesulfonate)

Crystal data



$M_r = 884.34$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.4105 (5) \text{ \AA}$

$b = 9.3500 (6) \text{ \AA}$

$c = 11.1693 (7) \text{ \AA}$

$\alpha = 108.489 (1)^\circ$

$\beta = 92.826 (1)^\circ$

$\gamma = 116.606 (1)^\circ$

$V = 725.58 (8) \text{ \AA}^3$

$Z = 1$

$F(000) = 436$

$D_x = 2.024 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3938 reflections

$\theta = 2.7\text{--}28.3^\circ$

$\mu = 1.58 \text{ mm}^{-1}$

$T = 173 \text{ K}$

Block, colorless

$0.35 \times 0.35 \times 0.25 \text{ mm}$

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.607, T_{\max} = 0.693$

4132 measured reflections

2791 independent reflections

2665 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.012$
 $\theta_{\text{max}} = 26.0^\circ, \theta_{\text{min}} = 2.0^\circ$
 $h = -9 \rightarrow 10$

$k = -11 \rightarrow 8$
 $l = -11 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.058$
 $S = 1.07$
2791 reflections
208 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
 $w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.5885P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.52 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.58 \text{ e } \text{\AA}^{-3}$

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.73116 (2)	0.42494 (2)	0.529910 (17)	0.02835 (8)
S1	0.71713 (7)	0.57867 (7)	0.27669 (5)	0.02346 (13)
F1	0.7558 (2)	0.4025 (2)	0.05757 (16)	0.0470 (4)
F2	0.4881 (2)	0.3730 (2)	0.05173 (16)	0.0458 (4)
F3	0.5706 (3)	0.2439 (2)	0.14581 (17)	0.0472 (4)
O1	0.5669 (3)	0.5441 (3)	0.33935 (19)	0.0453 (5)
O2	0.8665 (3)	0.5741 (3)	0.34139 (18)	0.0401 (4)
O3	0.7701 (3)	0.7179 (2)	0.2327 (2)	0.0432 (5)
N1	0.5191 (2)	0.1705 (2)	0.40024 (18)	0.0208 (4)
N2	1.0963 (2)	0.3571 (2)	0.29514 (18)	0.0214 (4)
N3	0.8870 (2)	0.2190 (2)	0.40206 (18)	0.0233 (4)
H3N	0.9469	0.3125	0.4732	0.028*
C1	0.3513 (3)	0.1454 (3)	0.3606 (2)	0.0246 (5)
H1	0.3303	0.2413	0.3882	0.030*
C2	0.2088 (3)	-0.0146 (3)	0.2816 (2)	0.0276 (5)
H2	0.0916	-0.0288	0.2561	0.033*
C3	0.2397 (3)	-0.1544 (3)	0.2398 (2)	0.0290 (5)
H3	0.1438	-0.2661	0.1859	0.035*
C4	0.4122 (3)	-0.1284 (3)	0.2781 (2)	0.0256 (5)
H4	0.4370	-0.2219	0.2494	0.031*
C5	0.5496 (3)	0.0359 (3)	0.3591 (2)	0.0201 (4)
C6	0.7364 (3)	0.0649 (3)	0.4082 (2)	0.0230 (4)

H6A	0.7481	0.0738	0.4992	0.028*
H6B	0.7467	-0.0372	0.3566	0.028*
C7	0.9368 (3)	0.2208 (3)	0.2875 (2)	0.0195 (4)
C8	0.8283 (3)	0.0890 (3)	0.1673 (2)	0.0236 (5)
H8	0.7182	-0.0083	0.1631	0.028*
C9	0.8834 (3)	0.1027 (3)	0.0562 (2)	0.0264 (5)
H9	0.8101	0.0155	-0.0257	0.032*
C10	1.0466 (3)	0.2440 (3)	0.0629 (2)	0.0271 (5)
H10	1.0864	0.2556	-0.0133	0.033*
C11	1.1477 (3)	0.3658 (3)	0.1834 (2)	0.0259 (5)
H11	1.2601	0.4618	0.1889	0.031*
C12	0.6282 (3)	0.3897 (3)	0.1256 (2)	0.0265 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02417 (11)	0.01720 (10)	0.02998 (12)	0.00595 (8)	-0.00098 (7)	-0.00025 (7)
S1	0.0221 (3)	0.0213 (3)	0.0212 (3)	0.0091 (2)	0.0029 (2)	0.0037 (2)
F1	0.0484 (10)	0.0486 (10)	0.0368 (9)	0.0236 (9)	0.0216 (8)	0.0059 (8)
F2	0.0425 (9)	0.0494 (10)	0.0325 (8)	0.0217 (8)	-0.0096 (7)	0.0038 (7)
F3	0.0636 (11)	0.0233 (8)	0.0445 (10)	0.0155 (8)	0.0077 (8)	0.0098 (7)
O1	0.0343 (10)	0.0484 (12)	0.0359 (11)	0.0150 (9)	0.0156 (9)	0.0019 (9)
O2	0.0359 (10)	0.0451 (11)	0.0313 (10)	0.0205 (9)	-0.0062 (8)	0.0060 (9)
O3	0.0574 (13)	0.0234 (9)	0.0423 (11)	0.0160 (9)	0.0063 (10)	0.0111 (8)
N1	0.0211 (9)	0.0183 (9)	0.0192 (9)	0.0073 (7)	0.0041 (7)	0.0062 (7)
N2	0.0179 (9)	0.0175 (9)	0.0250 (10)	0.0079 (7)	0.0044 (7)	0.0048 (7)
N3	0.0200 (9)	0.0216 (9)	0.0193 (9)	0.0063 (8)	0.0029 (7)	0.0030 (7)
C1	0.0248 (11)	0.0261 (12)	0.0235 (11)	0.0126 (10)	0.0051 (9)	0.0098 (9)
C2	0.0220 (11)	0.0331 (13)	0.0226 (11)	0.0095 (10)	0.0023 (9)	0.0107 (10)
C3	0.0258 (12)	0.0233 (12)	0.0222 (11)	0.0031 (10)	0.0018 (9)	0.0036 (9)
C4	0.0285 (12)	0.0187 (11)	0.0238 (11)	0.0088 (9)	0.0072 (9)	0.0050 (9)
C5	0.0232 (10)	0.0191 (10)	0.0173 (10)	0.0084 (9)	0.0070 (8)	0.0090 (8)
C6	0.0250 (11)	0.0224 (11)	0.0225 (11)	0.0116 (9)	0.0065 (9)	0.0096 (9)
C7	0.0173 (10)	0.0188 (10)	0.0218 (11)	0.0102 (8)	0.0039 (8)	0.0051 (9)
C8	0.0192 (10)	0.0209 (11)	0.0236 (11)	0.0063 (9)	0.0041 (9)	0.0054 (9)
C9	0.0250 (11)	0.0274 (12)	0.0201 (11)	0.0109 (10)	0.0021 (9)	0.0043 (9)
C10	0.0285 (12)	0.0284 (12)	0.0242 (11)	0.0131 (10)	0.0100 (9)	0.0104 (10)
C11	0.0232 (11)	0.0239 (11)	0.0304 (12)	0.0112 (9)	0.0094 (9)	0.0101 (10)
C12	0.0278 (11)	0.0250 (12)	0.0232 (11)	0.0117 (10)	0.0046 (9)	0.0071 (9)

Geometric parameters (\AA , ^\circ)

Ag1—N2 ⁱ	2.1500 (19)	C1—C2	1.381 (3)
Ag1—N1	2.1673 (19)	C1—H1	0.9500
Ag1—N3	2.8573 (19)	C2—C3	1.386 (4)
Ag1—O2	2.890 (2)	C2—H2	0.9500
Ag1—C11 ⁱ	3.006 (2)	C3—C4	1.380 (3)
Ag1—O1 ⁱⁱ	3.0402 (18)	C3—H3	0.9500

S1—O3	1.429 (2)	C4—C5	1.393 (3)
S1—O1	1.4337 (19)	C4—H4	0.9500
S1—O2	1.4420 (19)	C5—C6	1.511 (3)
S1—C12	1.825 (2)	C6—H6A	0.9900
F1—C12	1.329 (3)	C6—H6B	0.9900
F2—C12	1.323 (3)	C7—C8	1.406 (3)
F3—C12	1.327 (3)	C7—Ag1 ⁱ	3.131 (2)
O1—Ag1 ⁱⁱ	3.0402 (18)	C8—C9	1.369 (3)
N1—C5	1.340 (3)	C8—H8	0.9500
N1—C1	1.348 (3)	C9—C10	1.392 (3)
N2—C7	1.349 (3)	C9—H9	0.9500
N2—C11	1.355 (3)	C10—C11	1.371 (3)
N2—Ag1 ⁱ	2.1500 (19)	C10—H10	0.9500
N3—C7	1.369 (3)	C11—Ag1 ⁱ	3.006 (2)
N3—C6	1.456 (3)	C11—H11	0.9500
N3—H3N	0.8800		
N2 ⁱ —Ag1—N1	161.02 (7)	C5—C4—H4	120.3
N2 ⁱ —Ag1—N3	115.71 (6)	N1—C5—C4	121.6 (2)
N1—Ag1—N3	69.45 (6)	N1—C5—C6	118.06 (19)
N2 ⁱ —Ag1—O2	99.53 (6)	C4—C5—C6	120.3 (2)
N1—Ag1—O2	99.40 (6)	C4—C5—Ag1	158.27 (17)
N3—Ag1—O2	79.27 (6)	C6—C5—Ag1	81.36 (12)
N2 ⁱ —Ag1—O1 ⁱⁱ	81.91 (6)	N3—C6—C5	114.20 (18)
N1—Ag1—O1 ⁱⁱ	86.40 (6)	N3—C6—Ag1	62.26 (11)
N3—Ag1—O1 ⁱⁱ	149.79 (6)	C5—C6—Ag1	71.08 (12)
O2—Ag1—O1 ⁱⁱ	123.91 (6)	N3—C6—H6A	108.7
C11 ⁱ —Ag1—O1 ⁱⁱ	64.92 (6)	C5—C6—H6A	108.7
O3—S1—O1	116.39 (14)	Ag1—C6—H6A	83.1
O3—S1—O2	114.82 (13)	N3—C6—H6B	108.7
O1—S1—O2	113.51 (13)	C5—C6—H6B	108.7
O3—S1—C12	102.74 (12)	Ag1—C6—H6B	168.3
O1—S1—C12	104.03 (12)	H6A—C6—H6B	107.6
O2—S1—C12	102.98 (11)	N2—C7—N3	116.50 (19)
S1—O1—Ag1 ⁱⁱ	162.63 (14)	N2—C7—C8	121.1 (2)
S1—O2—Ag1	106.35 (10)	N3—C7—C8	122.42 (19)
C5—N1—C1	118.76 (19)	N3—C7—Ag1 ⁱ	82.48 (12)
C5—N1—Ag1	121.61 (15)	C8—C7—Ag1 ⁱ	155.01 (15)
C1—N1—Ag1	119.63 (15)	C9—C8—C7	119.2 (2)
C7—N2—C11	118.19 (19)	C9—C8—H8	120.4
C7—N2—Ag1 ⁱ	125.35 (15)	C7—C8—H8	120.4
C11—N2—Ag1 ⁱ	116.27 (15)	C8—C9—C10	120.2 (2)
C7—N3—C6	121.04 (18)	C8—C9—H9	119.9
C7—N3—H3N	119.5	C10—C9—H9	119.9
C6—N3—H3N	119.5	C11—C10—C9	117.6 (2)
N1—C1—C2	122.4 (2)	C11—C10—H10	121.2
C2—C1—Ag1	160.26 (18)	C9—C10—H10	121.2
N1—C1—H1	118.8	N2—C11—C10	123.7 (2)

C2—C1—H1	118.8	C10—C11—Ag ⁱ	163.26 (17)
Ag ⁱ —C1—H1	80.9	N2—C11—H11	118.1
C1—C2—C3	118.9 (2)	C10—C11—H11	118.1
C1—C2—H2	120.5	Ag ⁱ —C11—H11	78.4
C3—C2—H2	120.5	F2—C12—F3	106.8 (2)
C4—C3—C2	118.8 (2)	F2—C12—F1	107.4 (2)
C4—C3—H3	120.6	F3—C12—F1	107.8 (2)
C2—C3—H3	120.6	F2—C12—S1	111.64 (17)
C3—C4—C5	119.5 (2)	F3—C12—S1	112.18 (17)
C3—C4—H4	120.3	F1—C12—S1	110.72 (17)
N2 ⁱ —Ag ⁱ —N1—C5	-89.5 (3)	Ag ⁱ —N2—C7—C8	176.29 (16)
N2 ⁱ —Ag ⁱ —N1—C1	89.7 (3)	C6—N3—C7—N2	-168.59 (19)
C5—N1—C1—C2	1.4 (3)	C6—N3—C7—C8	11.8 (3)
Ag ⁱ —N1—C1—C2	-177.83 (17)	N2—C7—C8—C9	-2.1 (3)
N1—C1—C2—C3	-0.8 (4)	N3—C7—C8—C9	177.5 (2)
C1—C2—C3—C4	-0.5 (4)	C7—C8—C9—C10	1.2 (4)
C2—C3—C4—C5	1.2 (3)	C8—C9—C10—C11	0.3 (4)
C1—N1—C5—C4	-0.6 (3)	C7—N2—C11—C10	0.1 (3)
Ag ⁱ —N1—C5—C4	178.56 (16)	Ag ⁱ —N2—C11—C10	-175.23 (19)
C1—N1—C5—C6	-177.88 (19)	C9—C10—C11—N2	-0.9 (4)
Ag ⁱ —N1—C5—C6	1.3 (3)	O3—S1—C12—F2	-60.1 (2)
C3—C4—C5—N1	-0.6 (3)	O1—S1—C12—F2	61.6 (2)
C3—C4—C5—C6	176.6 (2)	O2—S1—C12—F2	-179.73 (18)
C7—N3—C6—C5	-77.7 (3)	O3—S1—C12—F3	-179.98 (18)
N1—C5—C6—N3	-46.9 (3)	O1—S1—C12—F3	-58.2 (2)
C4—C5—C6—N3	135.8 (2)	O2—S1—C12—F3	60.4 (2)
C11—N2—C7—N3	-178.18 (19)	O3—S1—C12—F1	59.5 (2)
Ag ⁱ —N2—C7—N3	-3.3 (3)	O1—S1—C12—F1	-178.74 (19)
C11—N2—C7—C8	1.4 (3)	O2—S1—C12—F1	-60.1 (2)

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

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

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
N3—H3N \cdots O2 ⁱ	0.88	2.16	2.925 (3)	145

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