

# catena-Poly[[[6-aminonaphthalene-1-sulfonato- $\kappa$ O]silver(I)]- $\mu$ -2,3,5,6-tetramethylpyrazine- $\kappa^2$ N:N']

Hai-Yan Liu, Ji-Cheng Ma and Ying-Ying Liu\*

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail: liuyy21@yahoo.com.cn

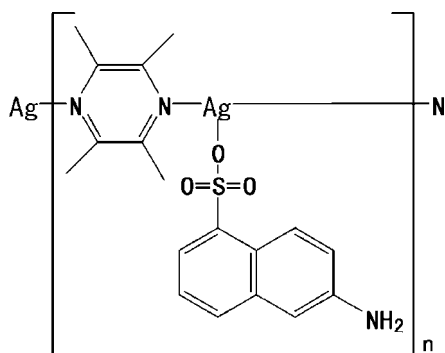
Received 5 October 2007; accepted 9 October 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.020;  $wR$  factor = 0.047; data-to-parameter ratio = 14.8.

In the title compound,  $[\text{Ag}(\text{C}_{10}\text{H}_8\text{NO}_3\text{S})(\text{C}_8\text{H}_{12}\text{N}_2)]_n$ , the  $\text{Ag}^+$  cation is three-coordinated by two N atoms from two 2,3,5,6-tetramethylpyrazine ligands and one O atom from a 7-aminonaphthalene-1-sulfonate anion. The 2,3,5,6-tetramethylpyrazine ligand acts as a bridging bidentate ligand, linking the  $\text{Ag}^+$  centres into a one-dimensional chain. The chains are interconnected *via* intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and  $\text{C}-\text{H}\cdots\pi$  interactions, resulting in the formation of a three-dimensional framework.

## Related literature

The bond distances and angles in the title compound are normal (Wu *et al.*, 2006).



## Experimental

### Crystal data

$[\text{Ag}(\text{C}_{10}\text{H}_8\text{NO}_3\text{S})(\text{C}_8\text{H}_{12}\text{N}_2)]$   
 $M_r = 466.30$

Monoclinic,  $Cc$   
 $a = 10.101$  (5) Å  
 $b = 10.631$  (6) Å  
 $c = 15.831$  (7) Å  
 $\beta = 96.180$  (19)°

$V = 1690.1$  (15) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 1.34$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.21 \times 0.16 \times 0.15$  mm

### Data collection

Bruker APEX CCD area-detector diffractometer  
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\min} = 0.765$ ,  $T_{\max} = 0.808$

8210 measured reflections  
3626 independent reflections  
3534 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.016$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$   
 $wR(F^2) = 0.047$   
 $S = 1.12$   
3626 reflections  
245 parameters  
4 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.51$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983), 1687 Friedel pairs  
Flack parameter:  $-0.001$  (14)

**Table 1**

Selected geometric parameters (Å, °).

Ag1—N1	2.279 (2)	Ag1—O1	2.5936 (19)
Ag1—N2	2.298 (2)		
N1—Ag1—N2	171.76 (6)	N2—Ag1—O1	85.19 (6)
N1—Ag1—O1	102.85 (6)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$Cg1$  is the centroid of the C1—C4/C10/C9 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H1N $\cdots$ O3 <sup>i</sup>	0.85 (2)	2.23 (3)	3.055 (3)	165 (4)
N3—H2N $\cdots$ O2 <sup>ii</sup>	0.83 (2)	2.43 (3)	3.197 (3)	155 (3)
C16—H16B $\cdots$ Cg1 <sup>iii</sup>	0.96	2.65	3.425 (3)	138

Symmetry codes: (i)  $x, -y + 1, z + \frac{1}{2}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$ ; (iii)  $x - \frac{1}{2}, y + \frac{1}{2}, z$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank the Analysis and Testing Foundation of Northeast Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2480).

## References

- Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison, Wisconsin, USA.  
Bruker (1999). *SAINTE*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.  
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.  
Sheldrick, G. M. (1996). *SADABS*. Version 2.03. University of Göttingen, Germany.  
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
Wu, H., Dong, X.-W. & Ma, J.-F. (2006). *Acta Cryst.* **E62**, m1227–m1228.

**supplementary materials**

*Acta Cryst.* (2007). E63, m3035 [ doi:10.1107/S1600536807049550 ]

***catena*-Poly[[*(*6-aminonaphthalene-1-sulfonato- $\kappa$ O)*silver*(I)]- $\mu$ -2,3,5,6-tetramethylpyrazine- $\kappa^2$ N:N']**

**H.-Y. Liu, J.-C. Ma and Y.-Y. Liu**

**Comment**

As part of an investigation of the transition metal application there is a need to prepare further examples of these compounds. In this paper, the structure of the title compound is described.

As shown in Fig. 1, the Ag<sup>I</sup> ion is three coordinated by two N atoms from two 2,3,5,6-tetramethylpyrazine ligands and one O atom from a 7-aminonaphthalene-1-sulfonate anion. Each 2,3,5,6-tetramethylpyrazine ligand coordinates to two Ag<sup>I</sup> cations through its two aromatic N atoms, thus acting as a bridging bidentate ligand. The Ag<sup>I</sup> cations are bridged by 2,3,5,6-tetramethylpyrazine ligands to a chain structure. In the chain, face-to-face  $\pi$ - $\pi$  interaction is observed between the naphthalene ring system and the adjacent pyrazine ring, with a ring centroid-to-centroid distance of 3.517 (1) Å. (Fig. 2). Intermolecular N—H $\cdots$ O hydrogen bonds (Table 2) involving the amino N atom and two sulfonate O atoms of two adjacent 7-aminonaphthalene-1-sulfonate anions link the chains into a three-dimensional framework (Fig. 3). A C—H $\cdots$  $\pi$  interaction (Table 2) between a methyl group of the 2,3,5,6-tetramethylpyrazine ligand and the C1—C4/C10/C9 benzene ring (centroid Cg1) of the adjacent naphthalene ring system further stabilize the three-dimensional framework.

**Experimental**

An aqueous solution (10 ml) of 7-aminonaphthalene-1-sulfonic acid (0.112 g, 0.5 mmol) was added to solid Ag<sub>2</sub>CO<sub>3</sub> (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO<sub>2</sub> was given off. 2,3,5,6-tetramethylpyrazine (0.068 g, 0.5 mmol) in methanol (5 ml) was then added and a white precipitate formed. The precipitate was dissolved by dropwise addition of an aqueous solution of NH<sub>3</sub> (14 M), and crystals of the title compound were obtained by slow evaporation of the solvent for several days at room temperature.

**Refinement**

H atoms of the amino group were located in a difference map and refined isotropically with  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{N})$ . C-bound H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$  for aromatic H atoms and C—H = 0.96 Å and  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms. The maximum residual density peak is 0.71 Å from atom Ag1.

## Figures

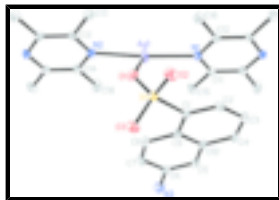


Fig. 1. A view of the local coordination of the Ag<sup>1</sup> cation in the title compound. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.



Fig. 2. Part of the polymeric chain in the title compound, showing face-to-face  $\pi$ - $\pi$  interactions as dashed lines.

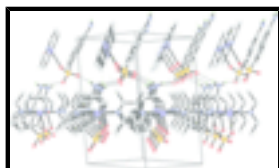


Fig. 3. Part of the crystal structure of the title compound, showing N—H...O hydrogen bonds (dashed lines). C-bound H-atoms have been omitted for clarity.

## **catena-Poly[[*(*(6-aminonaphthalene-1-sulfonato-*k*O)silver(I)]- $\mu$ -2,3,5,6-tetramethylpyrazine- $\kappa^2$ N:N']**

### Crystal data

[Ag(C<sub>10</sub>H<sub>8</sub>NO<sub>3</sub>S)(C<sub>8</sub>H<sub>12</sub>N<sub>2</sub>)]

$M_r = 466.30$

Monoclinic, *Cc*

Hall symbol: C -2yc

$a = 10.101$  (5) Å

$b = 10.631$  (6) Å

$c = 15.831$  (7) Å

$\beta = 96.180$  (19)°

$V = 1690.1$  (15) Å<sup>3</sup>

$Z = 4$

$F_{000} = 944$

$D_x = 1.833$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71069$  Å

Cell parameters from 8199 reflections

$\theta = 3.2$ – $27.5$ °

$\mu = 1.34$  mm<sup>-1</sup>

$T = 293$  (2) K

Block, yellow

$0.21 \times 0.16 \times 0.15$  mm

### Data collection

Bruker APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

$\omega$  scans

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

$T_{\min} = 0.765$ ,  $T_{\max} = 0.808$

8210 measured reflections

3626 independent reflections

3534 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 3.2$ °

$h = -12 \rightarrow 13$

$k = -13 \rightarrow 13$

$l = -20 \rightarrow 20$

Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.020$	$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.047$	$(\Delta/\sigma)_{\max} = 0.002$
$S = 1.12$	$\Delta\rho_{\max} = 0.51 \text{ e } \text{\AA}^{-3}$
3626 reflections	$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$
245 parameters	Extinction correction: none
4 restraints	Absolute structure: Flack (1983), with 1687 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: $-0.001 (14)$
Secondary atom site location: difference Fourier map	

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.404494 (13)	0.904978 (15)	0.914016 (11)	0.03466 (6)
C1	0.4695 (2)	0.61273 (18)	0.79933 (12)	0.0199 (4)
C2	0.3599 (2)	0.5415 (2)	0.77423 (14)	0.0275 (4)
H2	0.3126	0.5553	0.7214	0.033*
C3	0.3183 (2)	0.4473 (2)	0.82799 (17)	0.0334 (5)
H3	0.2428	0.3998	0.8109	0.040*
C4	0.3888 (3)	0.4256 (2)	0.9052 (2)	0.0306 (5)
H4	0.3600	0.3633	0.9403	0.037*
C5	0.5778 (2)	0.4698 (2)	1.01204 (13)	0.0252 (4)
H5	0.5502	0.4054	1.0458	0.030*
C6	0.6894 (2)	0.5382 (2)	1.03999 (13)	0.0246 (4)
C7	0.7290 (3)	0.6356 (3)	0.98737 (15)	0.0304 (5)
H7	0.8041	0.6828	1.0058	0.037*
C8	0.6608 (2)	0.6625 (2)	0.91078 (14)	0.0282 (4)

## supplementary materials

H8	0.6899	0.7274	0.8780	0.034*
C9	0.5449 (2)	0.59244 (18)	0.87993 (14)	0.0214 (4)
C10	0.5043 (2)	0.49545 (19)	0.93312 (13)	0.0228 (4)
C11	0.2410 (2)	0.6798 (2)	0.98876 (14)	0.0240 (4)
C12	0.1527 (2)	0.73938 (19)	0.85327 (13)	0.0237 (4)
C13	0.5543 (2)	1.1474 (2)	0.85442 (14)	0.0215 (4)
C14	0.6417 (2)	1.0872 (2)	0.98955 (14)	0.0246 (4)
C15	0.3439 (2)	0.6982 (2)	1.06260 (15)	0.0329 (5)
H15A	0.4058	0.7618	1.0491	0.049*
H15B	0.3906	0.6206	1.0750	0.049*
H15C	0.3016	0.7241	1.1112	0.049*
C16	0.1599 (2)	0.8227 (2)	0.77814 (14)	0.0317 (5)
H16A	0.2167	0.8931	0.7940	0.047*
H16B	0.0723	0.8525	0.7584	0.047*
H16C	0.1952	0.7763	0.7337	0.047*
C17	0.4499 (2)	1.1309 (2)	0.78121 (16)	0.0318 (5)
H17A	0.3824	1.0747	0.7970	0.048*
H17B	0.4895	1.0964	0.7338	0.048*
H17C	0.4107	1.2110	0.7657	0.048*
C18	0.6354 (3)	1.0027 (3)	1.06474 (16)	0.0399 (6)
H18A	0.5556	0.9532	1.0569	0.060*
H18B	0.6352	1.0527	1.1152	0.060*
H18C	0.7115	0.9480	1.0702	0.060*
N1	0.24569 (17)	0.75411 (17)	0.92050 (11)	0.0233 (3)
N2	0.55020 (18)	1.07168 (17)	0.92248 (11)	0.0234 (4)
N3	0.7676 (2)	0.5116 (2)	1.11496 (13)	0.0350 (5)
H2N	0.821 (3)	0.565 (3)	1.136 (2)	0.052*
H1N	0.730 (3)	0.463 (3)	1.147 (2)	0.052*
O1	0.50658 (17)	0.84893 (15)	0.77532 (10)	0.0309 (3)
O2	0.41660 (17)	0.72625 (17)	0.65422 (10)	0.0353 (4)
O3	0.64820 (15)	0.70373 (17)	0.70974 (10)	0.0313 (3)
S1	0.51364 (5)	0.73176 (5)	0.72854 (3)	0.02202 (10)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.03143 (8)	0.03442 (9)	0.03796 (9)	-0.01554 (8)	0.00295 (6)	-0.00011 (8)
C1	0.0198 (9)	0.0185 (9)	0.0214 (9)	0.0009 (7)	0.0016 (8)	-0.0010 (7)
C2	0.0232 (10)	0.0249 (10)	0.0330 (11)	-0.0013 (8)	-0.0042 (9)	-0.0052 (9)
C3	0.0262 (11)	0.0250 (11)	0.0478 (14)	-0.0111 (9)	-0.0021 (10)	-0.0014 (10)
C4	0.0301 (14)	0.0223 (9)	0.0398 (14)	-0.0104 (10)	0.0061 (11)	0.0013 (10)
C5	0.0314 (11)	0.0207 (10)	0.0244 (9)	-0.0020 (8)	0.0071 (8)	0.0031 (7)
C6	0.0300 (10)	0.0219 (10)	0.0216 (9)	0.0035 (8)	0.0011 (8)	-0.0011 (8)
C7	0.0295 (12)	0.0336 (13)	0.0270 (11)	-0.0130 (10)	-0.0023 (10)	0.0027 (10)
C8	0.0281 (10)	0.0273 (11)	0.0283 (9)	-0.0126 (8)	-0.0012 (9)	0.0046 (8)
C9	0.0208 (9)	0.0212 (10)	0.0221 (9)	-0.0024 (7)	0.0020 (8)	-0.0026 (7)
C10	0.0238 (9)	0.0193 (9)	0.0257 (10)	-0.0024 (8)	0.0041 (8)	-0.0036 (7)
C11	0.0220 (9)	0.0244 (10)	0.0257 (9)	0.0004 (8)	0.0028 (8)	-0.0073 (8)

C12	0.0216 (9)	0.0229 (10)	0.0268 (9)	0.0027 (8)	0.0037 (8)	-0.0020 (8)
C13	0.0178 (9)	0.0199 (11)	0.0266 (10)	0.0020 (8)	0.0010 (8)	-0.0038 (8)
C14	0.0235 (10)	0.0265 (11)	0.0240 (10)	-0.0016 (8)	0.0035 (9)	-0.0015 (8)
C15	0.0268 (11)	0.0403 (14)	0.0302 (11)	-0.0030 (10)	-0.0027 (9)	-0.0074 (10)
C16	0.0333 (11)	0.0292 (11)	0.0327 (11)	-0.0004 (9)	0.0044 (9)	0.0052 (9)
C17	0.0321 (11)	0.0260 (11)	0.0344 (11)	-0.0022 (9)	-0.0100 (10)	0.0000 (9)
C18	0.0465 (14)	0.0428 (14)	0.0293 (11)	-0.0143 (11)	-0.0007 (11)	0.0057 (10)
N1	0.0200 (8)	0.0235 (9)	0.0269 (8)	-0.0029 (6)	0.0051 (7)	-0.0063 (6)
N2	0.0212 (8)	0.0243 (9)	0.0246 (9)	-0.0014 (7)	0.0014 (7)	-0.0041 (6)
N3	0.0430 (12)	0.0343 (11)	0.0254 (9)	-0.0045 (9)	-0.0062 (9)	0.0040 (8)
O1	0.0371 (8)	0.0217 (8)	0.0348 (8)	-0.0009 (6)	0.0079 (7)	-0.0007 (6)
O2	0.0335 (8)	0.0437 (10)	0.0263 (7)	0.0006 (7)	-0.0075 (7)	0.0048 (7)
O3	0.0247 (7)	0.0401 (9)	0.0300 (8)	0.0036 (7)	0.0072 (6)	0.0015 (6)
S1	0.0213 (2)	0.0240 (2)	0.0205 (2)	0.00127 (18)	0.00097 (19)	0.00122 (18)

*Geometric parameters (Å, °)*

Ag1—N1	2.279 (2)	C12—C13 <sup>i</sup>	1.395 (3)
Ag1—N2	2.298 (2)	C12—C16	1.491 (3)
Ag1—O1	2.5936 (19)	C13—N2	1.349 (3)
C1—C2	1.364 (3)	C13—C12 <sup>ii</sup>	1.395 (3)
C1—C9	1.430 (3)	C13—C17	1.491 (3)
C1—S1	1.779 (2)	C14—N2	1.341 (3)
C2—C3	1.408 (3)	C14—C11 <sup>ii</sup>	1.406 (3)
C2—H2	0.93	C14—C18	1.498 (3)
C3—C4	1.367 (4)	C15—H15A	0.96
C3—H3	0.93	C15—H15B	0.96
C4—C10	1.414 (3)	C15—H15C	0.96
C4—H4	0.93	C16—H16A	0.96
C5—C6	1.373 (3)	C16—H16B	0.96
C5—C10	1.409 (3)	C16—H16C	0.96
C5—H5	0.93	C17—H17A	0.96
C6—N3	1.383 (3)	C17—H17B	0.96
C6—C7	1.414 (3)	C17—H17C	0.96
C7—C8	1.359 (3)	C18—H18A	0.96
C7—H7	0.93	C18—H18B	0.96
C8—C9	1.428 (3)	C18—H18C	0.96
C8—H8	0.93	N3—H2N	0.83 (2)
C9—C10	1.419 (3)	N3—H1N	0.85 (2)
C11—N1	1.343 (3)	O1—S1	1.4549 (18)
C11—C14 <sup>i</sup>	1.406 (3)	O2—S1	1.4492 (17)
C11—C15	1.491 (3)	O3—S1	1.4532 (17)
C12—N1	1.351 (3)		
N1—Ag1—N2	171.76 (6)	N2—C14—C18	118.1 (2)
N1—Ag1—O1	102.85 (6)	C11 <sup>ii</sup> —C14—C18	121.2 (2)
N2—Ag1—O1	85.19 (6)	C11—C15—H15A	109.5
C2—C1—C9	120.92 (19)	C11—C15—H15B	109.5
C2—C1—S1	117.51 (16)	H15A—C15—H15B	109.5

## supplementary materials

---

C9—C1—S1	121.58 (15)	C11—C15—H15C	109.5
C1—C2—C3	120.3 (2)	H15A—C15—H15C	109.5
C1—C2—H2	119.9	H15B—C15—H15C	109.5
C3—C2—H2	119.9	C12—C16—H16A	109.5
C4—C3—C2	120.0 (2)	C12—C16—H16B	109.5
C4—C3—H3	120.0	H16A—C16—H16B	109.5
C2—C3—H3	120.0	C12—C16—H16C	109.5
C3—C4—C10	121.6 (2)	H16A—C16—H16C	109.5
C3—C4—H4	119.2	H16B—C16—H16C	109.5
C10—C4—H4	119.2	C13—C17—H17A	109.5
C6—C5—C10	121.25 (19)	C13—C17—H17B	109.5
C6—C5—H5	119.4	H17A—C17—H17B	109.5
C10—C5—H5	119.4	C13—C17—H17C	109.5
C5—C6—N3	122.8 (2)	H17A—C17—H17C	109.5
C5—C6—C7	118.17 (19)	H17B—C17—H17C	109.5
N3—C6—C7	118.9 (2)	C14—C18—H18A	109.5
C8—C7—C6	122.1 (2)	C14—C18—H18B	109.5
C8—C7—H7	118.9	H18A—C18—H18B	109.5
C6—C7—H7	118.9	C14—C18—H18C	109.5
C7—C8—C9	120.9 (2)	H18A—C18—H18C	109.5
C7—C8—H8	119.6	H18B—C18—H18C	109.5
C9—C8—H8	119.6	C11—N1—C12	118.93 (19)
C10—C9—C8	117.01 (19)	C11—N1—Ag1	122.42 (14)
C10—C9—C1	118.60 (18)	C12—N1—Ag1	118.65 (15)
C8—C9—C1	124.4 (2)	C14—N2—C13	118.76 (19)
C5—C10—C4	120.9 (2)	C14—N2—Ag1	121.57 (14)
C5—C10—C9	120.55 (18)	C13—N2—Ag1	119.22 (14)
C4—C10—C9	118.5 (2)	C6—N3—H2N	120 (3)
N1—C11—C14 <sup>i</sup>	120.39 (19)	C6—N3—H1N	113 (2)
N1—C11—C15	118.1 (2)	H2N—N3—H1N	119 (4)
C14 <sup>i</sup> —C11—C15	121.5 (2)	S1—O1—Ag1	132.33 (10)
N1—C12—C13 <sup>i</sup>	120.4 (2)	O2—S1—O3	113.03 (10)
N1—C12—C16	118.0 (2)	O2—S1—O1	112.46 (10)
C13 <sup>i</sup> —C12—C16	121.5 (2)	O3—S1—O1	112.21 (11)
N2—C13—C12 <sup>ii</sup>	120.78 (19)	O2—S1—C1	106.81 (10)
N2—C13—C17	118.1 (2)	O3—S1—C1	106.66 (10)
C12 <sup>ii</sup> —C13—C17	121.1 (2)	O1—S1—C1	105.01 (10)
N2—C14—C11 <sup>ii</sup>	120.7 (2)		
C9—C1—C2—C3	0.7 (3)	C13 <sup>i</sup> —C12—N1—C11	-0.8 (3)
S1—C1—C2—C3	-178.85 (18)	C16—C12—N1—C11	-179.95 (19)
C1—C2—C3—C4	-0.9 (4)	C13 <sup>i</sup> —C12—N1—Ag1	179.48 (15)
C2—C3—C4—C10	-0.3 (4)	C16—C12—N1—Ag1	0.3 (2)
C10—C5—C6—N3	-176.6 (2)	O1—Ag1—N1—C11	125.56 (16)
C10—C5—C6—C7	0.0 (3)	O1—Ag1—N1—C12	-54.73 (16)
C5—C6—C7—C8	-0.3 (4)	C11 <sup>ii</sup> —C14—N2—C13	-0.6 (3)
N3—C6—C7—C8	176.5 (2)	C18—C14—N2—C13	179.8 (2)



C6—C7—C8—C9	0.0 (4)	C11 <sup>ii</sup> —C14—N2—Ag1	171.63 (15)
C7—C8—C9—C10	0.7 (4)	C18—C14—N2—Ag1	-8.0 (3)
C7—C8—C9—C1	-178.5 (2)	C12 <sup>ii</sup> —C13—N2—C14	0.6 (3)
C2—C1—C9—C10	0.7 (3)	C17—C13—N2—C14	-178.6 (2)
S1—C1—C9—C10	-179.75 (15)	C12 <sup>ii</sup> —C13—N2—Ag1	-171.77 (15)
C2—C1—C9—C8	179.8 (2)	C17—C13—N2—Ag1	9.0 (3)
S1—C1—C9—C8	-0.6 (3)	O1—Ag1—N2—C14	-121.18 (17)
C6—C5—C10—C4	-179.3 (2)	O1—Ag1—N2—C13	50.99 (16)
C6—C5—C10—C9	0.6 (3)	N1—Ag1—O1—S1	-24.43 (14)
C3—C4—C10—C5	-178.4 (2)	N2—Ag1—O1—S1	157.43 (14)
C3—C4—C10—C9	1.7 (4)	Ag1—O1—S1—O2	102.13 (14)
C8—C9—C10—C5	-0.9 (3)	Ag1—O1—S1—O3	-129.12 (12)
C1—C9—C10—C5	178.25 (19)	Ag1—O1—S1—C1	-13.64 (15)
C8—C9—C10—C4	179.0 (2)	C2—C1—S1—O2	-0.2 (2)
C1—C9—C10—C4	-1.9 (3)	C9—C1—S1—O2	-179.73 (17)
C14 <sup>i</sup> —C11—N1—C12	0.9 (3)	C2—C1—S1—O3	-121.29 (18)
C15—C11—N1—C12	-179.54 (19)	C9—C1—S1—O3	59.14 (19)
C14 <sup>i</sup> —C11—N1—Ag1	-179.44 (15)	C2—C1—S1—O1	119.45 (18)
C15—C11—N1—Ag1	0.2 (3)	C9—C1—S1—O1	-60.11 (19)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H1N $\cdots$ O3 <sup>iii</sup>	0.85 (2)	2.23 (3)	3.055 (3)	165 (4)
N3—H2N $\cdots$ O2 <sup>iv</sup>	0.83 (2)	2.43 (3)	3.197 (3)	155 (3)
C16—H16B $\cdots$ Cg1 <sup>v</sup>	0.96	2.65	3.425 (3)	138

Symmetry codes: (iii)  $x, -y+1, z+1/2$ ; (iv)  $x+1/2, -y+3/2, z+1/2$ ; (v)  $x-1/2, y+1/2, z$ .

Fig. 1

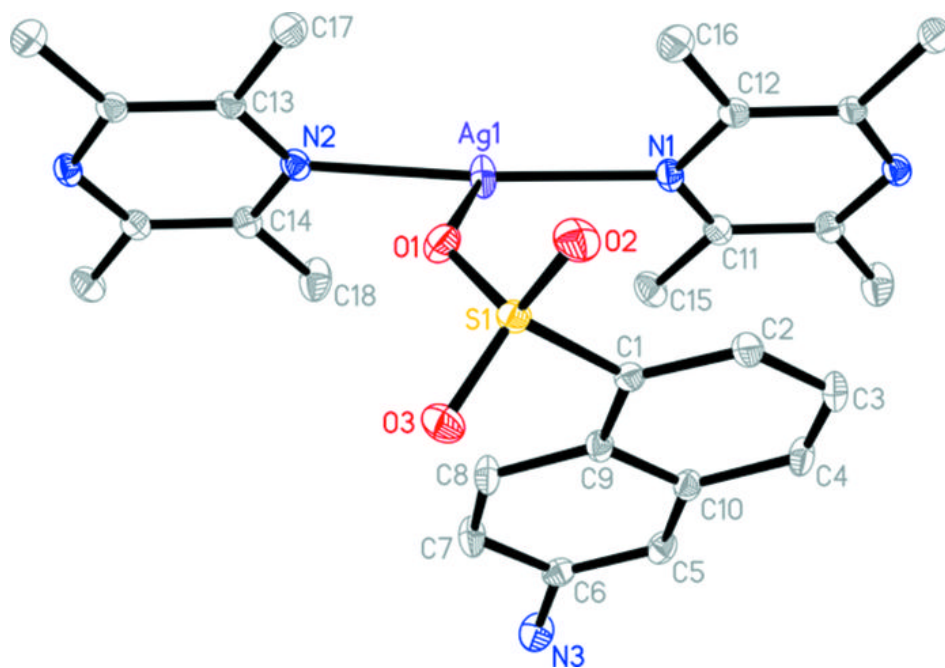


Fig. 2

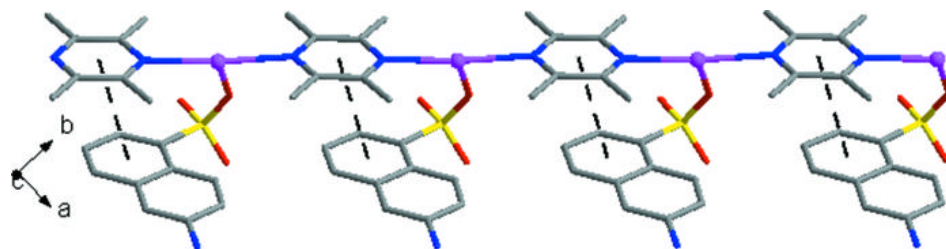


Fig. 3

