

catena-Poly[[*(2-amino-3,5-dimethylbenzenesulfonato-κO)silver(I)-μ-1,1'-(butane-1,4-diyl)diimidazole-κ²N³:N^{3'}*]]

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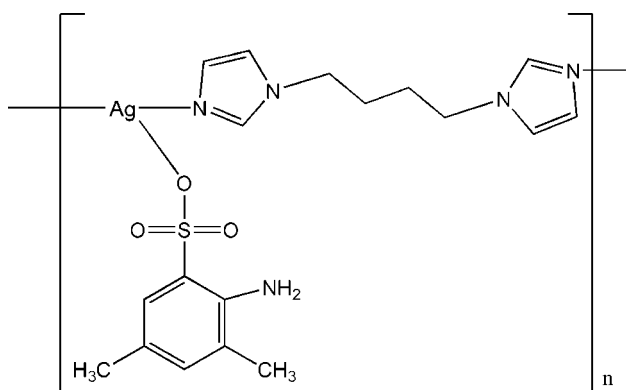
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 Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.038; wR factor = 0.100; data-to-parameter ratio = 17.6.

In the title compound, $[\text{Ag}(\text{C}_8\text{H}_{10}\text{NO}_3\text{S})(\text{C}_{10}\text{H}_{14}\text{N}_4)]$, each Ag^{I} cation is three-coordinated by two N atoms from two different 1,1'-(butane-1,4-diyl)diimidazole ligands (bbi), and one sulfonate O atom from one 2-amino-3,5-dimethylbenzenesulfonate (*L*) anion in a distorted trigonal-planar geometry. Each bbi molecule acts as a bidentate ligand that binds two Ag^{I} atoms, thus forming a one-dimensional chain. The *L* anions are attached on both sides of the chain through $\text{Ag}-\text{O}$ bonds. Finally, $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link the chains together, reinforcing the crystal cohesion.

Related literature

The related compound, $[\text{Ag}(L)(\text{bipy})]$ (*bipy* = 2,2'-bipyridine), has a mononuclear structure in which the Ag^{I} cation is three-coordinated by two N atoms from one *bipy* molecule and one N atom from a *L* anion in a highly distorted trigonal-planar geometry. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond helps to establish the molecular conformation (Liu *et al.*, 2006). For related literature, see: May & Shimizu (2005); Sun *et al.* (2004); You & Zhu (2004).



Experimental

Crystal data

$[\text{Ag}(\text{C}_8\text{H}_{10}\text{NO}_3\text{S})(\text{C}_{10}\text{H}_{14}\text{N}_4)]$
 $M_r = 498.35$
 Monoclinic, $P2_1/c$
 $a = 8.6632$ (17) Å
 $b = 17.239$ (3) Å
 $c = 13.789$ (3) Å
 $\beta = 93.11$ (3)°

$V = 2056.3$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.11$ mm⁻¹
 $T = 292$ (2) K
 $0.31 \times 0.27 \times 0.24$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
 $T_{\text{min}} = 0.703$, $T_{\text{max}} = 0.764$

17540 measured reflections
 4617 independent reflections
 2695 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.100$
 $S = 0.98$
 4617 reflections
 263 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.71$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.69$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1—N4	2.101 (3)	Ag1—O1	2.721 (3)
Ag1—N3 ⁱ	2.112 (3)		
N4—Ag1—O1	104.81 (10)	N4—Ag1—N3 ⁱ	169.75 (12)
O1—Ag1—N3 ⁱ	83.28 (10)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<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	0.83 (4)	2.34 (4)	2.985 (5)	136 (3)
N1—H1B \cdots O3 ⁱⁱ	0.92 (4)	2.40 (4)	3.252 (4)	154 (3)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2404).

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supplementary materials

Acta Cryst. (2007). E63, m1622-m1623 [doi:10.1107/S1600536807021897]

catena-Poly[[*(2-amino-3,5-dimethylbenzenesulfonato-κO)silver(I)-μ-1,1'-(butane-1,4-diyl)diimidazole-κ²N³:N^{3'}*]

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Comment

Recently, intense interest has been focused on silver(I) sulfonates due to their interesting structures and properties (May & Shimizu, 2005). Based on previous reports, the structure motif of most silver(I) sulfonates observed is a two-dimensional layer, which is similar to that of metal phosphonates (Sun *et al.*, 2004). So far, some silver(I) sulfonate compounds modified by nitrogen-based ligands that display different structure motifs depending upon the presence of secondary ligands have been reported (You *et al.*, 2004). However, the information on silver sulfonate coordination polymers are not yet well understood, especially, investigations of silver(I) sulfonates with neutral ligands are rather insufficient. We selected 2-amino-3,5-dimethylbenzenesulfonic acid (HL) as a sulfonate ligand and 1,1'-(1,4-butanediyl)-bis(imidazole) (bbi) as a secondary ligand, generating a new chain coordination polymer, [Ag(L)(bbi)], (I), which is reported here.

In compound (I), each Ag^I cation is three-coordinated by two N atoms from two different bbi ligands, and one sulfonate O atom from one *L* anion in a distorted trigonal-planar geometry (Fig. 1, Table 1). As shown in Fig. 2, each bbi moiety acts as a bidentate ligand that binds two Ag^I atoms, thus forming a one-dimensional chain. The *L* anions are attached on both sides of the chain through the Ag—O bonds. Moreover, N—H···O hydrogen bonds (Table 2) link the chains together, reinforcing the crystal cohesion of (I).

Experimental

To a mixture of HL (0.5 mmol) and NaOH (0.5 mmol) in water was added AgNO₃ (0.5 mmol) with constant stirring, to which was added bbi (0.5 mmol) in water. After the sample was stirred for 5 min, the precipitate was dissolved by dropwise addition of aqueous NH₃ solution. Colorless crystals of (I) were obtained from the filtrate by slow evaporation after standing in the dark for three days (45% yield).

Refinement

The H atoms bonded to N atom were located in a difference map and their positions were refined freely, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Figures

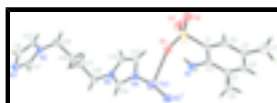


Fig. 1. The asymmetric unit of (I), expanded to show the silver coordination. Displacement ellipsoids are drawn at the 30% probability level. (arbitrary spheres for the H atoms). Symmetry code: (i) $x - 1, 1/2 - y, z - 1/2$.

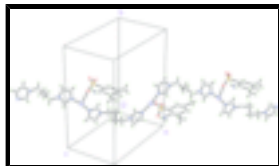


Fig. 2. View of the chain structure in (I). H atoms have been omitted.

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Crystal data

[Ag(C₈H₁₀NO₃S)(C₁₀H₁₄N₄)]

$M_r = 498.35$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.6632$ (17) Å

$b = 17.239$ (3) Å

$c = 13.789$ (3) Å

$\beta = 93.11$ (3)°

$V = 2056.3$ (7) Å³

$Z = 4$

$F_{000} = 1016$

$D_x = 1.610$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 13313 reflections

$\theta = 3.3$ – 27.5 °

$\mu = 1.11$ mm⁻¹

$T = 292$ (2) K

Block, colorless

$0.31 \times 0.27 \times 0.24$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: rotating anode

Monochromator: graphite

Detector resolution: 10.0 pixels mm⁻¹

$T = 292$ (2) K

ω scans

Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.703$, $T_{\max} = 0.764$

17540 measured reflections

4617 independent reflections

2695 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 1.9$ °

$h = -11 \rightarrow 10$

$k = -21 \rightarrow 22$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.100$

$S = 0.98$

4617 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: difmap and geom

H atoms treated by a mixture of
independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.71$ e Å⁻³

263 parameters

$$\Delta\rho_{\min} = -0.69 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.9861 (4)	0.11829 (16)	-0.1790 (2)	0.0349 (8)
C2	1.0868 (4)	0.11463 (17)	-0.0946 (2)	0.0363 (8)
C3	1.2453 (4)	0.12822 (18)	-0.1037 (3)	0.0403 (8)
C4	1.2984 (4)	0.14376 (19)	-0.1950 (3)	0.0469 (9)
H4	1.4037	0.1519	-0.2007	0.056*
C5	1.2009 (4)	0.14763 (19)	-0.2781 (3)	0.0466 (9)
C6	1.0449 (4)	0.13536 (17)	-0.2681 (2)	0.0426 (8)
H6	0.9774	0.1387	-0.3227	0.051*
C7	1.2654 (6)	0.1640 (3)	-0.3765 (3)	0.0840 (15)
H7A	1.3622	0.1909	-0.3673	0.126*
H7B	1.1936	0.1956	-0.4145	0.126*
H7C	1.2813	0.1160	-0.4097	0.126*
C8	1.3569 (4)	0.1259 (2)	-0.0155 (3)	0.0624 (11)
H8A	1.3278	0.1644	0.0304	0.094*
H8B	1.4596	0.1364	-0.0348	0.094*
H8C	1.3540	0.0755	0.0139	0.094*
C9	-0.1508 (4)	0.0935 (2)	0.4814 (3)	0.0509 (9)
H9A	-0.1969	0.0682	0.5319	0.061*
C10	-0.0880 (4)	0.0588 (2)	0.4058 (3)	0.0506 (10)
H10A	-0.0833	0.0057	0.3946	0.061*
C11	-0.0647 (4)	0.18262 (19)	0.3921 (3)	0.0482 (9)
H11A	-0.0394	0.2312	0.3682	0.058*
C12	0.6619 (4)	0.0826 (2)	0.1489 (3)	0.0503 (10)
H12	0.6945	0.0514	0.0990	0.060*
C13	0.5835 (4)	0.0580 (2)	0.2255 (3)	0.0498 (9)
H13	0.5521	0.0075	0.2374	0.060*
C14	0.6224 (4)	0.1819 (2)	0.2376 (3)	0.0455 (9)
H14	0.6216	0.2324	0.2613	0.055*
C15	0.0521 (4)	0.1066 (2)	0.2605 (3)	0.0557 (10)
H15A	0.0006	0.1361	0.2083	0.067*

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H15B	0.0506	0.0524	0.2414	0.067*
C16	0.2177 (4)	0.1334 (2)	0.2742 (3)	0.0597 (11)
H16A	0.2674	0.1268	0.2133	0.072*
H16B	0.2181	0.1884	0.2891	0.072*
C17	0.3117 (4)	0.0917 (3)	0.3527 (3)	0.0606 (11)
H17A	0.3181	0.0373	0.3355	0.073*
H17B	0.2584	0.0951	0.4127	0.073*
C18	0.4740 (4)	0.1231 (3)	0.3706 (3)	0.0646 (11)
H18A	0.4690	0.1761	0.3939	0.078*
H18B	0.5285	0.0923	0.4205	0.078*
N1	1.0317 (5)	0.1013 (2)	-0.0026 (2)	0.0518 (8)
N2	-0.0326 (3)	0.11565 (15)	0.3484 (2)	0.0419 (7)
N3	-0.1360 (3)	0.17177 (17)	0.4721 (2)	0.0485 (8)
N4	0.6856 (3)	0.16103 (17)	0.1567 (2)	0.0476 (7)
N5	0.5597 (3)	0.12121 (17)	0.2814 (2)	0.0445 (7)
O1	0.7257 (3)	0.16763 (13)	-0.1191 (2)	0.0567 (7)
O2	0.7185 (3)	0.09931 (16)	-0.2709 (2)	0.0682 (8)
O3	0.7705 (3)	0.02929 (13)	-0.1206 (2)	0.0617 (8)
S1	0.78366 (10)	0.10201 (5)	-0.17196 (7)	0.0420 (2)
Ag1	0.78216 (4)	0.23648 (2)	0.05684 (3)	0.07189 (16)
H1A	0.945 (5)	0.081 (2)	-0.003 (3)	0.052 (13)*
H1B	1.101 (4)	0.079 (2)	0.041 (3)	0.056 (12)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.043 (2)	0.0287 (16)	0.033 (2)	0.0022 (14)	0.0029 (16)	-0.0007 (13)
C2	0.044 (2)	0.0316 (17)	0.034 (2)	0.0016 (14)	0.0070 (16)	-0.0006 (13)
C3	0.044 (2)	0.0363 (18)	0.040 (2)	-0.0019 (15)	-0.0024 (17)	0.0019 (15)
C4	0.045 (2)	0.041 (2)	0.055 (3)	-0.0021 (15)	0.010 (2)	0.0000 (16)
C5	0.060 (3)	0.046 (2)	0.035 (2)	-0.0056 (17)	0.0146 (19)	-0.0003 (16)
C6	0.060 (2)	0.0356 (18)	0.032 (2)	-0.0013 (16)	0.0001 (17)	0.0003 (14)
C7	0.097 (4)	0.111 (4)	0.047 (3)	-0.029 (3)	0.026 (3)	0.003 (2)
C8	0.049 (2)	0.080 (3)	0.057 (3)	-0.008 (2)	-0.009 (2)	0.012 (2)
C9	0.050 (2)	0.060 (3)	0.043 (2)	0.0042 (18)	0.0026 (18)	0.0067 (18)
C10	0.055 (2)	0.037 (2)	0.059 (3)	0.0012 (17)	-0.001 (2)	0.0004 (17)
C11	0.060 (2)	0.0362 (19)	0.049 (3)	0.0074 (17)	0.007 (2)	-0.0004 (16)
C12	0.043 (2)	0.058 (2)	0.050 (3)	-0.0057 (18)	0.0050 (19)	-0.0118 (18)
C13	0.046 (2)	0.046 (2)	0.058 (3)	-0.0095 (17)	0.0064 (19)	0.0057 (18)
C14	0.039 (2)	0.045 (2)	0.052 (3)	-0.0072 (16)	-0.0029 (18)	-0.0025 (17)
C15	0.047 (2)	0.076 (3)	0.043 (2)	0.0123 (19)	0.0011 (18)	-0.0071 (19)
C16	0.055 (3)	0.083 (3)	0.041 (2)	0.007 (2)	0.014 (2)	0.008 (2)
C17	0.048 (2)	0.095 (3)	0.041 (2)	-0.002 (2)	0.0167 (19)	0.009 (2)
C18	0.046 (2)	0.107 (3)	0.041 (3)	-0.012 (2)	0.0067 (19)	-0.002 (2)
N1	0.051 (2)	0.070 (2)	0.034 (2)	-0.0012 (19)	0.0039 (17)	0.0069 (16)
N2	0.0392 (16)	0.0452 (17)	0.0414 (18)	0.0083 (13)	0.0012 (13)	-0.0061 (13)
N3	0.0490 (19)	0.054 (2)	0.043 (2)	0.0145 (14)	0.0036 (15)	-0.0046 (14)
N4	0.0407 (18)	0.0587 (19)	0.043 (2)	-0.0107 (14)	0.0018 (15)	0.0050 (14)

N5	0.0377 (17)	0.0597 (19)	0.0362 (18)	-0.0071 (14)	0.0031 (13)	-0.0034 (14)
O1	0.0463 (15)	0.0505 (15)	0.074 (2)	0.0030 (11)	0.0116 (14)	-0.0132 (13)
O2	0.0563 (17)	0.092 (2)	0.0547 (19)	-0.0096 (14)	-0.0140 (14)	-0.0007 (16)
O3	0.0518 (16)	0.0430 (14)	0.090 (2)	-0.0092 (12)	0.0051 (15)	0.0192 (13)
S1	0.0400 (5)	0.0395 (5)	0.0460 (6)	-0.0017 (4)	-0.0010 (4)	0.0007 (4)
Ag1	0.0656 (2)	0.0907 (3)	0.0585 (2)	-0.03257 (18)	-0.00434 (16)	0.02951 (18)

Geometric parameters (Å, °)

C1—C6	1.386 (4)	C12—H12	0.9300
C1—C2	1.418 (5)	C13—N5	1.357 (4)
C1—S1	1.784 (3)	C13—H13	0.9300
C2—N1	1.399 (4)	C14—N4	1.319 (4)
C2—C3	1.405 (5)	C14—N5	1.337 (4)
C3—C4	1.389 (5)	C14—H14	0.9300
C3—C8	1.513 (5)	C15—N2	1.460 (4)
C4—C5	1.388 (5)	C15—C16	1.509 (5)
C4—H4	0.9300	C15—H15A	0.9700
C5—C6	1.382 (5)	C15—H15B	0.9700
C5—C7	1.522 (5)	C16—C17	1.502 (6)
C6—H6	0.9300	C16—H16A	0.9700
C7—H7A	0.9600	C16—H16B	0.9700
C7—H7B	0.9600	C17—C18	1.515 (5)
C7—H7C	0.9600	C17—H17A	0.9700
C8—H8A	0.9600	C17—H17B	0.9700
C8—H8B	0.9600	C18—N5	1.472 (4)
C8—H8C	0.9600	C18—H18A	0.9700
C9—C10	1.343 (5)	C18—H18B	0.9700
C9—N3	1.362 (4)	N1—H1A	0.83 (4)
C9—H9A	0.9300	N1—H1B	0.92 (4)
C10—N2	1.363 (4)	O1—S1	1.450 (2)
C10—H10A	0.9300	O2—S1	1.448 (3)
C11—N3	1.307 (4)	O3—S1	1.447 (2)
C11—N2	1.338 (4)	Ag1—N4	2.101 (3)
C11—H11A	0.9300	Ag1—N3 ⁱ	2.112 (3)
C12—C13	1.354 (5)	Ag1—O1	2.721 (3)
C12—N4	1.370 (4)		
C6—C1—C2	119.9 (3)	N2—C15—C16	112.3 (3)
C6—C1—S1	119.4 (3)	N2—C15—H15A	109.1
C2—C1—S1	120.7 (2)	C16—C15—H15A	109.1
N1—C2—C3	119.5 (3)	N2—C15—H15B	109.1
N1—C2—C1	121.8 (3)	C16—C15—H15B	109.1
C3—C2—C1	118.6 (3)	H15A—C15—H15B	107.9
C4—C3—C2	119.1 (3)	C17—C16—C15	114.7 (3)
C4—C3—C8	120.3 (3)	C17—C16—H16A	108.6
C2—C3—C8	120.5 (3)	C15—C16—H16A	108.6
C5—C4—C3	122.7 (3)	C17—C16—H16B	108.6
C5—C4—H4	118.6	C15—C16—H16B	108.6
C3—C4—H4	118.6	H16A—C16—H16B	107.6

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C6—C5—C4	117.7 (3)	C16—C17—C18	114.1 (3)
C6—C5—C7	121.8 (4)	C16—C17—H17A	108.7
C4—C5—C7	120.5 (4)	C18—C17—H17A	108.7
C5—C6—C1	122.0 (3)	C16—C17—H17B	108.7
C5—C6—H6	119.0	C18—C17—H17B	108.7
C1—C6—H6	119.0	H17A—C17—H17B	107.6
C5—C7—H7A	109.5	N5—C18—C17	111.2 (3)
C5—C7—H7B	109.5	N5—C18—H18A	109.4
H7A—C7—H7B	109.5	C17—C18—H18A	109.4
C5—C7—H7C	109.5	N5—C18—H18B	109.4
H7A—C7—H7C	109.5	C17—C18—H18B	109.4
H7B—C7—H7C	109.5	H18A—C18—H18B	108.0
C3—C8—H8A	109.5	C2—N1—H1A	115 (3)
C3—C8—H8B	109.5	C2—N1—H1B	115 (2)
H8A—C8—H8B	109.5	H1A—N1—H1B	113 (4)
C3—C8—H8C	109.5	C11—N2—C10	105.7 (3)
H8A—C8—H8C	109.5	C11—N2—C15	126.3 (3)
H8B—C8—H8C	109.5	C10—N2—C15	127.9 (3)
C10—C9—N3	109.0 (3)	C11—N3—C9	105.8 (3)
C10—C9—H9A	125.5	C11—N3—Ag1 ⁱⁱ	123.2 (2)
N3—C9—H9A	125.5	C9—N3—Ag1 ⁱⁱ	130.8 (3)
C9—C10—N2	107.5 (3)	C14—N4—C12	105.5 (3)
C9—C10—H10A	126.3	C14—N4—Ag1	125.7 (2)
N2—C10—H10A	126.3	C12—N4—Ag1	128.5 (3)
N3—C11—N2	112.1 (3)	C14—N5—C13	107.1 (3)
N3—C11—H11A	124.0	C14—N5—C18	126.5 (3)
N2—C11—H11A	124.0	C13—N5—C18	126.3 (3)
C13—C12—N4	109.1 (3)	O3—S1—O2	113.33 (17)
C13—C12—H12	125.4	O3—S1—O1	113.01 (17)
N4—C12—H12	125.4	O2—S1—O1	111.77 (17)
C12—C13—N5	106.8 (3)	O3—S1—C1	105.46 (15)
C12—C13—H13	126.6	O2—S1—C1	106.71 (16)
N5—C13—H13	126.6	O1—S1—C1	105.84 (14)
N4—C14—N5	111.5 (3)	N4—Ag1—O1	104.81 (10)
N4—C14—H14	124.3	O1—Ag1—N3 ⁱ	83.28 (10)
N5—C14—H14	124.3	N4—Ag1—N3 ⁱ	169.75 (12)
C6—C1—C2—N1	176.8 (3)	C16—C15—N2—C11	64.0 (5)
S1—C1—C2—N1	-2.6 (4)	C16—C15—N2—C10	-112.3 (4)
C6—C1—C2—C3	-0.3 (4)	N2—C11—N3—C9	0.2 (4)
S1—C1—C2—C3	-179.7 (2)	N2—C11—N3—Ag1 ⁱⁱ	-176.2 (2)
N1—C2—C3—C4	-178.0 (3)	C10—C9—N3—C11	-0.2 (4)
C1—C2—C3—C4	-0.8 (4)	C10—C9—N3—Ag1 ⁱⁱ	175.7 (3)
N1—C2—C3—C8	2.0 (5)	N5—C14—N4—C12	-0.2 (4)
C1—C2—C3—C8	179.2 (3)	N5—C14—N4—Ag1	174.7 (2)
C2—C3—C4—C5	1.0 (5)	C13—C12—N4—C14	0.4 (4)
C8—C3—C4—C5	-179.1 (3)	C13—C12—N4—Ag1	-174.2 (3)
C3—C4—C5—C6	0.0 (5)	N4—C14—N5—C13	-0.1 (4)

C3—C4—C5—C7	-179.4 (3)	N4—C14—N5—C18	-177.3 (3)
C4—C5—C6—C1	-1.2 (5)	C12—C13—N5—C14	0.4 (4)
C7—C5—C6—C1	178.2 (3)	C12—C13—N5—C18	177.6 (3)
C2—C1—C6—C5	1.3 (5)	C17—C18—N5—C14	121.1 (4)
S1—C1—C6—C5	-179.2 (2)	C17—C18—N5—C13	-55.5 (5)
N3—C9—C10—N2	0.2 (4)	C6—C1—S1—O3	129.0 (3)
N4—C12—C13—N5	-0.5 (4)	C2—C1—S1—O3	-51.5 (3)
N2—C15—C16—C17	59.2 (5)	C6—C1—S1—O2	8.2 (3)
C15—C16—C17—C18	-175.8 (3)	C2—C1—S1—O2	-172.3 (2)
C16—C17—C18—N5	-57.1 (5)	C6—C1—S1—O1	-111.0 (3)
N3—C11—N2—C10	0.0 (4)	C2—C1—S1—O1	68.5 (3)
N3—C11—N2—C15	-177.0 (3)	C14—N4—Ag1—N3 ⁱ	-5.9 (8)
C9—C10—N2—C11	-0.1 (4)	C12—N4—Ag1—N3 ⁱ	167.8 (6)
C9—C10—N2—C15	176.8 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O3	0.83 (4)	2.34 (4)	2.985 (5)	136 (3)
N1—H1B \cdots O3 ⁱⁱⁱ	0.92 (4)	2.40 (4)	3.252 (4)	154 (3)

Symmetry codes: (iii) $-x+2, -y, -z$.

Fig. 1

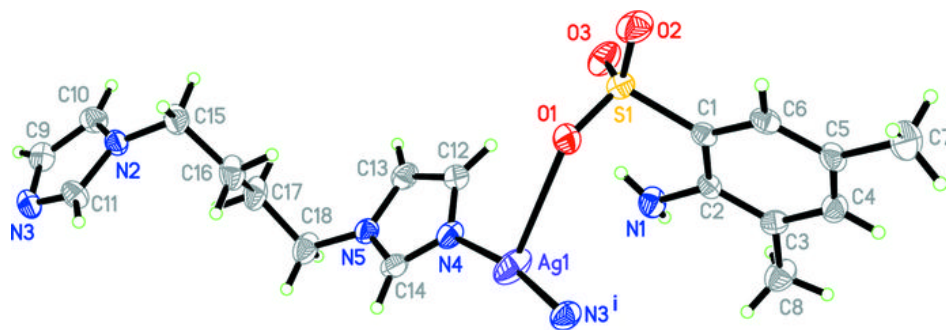


Fig. 2

