

catena-Poly[[silver(I)- μ -1,2-bis[(1*H*-imidazol-1-yl)methyl]benzene- κ^2 N³:N^{3'}] 2-amino-3,5-dimethylbenzenesulfonate]

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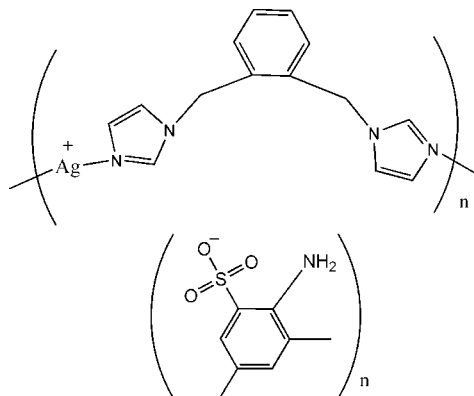
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.050; wR factor = 0.147; data-to-parameter ratio = 17.4.

The title compound, $\{[\text{Ag}(\text{C}_{14}\text{H}_{14}\text{N}_2)](\text{C}_8\text{H}_{10}\text{NO}_3\text{S})\}_n$, adopts a polymeric chain structure, where each Ag^{I} cation binds two N atoms from two different 1,2-bis[(1*H*-imidazol-1-yl)methyl]benzene (IBI) ligands in a linear coordination geometry. Each IBI ligand bridges two neighbouring Ag^{I} atoms to form the polymer chain. The 2-amino-3,5-dimethylbenzenesulfonate counter-ion does not coordinate to the Ag^{I} centre but forms an intramolecular N—H \cdots O hydrogen bond.

Related literature

For information on sulfonates as ligands, see Cote & Shimizu (2003). For related structures of silver sulfonates, see Li *et al.* (2006).



Experimental

Crystal data

$[\text{Ag}(\text{C}_{14}\text{H}_{14}\text{N}_2)](\text{C}_8\text{H}_{10}\text{NO}_3\text{S})$	$a = 10.683$ (2) Å
$M_r = 546.39$	$b = 13.987$ (3) Å
Monoclinic, $P2_1/c$	$c = 15.385$ (3) Å

$\beta = 102.07$ (3) $^\circ$
 $V = 2248.1$ (8) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 1.02$ mm⁻¹
 $T = 293$ (2) K
 $0.27 \times 0.21 \times 0.19$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.755$, $T_{\text{max}} = 0.824$

20972 measured reflections
 5122 independent reflections
 3779 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.147$
 $S = 1.08$
 5122 reflections
 295 parameters
 3 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.69$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.08$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1—N1	2.115 (3)	Ag1—N2 ⁱ	2.124 (3)
N1—Ag1—N2 ⁱ	170.93 (13)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—HN2 \cdots O2	0.863 (10)	2.36 (5)	2.924 (7)	123 (5)

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: SJ2368).

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supplementary materials

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***catena*-Poly[[silver(I)- μ -1,2-bis[(1*H*-imidazol-1-yl)methyl]benzene- $\kappa^2 N^3:N^{3'}$] 2-amino-3,5-dimethylbenzenesulfonate]**

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Comment

Sulfonates are generally perceived to be weaker ligands with low coordinating ability (Cote & Shimizu, 2003). Some silver(I) sulfonate compounds, modified by secondary nitrogen-based ligands, have been documented (Li *et al.*, 2006). In most of these silver(I) sulfonate complexes, the sulfonate ligand acts solely as a counter-anion with no coordination to the Ag^I centre. Herein, we present a new sulfonate coordination polymer, namely [Ag(IBM)] \cdot L (I), where IBM = 1,2-bis((1*H*-imidazol-1-yl)methyl)benzene and HL = 2-amino-3,5-dimethylbenzenesulfonic acid.

In (I) the Ag^I cation is coordinated by N atoms from two different IBM ligands in a linear coordination geometry (Fig. 1). The Ag—N (IBM) distance in (I), Table 1, is similar to that in several related compounds (Li *et al.*, 2006). The IBM ligand bridges two neighboring Ag^I atoms, forming a polymeric chain structure (Fig. 2). Notably, the L[−] ligand does not coordinate to the Ag^I center, acting only as a counter-anion and forming an intramolecular N—H \cdots O hydrogen bond, Table 2.

Experimental

An aqueous solution (15 ml) of 2-amino-3,5-dimethylbenzenesulfonic acid (1 mmol) was added to solid Ag₂CO₃ (0.5 mmol) and stirred for several minutes until no further CO₂ was given off. 1-(3-(1*H*-imidazol-1-yl)methyl)benzyl-1*H*-imidazole (1 mmol) was then added and a precipitate was formed. The precipitate was dissolved in ammonium hydroxide. Colorless crystals of (I) were obtained by evaporation of this solution for several days at room temperature.

Refinement

H atoms bound to N atoms were located in a difference map and refined freely, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. H atoms bonded to C atoms were positioned geometrically with and refined as riding, with $d(\text{C—H}) = 0.93 \text{ \AA}$, $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for aromatic 0.97 \AA , $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for CH₂ and 0.96 \AA , $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ for CH₃ atoms.

Figures

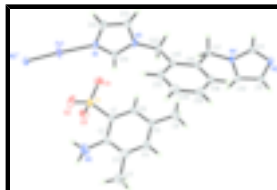


Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) $x, y - 1, z$.

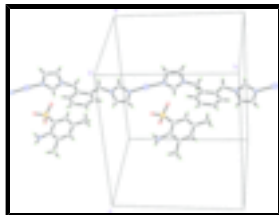


Fig. 2. A view of the chain structure of (I).

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Crystal data

[Ag(C₁₄H₁₄N₂)](C₈H₁₀NO₃S)

$M_r = 546.39$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.683$ (2) Å

$b = 13.987$ (3) Å

$c = 15.385$ (3) Å

$\beta = 102.07$ (3)°

$V = 2248.1$ (8) Å³

$Z = 4$

$F_{000} = 1112$

$D_x = 1.614$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 15895 reflections

$\theta = 3.0$ – 27.5 °

$\mu = 1.02$ mm⁻¹

$T = 293$ (2) K

Block, colourless

$0.27 \times 0.21 \times 0.19$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: rotating anode

Monochromator: graphite

Detector resolution: 10.0 pixels mm⁻¹

$T = 293$ (2) K

ω scans

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

$T_{\min} = 0.755$, $T_{\max} = 0.824$

20972 measured reflections

5122 independent reflections

3779 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 3.1$ °

$h = -12 \rightarrow 13$

$k = -18 \rightarrow 18$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.147$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0791P)^2 + 1.8517P]$$

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

$S = 1.08$ $(\Delta/\sigma)_{\max} = 0.001$
 5122 reflections $\Delta\rho_{\max} = 1.69 \text{ e } \text{\AA}^{-3}$
 295 parameters $\Delta\rho_{\min} = -1.08 \text{ e } \text{\AA}^{-3}$
 3 restraints Extinction correction: none
 Primary atom site location: structure-invariant direct methods

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	0.80506 (3)	0.22447 (2)	0.46567 (3)	0.05751 (16)
C1	0.7721 (4)	0.4262 (3)	0.7408 (2)	0.0417 (8)
C2	0.6586 (4)	0.4087 (3)	0.7712 (3)	0.0485 (10)
C3	0.5829 (4)	0.4850 (4)	0.7852 (3)	0.0558 (11)
C4	0.6187 (5)	0.5765 (3)	0.7683 (3)	0.0577 (11)
H4	0.5666	0.6271	0.7776	0.069*
C5	0.7290 (5)	0.5963 (3)	0.7381 (3)	0.0521 (10)
C6	0.8072 (4)	0.5209 (3)	0.7249 (2)	0.0462 (9)
H6	0.8827	0.5327	0.7056	0.055*
C7	0.4636 (6)	0.4682 (5)	0.8230 (5)	0.0911 (19)
H7A	0.4524	0.4008	0.8305	0.137*
H7B	0.3901	0.4935	0.7828	0.137*
H7C	0.4733	0.4996	0.8795	0.137*
C8	0.7649 (7)	0.6982 (4)	0.7215 (4)	0.0848 (19)
H8A	0.7003	0.7408	0.7339	0.127*
H8B	0.7715	0.7052	0.6606	0.127*
H8C	0.8457	0.7134	0.7596	0.127*
C12	0.8000 (5)	0.4069 (3)	0.3505 (3)	0.0607 (12)
H12	0.7853	0.3707	0.2986	0.073*
C13	0.8194 (5)	0.5016 (3)	0.3547 (3)	0.0602 (12)
H13	0.8214	0.5424	0.3073	0.072*
C14	0.8266 (4)	0.4461 (3)	0.4867 (3)	0.0416 (8)
H14	0.8346	0.4433	0.5480	0.050*
C15	0.7291 (3)	0.6783 (2)	0.4694 (2)	0.0359 (7)
C16	0.7329 (3)	0.7772 (2)	0.4811 (2)	0.0328 (7)
C17	0.8609 (3)	0.8280 (2)	0.4959 (3)	0.0367 (8)

supplementary materials

H17A	0.9213	0.7942	0.5413	0.044*
H17B	0.8928	0.8257	0.4414	0.044*
C18	0.6192 (4)	0.8265 (3)	0.4773 (3)	0.0445 (9)
H18	0.6211	0.8924	0.4857	0.053*
C19	0.5030 (4)	0.7791 (3)	0.4613 (4)	0.0589 (12)
H19	0.4275	0.8132	0.4584	0.071*
C20	0.4992 (4)	0.6823 (4)	0.4497 (4)	0.0634 (13)
H20	0.4211	0.6505	0.4390	0.076*
C21	0.6116 (4)	0.6316 (3)	0.4540 (3)	0.0537 (10)
H21	0.6085	0.5656	0.4465	0.064*
C22	0.8532 (4)	0.6233 (2)	0.4755 (3)	0.0425 (8)
H22A	0.9071	0.6578	0.4426	0.051*
H22B	0.8978	0.6209	0.5372	0.051*
N1	0.8051 (3)	0.3716 (2)	0.4339 (2)	0.0429 (7)
N3	0.8356 (3)	0.5266 (2)	0.4413 (2)	0.0388 (7)
N5	0.6217 (5)	0.3171 (3)	0.7929 (4)	0.0778 (13)
O1	0.9699 (4)	0.3667 (3)	0.6837 (2)	0.0685 (9)
O2	0.7907 (4)	0.2586 (3)	0.6756 (3)	0.0724 (10)
O3	0.9261 (3)	0.2952 (2)	0.8160 (2)	0.0543 (7)
S1	0.87311 (11)	0.32912 (7)	0.72741 (6)	0.0452 (2)
N4	0.8549 (3)	0.92730 (19)	0.52284 (19)	0.0332 (6)
C11	0.8364 (4)	1.0041 (3)	0.4692 (2)	0.0370 (8)
H11	0.8298	1.0020	0.4080	0.044*
N2	0.8289 (3)	1.0823 (2)	0.5148 (2)	0.0401 (7)
C9	0.8436 (4)	1.0544 (3)	0.6015 (3)	0.0468 (9)
H9	0.8426	1.0951	0.6492	0.056*
C10	0.8597 (4)	0.9588 (3)	0.6074 (3)	0.0455 (9)
H10	0.8717	0.9219	0.6587	0.055*
HN1	0.569 (3)	0.2884 (16)	0.819 (3)	0.068*
HN2	0.642 (6)	0.265 (2)	0.769 (4)	0.068*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0623 (3)	0.02041 (17)	0.0961 (3)	0.00368 (12)	0.0308 (2)	0.01127 (14)
C1	0.057 (2)	0.0355 (19)	0.0313 (17)	0.0008 (16)	0.0051 (15)	-0.0009 (15)
C2	0.062 (3)	0.041 (2)	0.040 (2)	-0.0128 (18)	0.0033 (17)	0.0023 (17)
C3	0.052 (3)	0.068 (3)	0.047 (2)	0.000 (2)	0.0098 (18)	0.001 (2)
C4	0.072 (3)	0.049 (2)	0.051 (2)	0.019 (2)	0.011 (2)	0.003 (2)
C5	0.082 (3)	0.035 (2)	0.040 (2)	0.0051 (19)	0.013 (2)	0.0043 (17)
C6	0.065 (3)	0.040 (2)	0.0344 (19)	-0.0027 (18)	0.0128 (17)	0.0016 (16)
C7	0.067 (4)	0.103 (5)	0.111 (5)	0.000 (3)	0.036 (3)	0.012 (4)
C8	0.148 (6)	0.036 (2)	0.075 (4)	-0.002 (3)	0.032 (4)	0.008 (2)
C12	0.105 (4)	0.033 (2)	0.047 (2)	-0.007 (2)	0.023 (2)	-0.0101 (19)
C13	0.106 (4)	0.032 (2)	0.045 (2)	-0.005 (2)	0.023 (2)	0.0028 (18)
C14	0.057 (2)	0.0232 (17)	0.045 (2)	0.0030 (14)	0.0111 (17)	0.0020 (15)
C15	0.0398 (19)	0.0262 (16)	0.0424 (19)	-0.0011 (13)	0.0102 (15)	-0.0016 (14)
C16	0.0402 (19)	0.0254 (16)	0.0337 (17)	0.0001 (13)	0.0100 (13)	0.0006 (13)

C17	0.0408 (19)	0.0198 (15)	0.050 (2)	0.0014 (13)	0.0106 (15)	-0.0044 (14)
C18	0.044 (2)	0.0316 (18)	0.060 (2)	0.0057 (15)	0.0156 (18)	-0.0015 (17)
C19	0.036 (2)	0.061 (3)	0.082 (3)	0.0062 (19)	0.017 (2)	-0.004 (2)
C20	0.038 (2)	0.062 (3)	0.091 (4)	-0.012 (2)	0.014 (2)	-0.007 (3)
C21	0.048 (2)	0.036 (2)	0.078 (3)	-0.0099 (17)	0.014 (2)	-0.008 (2)
C22	0.046 (2)	0.0205 (16)	0.061 (2)	0.0001 (14)	0.0115 (17)	-0.0042 (16)
N1	0.059 (2)	0.0200 (14)	0.0521 (18)	0.0001 (13)	0.0167 (15)	-0.0022 (13)
N3	0.0522 (19)	0.0200 (14)	0.0448 (17)	0.0013 (12)	0.0116 (14)	-0.0011 (12)
N5	0.075 (3)	0.056 (3)	0.106 (4)	-0.015 (2)	0.025 (3)	0.004 (3)
O1	0.093 (3)	0.059 (2)	0.064 (2)	0.0174 (18)	0.0403 (18)	0.0161 (16)
O2	0.079 (2)	0.0484 (18)	0.078 (2)	0.0095 (17)	-0.0085 (18)	-0.0262 (17)
O3	0.0555 (18)	0.0563 (18)	0.0488 (16)	0.0018 (14)	0.0056 (13)	0.0192 (14)
S1	0.0616 (6)	0.0342 (5)	0.0385 (5)	0.0043 (4)	0.0073 (4)	0.0014 (4)
N4	0.0432 (16)	0.0206 (13)	0.0367 (15)	-0.0002 (11)	0.0105 (12)	-0.0020 (11)
C11	0.048 (2)	0.0249 (16)	0.0382 (18)	0.0007 (14)	0.0098 (15)	0.0016 (14)
N2	0.0519 (19)	0.0213 (14)	0.0497 (18)	-0.0009 (12)	0.0168 (14)	0.0003 (13)
C9	0.068 (3)	0.0287 (18)	0.046 (2)	0.0009 (17)	0.0170 (19)	-0.0112 (16)
C10	0.066 (3)	0.0343 (19)	0.038 (2)	0.0037 (17)	0.0163 (18)	0.0013 (16)

Geometric parameters (Å, °)

Ag1—N1	2.115 (3)	C15—C22	1.519 (5)
Ag1—N2 ⁱ	2.124 (3)	C16—C18	1.387 (5)
C1—C2	1.410 (6)	C16—C17	1.515 (5)
C1—C6	1.412 (6)	C17—N4	1.454 (4)
C1—S1	1.773 (4)	C17—H17A	0.9700
C2—C3	1.383 (6)	C17—H17B	0.9700
C2—N5	1.401 (6)	C18—C19	1.383 (6)
C3—C4	1.376 (7)	C18—H18	0.9300
C3—C7	1.525 (7)	C19—C20	1.365 (7)
C4—C5	1.383 (7)	C19—H19	0.9300
C4—H4	0.9300	C20—C21	1.385 (7)
C5—C6	1.386 (6)	C20—H20	0.9300
C5—C8	1.512 (7)	C21—H21	0.9300
C6—H6	0.9300	C22—N3	1.448 (4)
C7—H7A	0.9600	C22—H22A	0.9700
C7—H7B	0.9600	C22—H22B	0.9700
C7—H7C	0.9600	N5—HN1	0.858 (10)
C8—H8A	0.9600	N5—HN2	0.863 (10)
C8—H8B	0.9600	O1—S1	1.445 (3)
C8—H8C	0.9600	O2—S1	1.446 (4)
C12—C13	1.341 (6)	O3—S1	1.443 (3)
C12—N1	1.365 (6)	N4—C11	1.343 (5)
C12—H12	0.9300	N4—C10	1.365 (5)
C13—N3	1.353 (5)	C11—N2	1.311 (5)
C13—H13	0.9300	C11—H11	0.9300
C14—N1	1.312 (5)	N2—C9	1.368 (5)
C14—N3	1.339 (5)	N2—Ag1 ⁱⁱ	2.124 (3)
C14—H14	0.9300	C9—C10	1.348 (5)

supplementary materials

C15—C21	1.390 (5)	C9—H9	0.9300
C15—C16	1.396 (5)	C10—H10	0.9300
N1—Ag1—N2 ⁱ	170.93 (13)	C16—C17—H17B	108.9
C2—C1—C6	119.9 (4)	H17A—C17—H17B	107.7
C2—C1—S1	119.4 (3)	C19—C18—C16	121.0 (4)
C6—C1—S1	120.6 (3)	C19—C18—H18	119.5
C3—C2—N5	117.7 (4)	C16—C18—H18	119.5
C3—C2—C1	119.3 (4)	C20—C19—C18	120.0 (4)
N5—C2—C1	122.9 (4)	C20—C19—H19	120.0
C4—C3—C2	119.6 (4)	C18—C19—H19	120.0
C4—C3—C7	120.2 (5)	C19—C20—C21	120.0 (4)
C2—C3—C7	120.2 (5)	C19—C20—H20	120.0
C3—C4—C5	122.7 (4)	C21—C20—H20	120.0
C3—C4—H4	118.6	C20—C21—C15	120.7 (4)
C5—C4—H4	118.6	C20—C21—H21	119.6
C4—C5—C6	118.6 (4)	C15—C21—H21	119.6
C4—C5—C8	120.6 (5)	N3—C22—C15	113.8 (3)
C6—C5—C8	120.7 (5)	N3—C22—H22A	108.8
C5—C6—C1	119.9 (4)	C15—C22—H22A	108.8
C5—C6—H6	120.1	N3—C22—H22B	108.8
C1—C6—H6	120.1	C15—C22—H22B	108.8
C3—C7—H7A	109.5	H22A—C22—H22B	107.7
C3—C7—H7B	109.5	C14—N1—C12	105.2 (3)
H7A—C7—H7B	109.5	C14—N1—Ag1	129.7 (3)
C3—C7—H7C	109.5	C12—N1—Ag1	124.5 (3)
H7A—C7—H7C	109.5	C14—N3—C13	106.7 (3)
H7B—C7—H7C	109.5	C14—N3—C22	127.9 (3)
C5—C8—H8A	109.5	C13—N3—C22	125.3 (3)
C5—C8—H8B	109.5	C2—N5—HN1	141.7 (17)
H8A—C8—H8B	109.5	C2—N5—HN2	124 (4)
C5—C8—H8C	109.5	HN1—N5—HN2	93 (4)
H8A—C8—H8C	109.5	O3—S1—O1	112.4 (2)
H8B—C8—H8C	109.5	O3—S1—O2	111.7 (2)
C13—C12—N1	109.6 (4)	O1—S1—O2	113.9 (2)
C13—C12—H12	125.2	O3—S1—C1	105.71 (19)
N1—C12—H12	125.2	O1—S1—C1	106.67 (19)
C12—C13—N3	106.9 (4)	O2—S1—C1	105.7 (2)
C12—C13—H13	126.6	C11—N4—C10	107.4 (3)
N3—C13—H13	126.6	C11—N4—C17	126.7 (3)
N1—C14—N3	111.6 (3)	C10—N4—C17	125.8 (3)
N1—C14—H14	124.2	N2—C11—N4	110.9 (3)
N3—C14—H14	124.2	N2—C11—H11	124.6
C21—C15—C16	119.2 (3)	N4—C11—H11	124.6
C21—C15—C22	121.2 (3)	C11—N2—C9	106.0 (3)
C16—C15—C22	119.5 (3)	C11—N2—Ag1 ⁱⁱ	127.4 (3)
C18—C16—C15	119.1 (3)	C9—N2—Ag1 ⁱⁱ	126.5 (2)
C18—C16—C17	121.9 (3)	C10—C9—N2	109.6 (3)
C15—C16—C17	119.0 (3)	C10—C9—H9	125.2

N4—C17—C16	113.5 (3)	N2—C9—H9	125.2
N4—C17—H17A	108.9	C9—C10—N4	106.1 (3)
C16—C17—H17A	108.9	C9—C10—H10	126.9
N4—C17—H17B	108.9	N4—C10—H10	126.9
C6—C1—C2—C3	0.0 (6)	C16—C15—C22—N3	-165.8 (3)
S1—C1—C2—C3	177.2 (3)	N3—C14—N1—C12	-0.1 (5)
C6—C1—C2—N5	-176.4 (4)	N3—C14—N1—Ag1	171.3 (3)
S1—C1—C2—N5	0.8 (6)	C13—C12—N1—C14	0.4 (6)
N5—C2—C3—C4	177.3 (5)	C13—C12—N1—Ag1	-171.5 (4)
C1—C2—C3—C4	0.7 (6)	N2 ⁱ —Ag1—N1—C14	-35.2 (10)
N5—C2—C3—C7	0.0 (7)	N2 ⁱ —Ag1—N1—C12	134.7 (7)
C1—C2—C3—C7	-176.6 (4)	N1—C14—N3—C13	-0.3 (5)
C2—C3—C4—C5	-0.4 (7)	N1—C14—N3—C22	177.1 (4)
C7—C3—C4—C5	176.9 (5)	C12—C13—N3—C14	0.6 (6)
C3—C4—C5—C6	-0.5 (7)	C12—C13—N3—C22	-177.0 (4)
C3—C4—C5—C8	-179.3 (5)	C15—C22—N3—C14	-94.2 (5)
C4—C5—C6—C1	1.2 (6)	C15—C22—N3—C13	82.8 (5)
C8—C5—C6—C1	179.9 (4)	C2—C1—S1—O3	-68.3 (3)
C2—C1—C6—C5	-0.9 (6)	C6—C1—S1—O3	108.9 (3)
S1—C1—C6—C5	-178.1 (3)	C2—C1—S1—O1	171.8 (3)
N1—C12—C13—N3	-0.6 (6)	C6—C1—S1—O1	-11.0 (4)
C21—C15—C16—C18	0.2 (5)	C2—C1—S1—O2	50.2 (4)
C22—C15—C16—C18	-178.6 (4)	C6—C1—S1—O2	-132.5 (4)
C21—C15—C16—C17	-178.7 (4)	C16—C17—N4—C11	-92.5 (4)
C22—C15—C16—C17	2.5 (5)	C16—C17—N4—C10	83.4 (5)
C18—C16—C17—N4	11.5 (5)	C10—N4—C11—N2	-0.2 (4)
C15—C16—C17—N4	-169.6 (3)	C17—N4—C11—N2	176.3 (3)
C15—C16—C18—C19	-0.7 (6)	N4—C11—N2—C9	0.2 (4)
C17—C16—C18—C19	178.2 (4)	N4—C11—N2—Ag1 ⁱⁱ	178.3 (2)
C16—C18—C19—C20	0.6 (7)	C11—N2—C9—C10	-0.1 (5)
C18—C19—C20—C21	0.0 (8)	Ag1 ⁱⁱ —N2—C9—C10	-178.3 (3)
C19—C20—C21—C15	-0.5 (8)	N2—C9—C10—N4	0.0 (5)
C16—C15—C21—C20	0.4 (7)	C11—N4—C10—C9	0.1 (5)
C22—C15—C21—C20	179.2 (4)	C17—N4—C10—C9	-176.4 (4)
C21—C15—C22—N3	15.4 (6)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—HN2 \cdots O2	0.863 (10)	2.36 (5)	2.924 (7)	123 (5)

Fig. 1

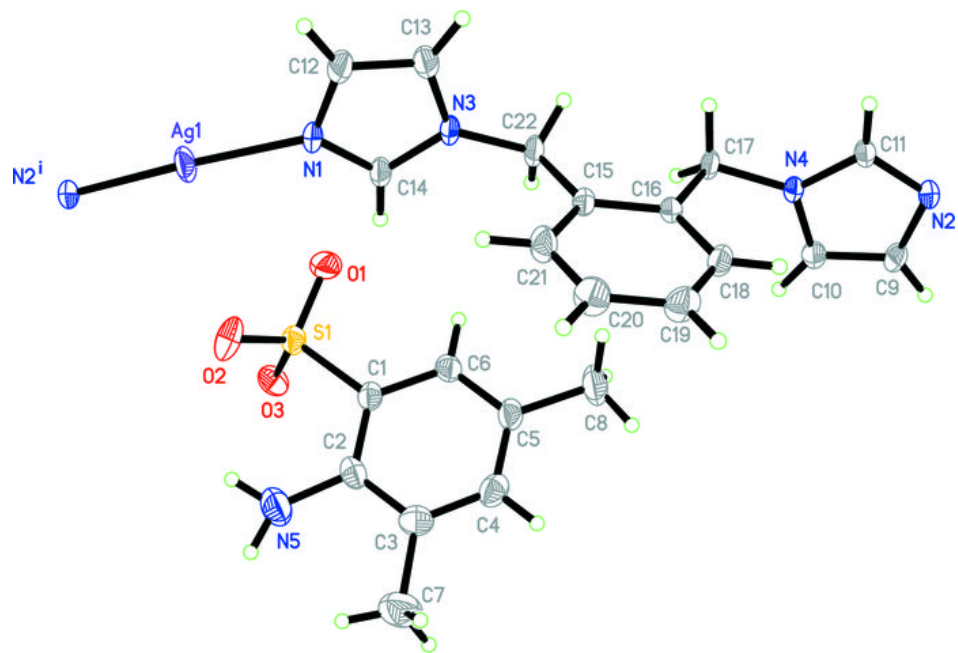


Fig. 2

