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Poly[[(μ_2-2-amino-4,5-dimethybenzenesulfonato-κ^2N:O)(μ_2-2-methylpyrazine-κ^2N:N')silver(I)] monohydrate]

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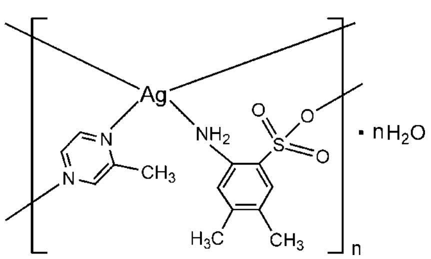
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.007 Å; H-atom completeness 89%; R factor = 0.032; wR factor = 0.084; data-to-parameter ratio = 17.7.

In the title compound, $\{[Ag(C_8H_{10}NO_3S)(C_7H_6N_2)]\cdot H_2O\}_n$, each Ag^I cation is four-coordinated by three N atoms from two different 2-methylpyrazine ligands and one –NH_2 group of a 2-amino-4,5-dimethybenzenesulfonate ligand, and by one sulfonate O atom, in a distorted tetrahedral coordination geometry. The Ag^I centres are bridged by both types of ligands, forming a two-dimensional network. N—H···O hydrogen bonds and O···O interactions complete the structure.

Related literature

For related literature, see: Cote & Shimizu (2004); Li *et al.* (2005); Liu *et al.* (2007).



Experimental

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_7H_6N_2)]\cdot H_2O$
M_r = 420.23
Orthorhombic, $P2_12_12_1$
a = 7.2340 (4) Å
b = 11.7610 (5) Å
c = 18.913 (1) Å
V = 1609.10 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 292 (2) K
0.35 × 0.29 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.615, T_{max} = 0.711
13881 measured reflections
3667 independent reflections
3083 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.02
3667 reflections
207 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}
Absolute structure: Flack (1983), 1369 Friedel pairs
Flack parameter: 0.00 (3)

Table 1
Selected geometric parameters (Å, °).

Ag1—N2	2.243 (3)	Ag1—N3^i	2.469 (4)
Ag1—N1	2.301 (4)	Ag1—O3^{ii}	2.525 (3)
N2—Ag1—N1	141.78 (13)	N2—Ag1—O3^{ii}	125.98 (12)
N2—Ag1—N3^i	102.19 (12)	N1—Ag1—O3^{ii}	87.53 (14)
N1—Ag1—N3^i	98.44 (13)	N3^i—Ag1—O3^{ii}	84.57 (12)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H2N···O2	0.82 (3)	2.36 (4)	2.982 (5)	133 (4)
N1—H1N···O1W^{ii}	0.82 (5)	2.15 (5)	2.946 (5)	164 (5)

Symmetry code: (ii) $x+1, y, z$.

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: CI2532).

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supplementary materials

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Poly[[(μ_2-2-amino-4,5-dimethybenzenesulfonato-κ^2*N*:*O*)(μ_2-2-methylpyrazine-κ^2*N*:*N'*)silver(I)] monohydrate]

X.-W. Dong and **Y.-J. Li**

Comment

Silver(I) sulfonate coordination polymers have received much attention for their interesting structural features and potential applications (Cote & Shimizu, 2004). Recently, silver(I) sulfonate compounds with nitrogen-based secondary ligands have been reported (Li *et al.*, 2005). We report here the crystal structure of the title compound.

Selected geometric parameters are listed in Table 1. The Ag^I cation is four-coordinated by three N atoms from two different 2-methylpyrazine ligands and one $-NH_2$ group of anion, and one sulfonate O atom in a distorted tetrahedral coordination geometry (Fig.1). The Ag—N distances in the title compound are similar to those in related compounds (Liu *et al.*, 2007). The Ag^I centers are doubly bridged by both types of ligands to form a two-dimensional network (Fig.2), which are linked *via* N—H···O hydrogen bonds (Table 2) and O···O interacitons into a three-dimensional framework (Fig.3).

Experimental

An aqueous solution (10 ml) of 2-amino-4,5-dimethylbenzenesulfonic acid (1 mmol) was added to solid Ag_2CO_3 (0.5 mmol) and stirred for several minutes until no further CO_2 was given off. 2-Methylpyrazine (1 mmol) was then added and a precipitate was formed. The precipitate was dissolved by ammonium hydroxide. Crystals of the title compound were obtained by slow evaporation of the solution at room temperature for 7 d.

Refinement

All H atoms on C atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H)= 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}) The amino H-atoms were located in a difference Fourier map and its positional parameters were refined, With the N—H distances restrained to 0.82 (2) Å, and with U_{iso}(H) = 1.2U_{eq}(N). H atoms bonded to water molecules could not be located and were therefore omitted.

Figures

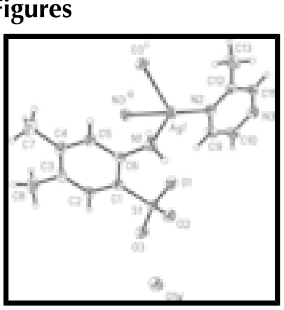

Fig. 1. The coordination environment of atom Ag1 in the title compound, showing 30% probability displacement ellipsoids [Symmetry codes: (i) -*x* + 1, *y* + 1/2, -*z* + 1/2; (ii) *x* + 1, *y*, *z*].

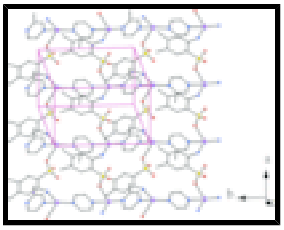

Fig. 2. View of a two-dimensional network in the title compound.

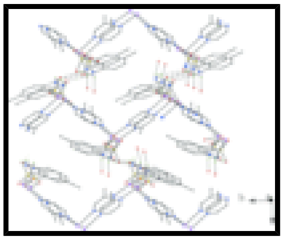

Fig. 3. Part of the three-dimensional network of the title compound. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen-bonding interactions have been omitted.

Poly[[(μ$_2$-2-amino-4,5-dimethybenzenesulfonato-κ^2*N*:*O*)(μ$_2$-2- methylpyrazine-κ^2*N*:*N*')silver(I)] monohydrate]

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_7H_6N_2)]\cdot H_2O$	F_{000} = 848
M_r = 420.23	D_x = 1.735 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo *K*α radiation λ = 0.71069 Å
Hall symbol: P 2ac 2ab	Cell parameters from 3667 reflections
a = 7.2340 (4) Å	θ = 2.0–27.5°
b = 11.7610 (5) Å	μ = 1.40 mm^{-1}
c = 18.913 (1) Å	*T* = 292 (2) K
V = 1609.10 (14) Å^3	Block, yellow
Z = 4	0.35 × 0.29 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	3667 independent reflections
Radiation source: fine-focus sealed tube	3083 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.053
T = 292(2) K	θ_{max} = 27.5°
ω scans	θ_{min} = 2.0°
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -9 \rightarrow 9$
T_{min} = 0.615, T_{max} = 0.711	$k = -15 \rightarrow 15$
13881 measured reflections	$l = -24 \rightarrow 24$

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

$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.085$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.50$ e Å^{-3}
3667 reflections	$\Delta\rho_{min} = -0.58$ e Å^{-3}
207 parameters	Extinction correction: none
4 restraints	Absolute structure: Flack (1983), with 1369 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.00 (3)
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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.57509 (5)	0.32306 (3)	0.368222 (17)	0.04386 (11)
C1	0.1920 (5)	0.5165 (3)	0.4190 (2)	0.0308 (8)
C2	0.1248 (6)	0.6189 (4)	0.3919 (2)	0.0393 (10)
H2	0.0045	0.6211	0.3746	0.047*
C3	0.2286 (7)	0.7160 (4)	0.3898 (2)	0.0444 (11)
C4	0.4079 (8)	0.7131 (4)	0.4174 (2)	0.0455 (11)
C5	0.4746 (6)	0.6123 (4)	0.4454 (2)	0.0408 (10)
H5	0.5927	0.6113	0.4647	0.049*
C6	0.3719 (5)	0.5128 (3)	0.4457 (2)	0.0316 (9)
C7	0.5321 (8)	0.8154 (5)	0.4164 (3)	0.0684 (16)
H7A	0.4744	0.8765	0.4418	0.103*
H7B	0.5535	0.8383	0.3684	0.103*
H7C	0.6478	0.7967	0.4384	0.103*
C8	0.1486 (9)	0.8237 (4)	0.3565 (3)	0.0723 (16)
H8A	0.1767	0.8879	0.3859	0.108*
H8B	0.0169	0.8160	0.3521	0.108*
H8C	0.2018	0.8347	0.3105	0.108*
C9	0.3884 (6)	0.1510 (4)	0.2665 (2)	0.0455 (12)
H10	0.2963	0.2058	0.2704	0.055*
C10	0.3556 (7)	0.0582 (4)	0.2262 (3)	0.0493 (12)
H11	0.2415	0.0505	0.2040	0.059*

C11	0.6419 (6)	−0.0062 (4)	0.2511 (2)	0.0413 (10)
H12	0.7349	−0.0602	0.2459	0.050*
C12	0.6755 (6)	0.0873 (4)	0.2934 (2)	0.0410 (10)
C13	0.8545 (8)	0.1001 (6)	0.3321 (4)	0.078 (2)
H24A	0.8528	0.1694	0.3590	0.117*
H24B	0.9545	0.1024	0.2988	0.117*
H24C	0.8712	0.0368	0.3635	0.117*
N1	0.4536 (5)	0.4089 (3)	0.46717 (18)	0.0371 (8)
N2	0.5462 (5)	0.1673 (3)	0.30075 (16)	0.0366 (8)
N3	0.4829 (5)	−0.0226 (3)	0.21749 (19)	0.0435 (9)
O1	0.1454 (4)	0.3189 (3)	0.36351 (17)	0.0529 (8)
O2	0.0582 (5)	0.3433 (3)	0.48525 (17)	0.0518 (8)
O3	−0.1281 (4)	0.4287 (3)	0.3932 (2)	0.0573 (9)
O1W	−0.2470 (5)	0.4027 (3)	0.57266 (16)	0.0484 (8)
S1	0.05493 (14)	0.39276 (9)	0.41453 (6)	0.0369 (2)
H1N	0.539 (7)	0.421 (4)	0.495 (2)	0.055*
H2N	0.383 (6)	0.362 (3)	0.485 (2)	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.04702 (19)	0.03504 (16)	0.04951 (17)	0.00277 (16)	−0.00239 (16)	−0.00726 (15)
C1	0.029 (2)	0.030 (2)	0.0339 (19)	−0.0029 (17)	0.0002 (16)	0.0016 (16)
C2	0.036 (2)	0.036 (2)	0.046 (2)	0.0036 (18)	−0.0017 (17)	−0.0005 (18)
C3	0.057 (3)	0.030 (2)	0.046 (2)	0.003 (2)	−0.003 (2)	0.0004 (18)
C4	0.054 (3)	0.037 (2)	0.045 (2)	−0.011 (2)	0.001 (2)	−0.0067 (18)
C5	0.036 (2)	0.041 (2)	0.045 (2)	−0.006 (2)	0.0013 (18)	−0.0043 (18)
C6	0.027 (2)	0.034 (2)	0.0334 (19)	0.0037 (17)	−0.0002 (15)	−0.0014 (16)
C7	0.078 (4)	0.050 (3)	0.077 (3)	−0.026 (3)	−0.005 (3)	0.002 (3)
C8	0.087 (4)	0.033 (2)	0.097 (4)	0.002 (3)	−0.014 (3)	0.012 (3)
C9	0.038 (3)	0.049 (3)	0.049 (2)	0.009 (2)	−0.0029 (19)	−0.012 (2)
C10	0.040 (2)	0.058 (3)	0.050 (3)	0.007 (2)	−0.012 (2)	−0.016 (2)
C11	0.038 (2)	0.036 (2)	0.050 (2)	0.0044 (19)	−0.001 (2)	−0.007 (2)
C12	0.039 (2)	0.038 (2)	0.046 (2)	−0.001 (2)	0.000 (2)	−0.001 (2)
C13	0.050 (3)	0.066 (4)	0.118 (5)	0.006 (3)	−0.031 (3)	−0.032 (4)
N1	0.031 (2)	0.0407 (19)	0.0398 (18)	0.0009 (16)	−0.0075 (16)	0.0044 (15)
N2	0.0350 (19)	0.0370 (18)	0.0377 (16)	−0.0004 (19)	0.0021 (14)	−0.0052 (15)
N3	0.047 (2)	0.041 (2)	0.0423 (19)	−0.0042 (19)	−0.0043 (17)	−0.0079 (16)
O1	0.0533 (18)	0.0402 (16)	0.0653 (19)	−0.0123 (17)	0.0106 (17)	−0.0140 (19)
O2	0.0434 (18)	0.049 (2)	0.0626 (18)	−0.0032 (17)	0.0058 (15)	0.0194 (15)
O3	0.0284 (16)	0.048 (2)	0.095 (3)	−0.0068 (14)	−0.0196 (16)	0.0175 (18)
O1W	0.0428 (18)	0.0499 (19)	0.0526 (18)	0.0038 (16)	−0.0054 (15)	0.0033 (15)
S1	0.0255 (5)	0.0328 (5)	0.0524 (6)	−0.0029 (4)	−0.0004 (5)	0.0053 (4)

Geometric parameters (Å, °)

Ag1—N2	2.243 (3)	C8—H8C	0.96
Ag1—N1	2.301 (4)	C9—N2	1.326 (6)

Ag1—N3^{i}	2.469 (4)	C9—C10	1.353 (7)
Ag1—O3^{ii}	2.525 (3)	C9—H10	0.9300
C1—C2	1.396 (6)	C10—N3	1.333 (6)
C1—C6	1.396 (6)	C10—H11	0.93
C1—S1	1.763 (4)	C11—N3	1.329 (5)
C2—C3	1.368 (6)	C11—C12	1.381 (6)
C2—H2	0.93	C11—H12	0.93
C3—C4	1.399 (8)	C12—N2	1.334 (6)
C3—C8	1.528 (7)	C12—C13	1.495 (7)
C4—C5	1.386 (6)	C13—H24A	0.96
C4—C7	1.501 (7)	C13—H24B	0.96
C5—C6	1.386 (6)	C13—H24C	0.96
C5—H5	0.93	N1—H1N	0.82 (5)
C6—N1	1.417 (5)	N1—H2N	0.82 (3)
C7—H7A	0.96	N3—Ag1^{iii}	2.469 (4)
C7—H7B	0.96	O1—S1	1.454 (3)
C7—H7C	0.96	O2—S1	1.459 (3)
C8—H8A	0.96	O3—S1	1.448 (3)
C8—H8B	0.96	O3—Ag1^{iv}	2.525 (3)
N2—Ag1—N1	141.78 (13)	N2—C9—H10	118.6
N2—Ag1—N3^{i}	102.19 (12)	C10—C9—H10	118.6
N1—Ag1—N3^{i}	98.44 (13)	N3—C10—C9	121.6 (4)
N2—Ag1—O3^{ii}	125.98 (12)	N3—C10—H11	119.2
N1—Ag1—O3^{ii}	87.53 (14)	C9—C10—H11	119.2
N3^{i}—Ag1—O3^{ii}	84.57 (12)	N3—C11—C12	123.1 (4)
C2—C1—C6	119.0 (4)	N3—C11—H12	118.5
C2—C1—S1	119.9 (3)	C12—C11—H12	118.5
C6—C1—S1	121.0 (3)	N2—C12—C11	119.9 (4)
C3—C2—C1	122.7 (4)	N2—C12—C13	119.0 (4)
C3—C2—H2	118.7	C11—C12—C13	121.1 (4)
C1—C2—H2	118.7	C12—C13—H24A	109.5
C2—C3—C4	118.6 (4)	C12—C13—H24B	109.5
C2—C3—C8	119.8 (5)	H24A—C13—H24B	109.5
C4—C3—C8	121.7 (4)	C12—C13—H24C	109.5
C5—C4—C3	119.1 (4)	H24A—C13—H24C	109.5
C5—C4—C7	118.8 (5)	H24B—C13—H24C	109.5
C3—C4—C7	122.1 (4)	C6—N1—Ag1	107.7 (2)
C4—C5—C6	122.5 (4)	C6—N1—H1N	111 (4)
C4—C5—H5	118.7	Ag1—N1—H1N	108 (3)
C6—C5—H5	118.7	C6—N1—H2N	116 (3)
C5—C6—C1	118.1 (4)	Ag1—N1—H2N	107 (3)
C5—C6—N1	120.4 (4)	H1N—N1—H2N	108 (4)
C1—C6—N1	121.3 (4)	C9—N2—C12	116.8 (4)
C4—C7—H7A	109.5	C9—N2—Ag1	118.4 (3)
C4—C7—H7B	109.5	C12—N2—Ag1	124.8 (3)
H7A—C7—H7B	109.5	C11—N3—C10	115.8 (4)
C4—C7—H7C	109.5	C11—N3—Ag1^{iii}	124.6 (3)

H7A—C7—H7C	109.5	C10—N3—Ag1^{iii}	119.2 (3)
H7B—C7—H7C	109.5	S1—O3—Ag1^{iv}	133.33 (19)
C3—C8—H8A	109.5	O3—S1—O1	113.6 (2)
C3—C8—H8B	109.5	O3—S1—O2	112.8 (2)
H8A—C8—H8B	109.5	O1—S1—O2	111.3 (2)
C3—C8—H8C	109.5	O3—S1—C1	106.66 (19)
H8A—C8—H8C	109.5	O1—S1—C1	105.76 (18)
H8B—C8—H8C	109.5	O2—S1—C1	106.0 (2)
N2—C9—C10	122.8 (4)		

C6—C1—C2—C3	0.6 (6)	C10—C9—N2—Ag1	−178.1 (4)
S1—C1—C2—C3	−175.8 (4)	C11—C12—N2—C9	0.6 (6)
C1—C2—C3—C4	−1.5 (7)	C13—C12—N2—C9	−178.7 (5)
C1—C2—C3—C8	177.4 (5)	C11—C12—N2—Ag1	179.1 (3)
C2—C3—C4—C5	0.4 (7)	C13—C12—N2—Ag1	−0.2 (6)
C8—C3—C4—C5	−178.4 (5)	N1—Ag1—N2—C9	63.6 (4)
C2—C3—C4—C7	179.3 (5)	N3^{i}—Ag1—N2—C9	−57.6 (3)
C8—C3—C4—C7	0.4 (7)	O3^{ii}—Ag1—N2—C9	−149.7 (3)
C3—C4—C5—C6	1.6 (7)	N1—Ag1—N2—C12	−114.9 (3)
C7—C4—C5—C6	−177.3 (4)	N3^{i}—Ag1—N2—C12	124.0 (3)
C4—C5—C6—C1	−2.5 (6)	O3^{ii}—Ag1—N2—C12	31.8 (4)
C4—C5—C6—N1	172.5 (4)	C12—C11—N3—C10	0.8 (7)
C2—C1—C6—C5	1.4 (6)	C12—C11—N3—Ag1^{iii}	173.4 (3)
S1—C1—C6—C5	177.7 (3)	C9—C10—N3—C11	0.4 (7)
C2—C1—C6—N1	−173.6 (4)	C9—C10—N3—Ag1^{iii}	−172.7 (4)
S1—C1—C6—N1	2.8 (5)	Ag1^{iv}—O3—S1—O1	62.2 (4)
N2—C9—C10—N3	−1.1 (8)	Ag1^{iv}—O3—S1—O2	−65.6 (4)
N3—C11—C12—N2	−1.3 (7)	Ag1^{iv}—O3—S1—C1	178.4 (3)
N3—C11—C12—C13	177.9 (5)	C2—C1—S1—O3	−10.7 (4)
C5—C6—N1—Ag1	−90.6 (4)	C6—C1—S1—O3	172.9 (3)
C1—C6—N1—Ag1	84.2 (4)	C2—C1—S1—O1	110.6 (3)
N2—Ag1—N1—C6	−116.6 (3)	C6—C1—S1—O1	−65.8 (4)
N3^{i}—Ag1—N1—C6	5.7 (3)	C2—C1—S1—O2	−131.2 (3)
O3^{ii}—Ag1—N1—C6	89.8 (3)	C6—C1—S1—O2	52.5 (4)
C10—C9—N2—C12	0.5 (7)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H2N···O2	0.82 (3)	2.36 (4)	2.982 (5)	133 (4)
N1—H1N···O1W^{ii}	0.82 (5)	2.15 (5)	2.946 (5)	164 (5)

Symmetry codes: (ii) *x*+1, *y*, *z*.

Fig. 1

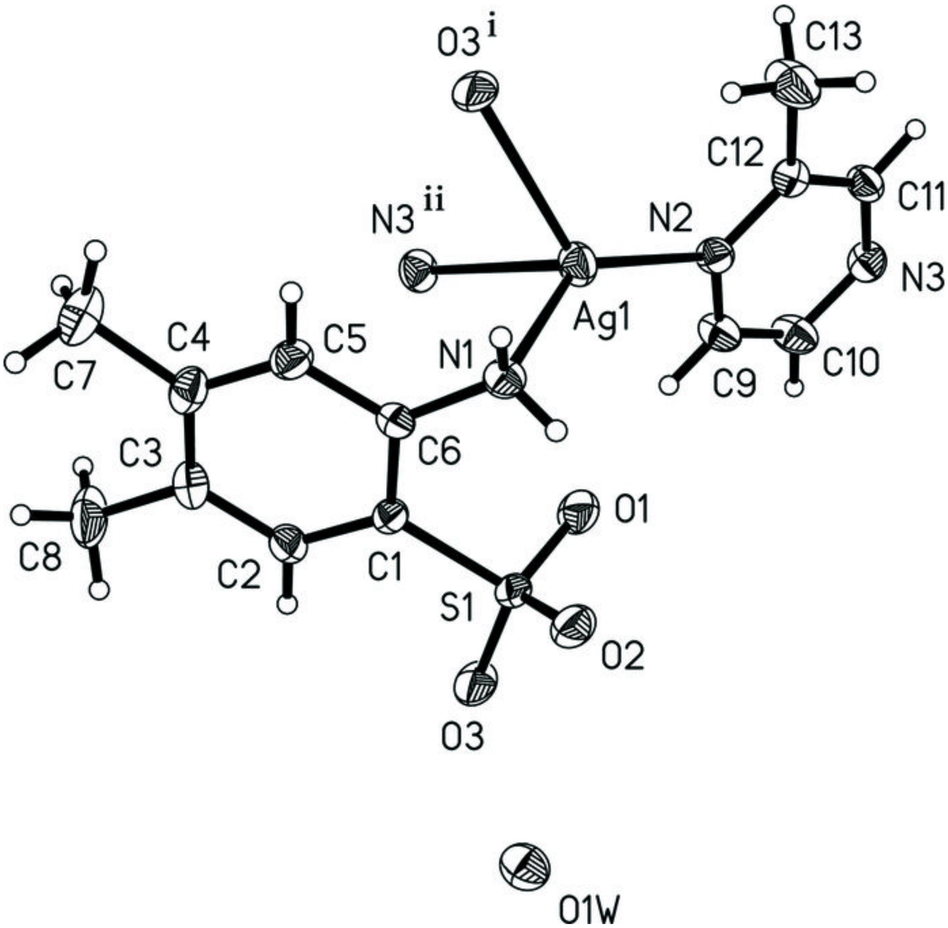
O3 i
C13
C12
C11
N3 ii
N2
N3
Ag1
C7
C4
C5
N1
C10
C9
C3
C6
O1
C8
C2
C1
S1
O2
O3
O1W

Fig. 2

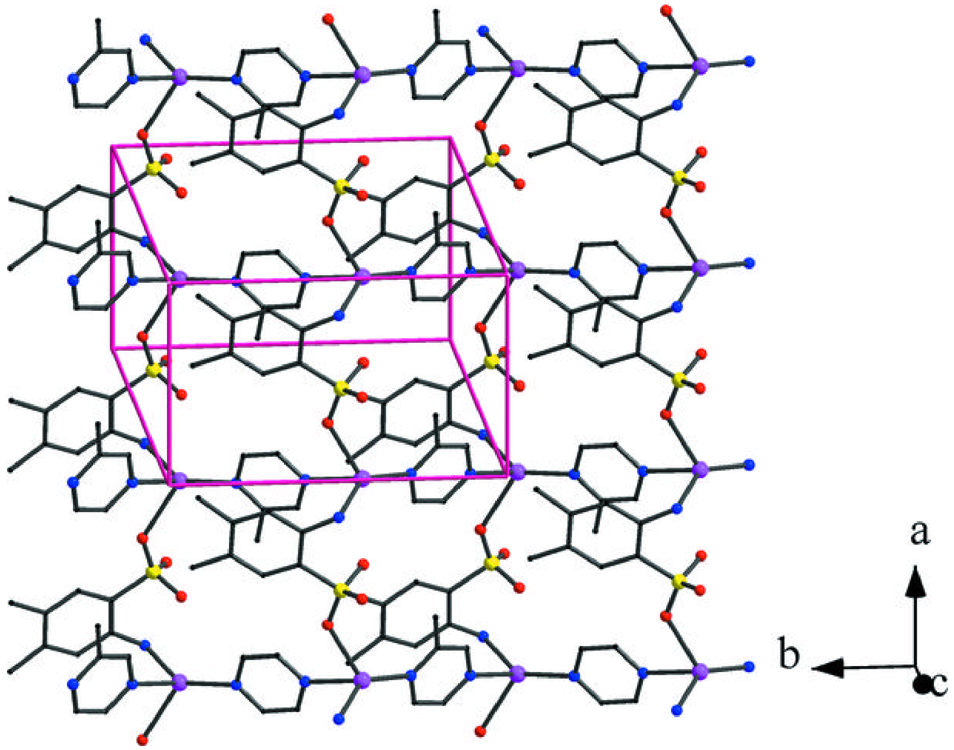

Fig. 3