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catena-Poly[[[aquasilver(I)]-μ-2,3-dimethylpyrazine-κ^2N:N'] 4-amino-2,5-dichlorobenzenesulfonate]

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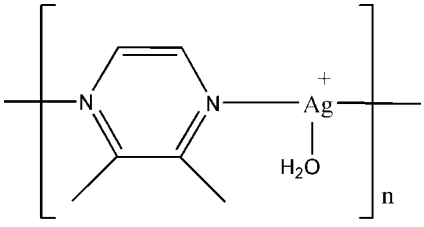
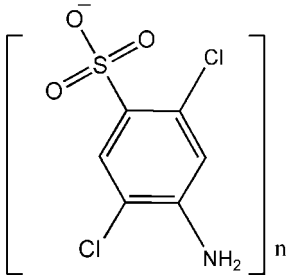
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; R factor = 0.074; wR factor = 0.194; data-to-parameter ratio = 16.0.

In the title compound, $\{[Ag(C_6H_8N_2)(H_2O)](C_6H_4Cl_2NO_3S)\}_n$, the Ag^I ion is three-coordinated by two N atoms from two symmetry-related 2,3-dimethylpyrazine (dmp) ligands, and one water O atom in a distorted trigonal–planar geometry. The dmp ligands bridge Ag^I ions to form a one-dimensional chain structure with charge-balancing 4-amino-2,5-dichlorobenzenesulfonate anions. In the crystal structure, intermolecular O—H···O and N—H···O hydrogen bonds form a two-dimensional network.

Related literature

For general background, see: Yaghi & Li (1995). For studies of silver sulfonates, see: Cote & Shimizu (2003); Li *et al.* (2006); Liu *et al.* (2007).





Experimental

Crystal data

$[Ag(C_6H_8N_2)(H_2O)](C_6H_4Cl_2NO_3S)$
M_r = 475.09
Monoclinic, $P2_1/n$
a = 7.162 (4) Å
b = 16.298 (9) Å
c = 13.721 (6) Å
β = 103.26 (2)°
V = 1558.9 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.79 mm^{-1}
T = 293 (2) K
0.28 × 0.22 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.597, T_{max} = 0.710
14717 measured reflections
3520 independent reflections
2932 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.194
S = 1.14
3520 reflections
220 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 2.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.184 (7)	Ag1—O1*W*	2.542 (8)
Ag1—N2^{i}	2.216 (6)		
N1—Ag1—N2^{i}	170.7 (2)	N2^{i}—Ag1—O1*W*	92.0 (2)
N1—Ag1—O1*W*	97.3 (3)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H*W*11···O3^{ii}	0.85 (10)	2.15 (10)	2.977 (10)	164 (13)
N3—HN2···O1^{iii}	0.85 (7)	2.34 (8)	3.040 (10)	140 (11)
O1*W*—H*W*12···O2	0.85 (7)	1.90 (4)	2.725 (11)	162 (12)

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

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: LH2525).

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supplementary materials

Acta Cryst. (2007). E**63**, m2734-m2735 [**doi:10.1107/S160053680704977X**]

catena-Poly[[[aquasilver(I)]-μ-2,3-dimethylpyrazine-κ^2N:N'] 4-amino-2,5-dichlorobenzenesulfonate]

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

Comment

Metal–organic coordination polymers have received much attention for their interesting structural features and potential application in optical devices, enantiomer separation, chiral synthesis and selective catalysis (Yaghi & Li, 1995). In particular, silver(I) sulfonates have attracted intense interest from chemists (Cote & Shimizu, 2003). So far, some silver(I) sulfonate compounds with nitrogen-based secondary ligands have been observed in the literature (Li *et al.*, 2006). Herein, we present a new sulfonate coordination polymer, namely [Ag(dmp)(H_2O)]·*L* (I), where dmp = 2,3-dimethylprazine and HL = 4-amino-2,5-dichlorobenzenesulfonic acid.

In the title compound, the unique Ag^I ion is three-coordinated by two N atoms from two symmetry realted dmp ligands, and one water O atom in a distorted trigonal-planar geometry (Fig. 1). The Ag—N distance is similar to those in reported compounds (Liu *et al.*, 2007). The dmp ligands bridge neighboring Ag^I ions to form a chain structure (Fig. 2). The *L* ligand acts as a counter anion. Finally, the O—H···O and N—H···O hydrogen bonds complete the structure.

Experimental

An aqueous solution (9 ml) of 4-amino-2,5-dichlorobenzenesulfonic 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. 2,3-dimethylprazine (1 mmol) was then added and a precipitate was formed. The precipitate was dissolved by ammonium hydroxide. Crystals of were obtained by evaporation of the solution for several days at room temperature.

Refinement

H atoms of 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) for methyl. H atoms bonded to atom N3 were located in a difference map and refined freely, but with U_{iso}(H) = 1.5U_{eq}(N). The water H atoms were located from a difference map and refined freely with U_{iso}(H) = 1.5U_{eq}(O). Restraints were applied to the N—H and O—H distances.

Figures

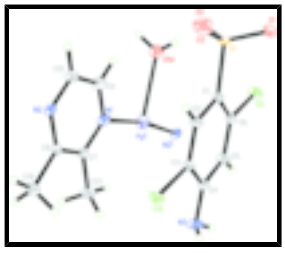

Fig. 1. The asymmetric unit with symmetry complete Ag^{I} coordination, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) $x-1, y, z$.

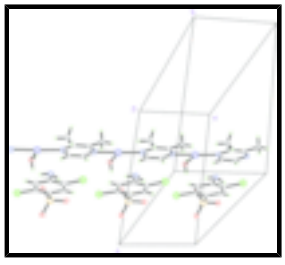

Fig. 2. View of the one-dimensional chain structure.

catena-Poly[[[aquasilver(I)]-μ-2,3-dimethylpyrazine-κ^2*N*:*N*'] 4-amino-2,5-dichlorobenzenesulfonate]

Crystal data

$[Ag(C_6H_8N_2)(H_2O)](C_6H_4Cl_2NO_3S)$	F_{000} = 944
M_r = 475.09	D_x = 2.024 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2yn	Cell parameters from 12993 reflections
a = 7.162 (4) Å	θ = 3.0–27.5º
b = 16.298 (9) Å	μ = 1.79 mm^{-1}
c = 13.721 (6) Å	T = 293 (2) K
β = 103.26 (2)º	Block, colourless
V = 1558.9 (14) Å^3	0.28 × 0.22 × 0.19 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	3520 independent reflections
Radiation source: rotating anode	2932 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.1º
ω scans	h = −9→9
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −21→21
T_{min} = 0.597, T_{max} = 0.710	l = −17→17
14717 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.074$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.194$	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 23.775P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{max} < 0.001$
3520 reflections	$\Delta\rho_{max} = 2.58$ e Å^{-3}
220 parameters	$\Delta\rho_{min} = -0.93$ e Å^{-3}
5 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	−0.29399 (9)	0.23016 (5)	0.46242 (6)	0.0406 (2)
Cl1	−0.4029 (3)	0.11290 (13)	0.70107 (19)	0.0383 (5)
S1	0.0264 (3)	0.03566 (11)	0.70936 (15)	0.0269 (4)
Cl2	0.2908 (3)	0.34574 (12)	0.72206 (17)	0.0351 (5)
C7	0.1131 (11)	0.3127 (5)	0.4664 (6)	0.0251 (15)
C8	0.3063 (10)	0.3119 (5)	0.4708 (6)	0.0237 (14)
O1	−0.0284 (10)	−0.0027 (4)	0.7928 (5)	0.0393 (14)
O3	0.2262 (10)	0.0319 (4)	0.7124 (6)	0.0466 (17)
C6	−0.2032 (11)	0.1760 (5)	0.7083 (6)	0.0262 (15)
C4	−0.0839 (11)	0.3161 (5)	0.7147 (6)	0.0261 (15)
O2	−0.0909 (12)	0.0070 (4)	0.6145 (6)	0.056 (2)
N2	0.4000 (8)	0.2405 (4)	0.4677 (5)	0.0238 (13)
C1	−0.0228 (10)	0.1426 (4)	0.7134 (6)	0.0232 (14)
N3	−0.1112 (11)	0.3970 (4)	0.7135 (7)	0.0383 (17)
HN2	−0.225 (7)	0.401 (8)	0.722 (9)	0.057*
HN1	−0.013 (10)	0.414 (7)	0.756 (7)	0.057*

C3	0.0991 (10)	0.2810 (4)	0.7199 (6)	0.0239 (14)
N1	0.0099 (10)	0.2414 (5)	0.4624 (5)	0.0322 (15)
C2	0.1272 (12)	0.1976 (5)	0.7203 (6)	0.0284 (16)
H2	0.2505	0.1774	0.7253	0.034*
C19	0.4244 (13)	0.3885 (6)	0.4822 (8)	0.040 (2)
H19A	0.5553	0.3747	0.4834	0.061*
H19B	0.4182	0.4154	0.5436	0.061*
H19C	0.3757	0.4245	0.4268	0.061*
C10	0.2999 (13)	0.1707 (5)	0.4620 (7)	0.0343 (18)
H10	0.3607	0.1207	0.4587	0.041*
C5	−0.2334 (12)	0.2593 (5)	0.7078 (6)	0.0314 (17)
H5	−0.3574	0.2787	0.7026	0.038*
C9	0.1084 (12)	0.1724 (6)	0.4612 (7)	0.0351 (18)
H9	0.0439	0.1228	0.4598	0.042*
C23	0.0026 (14)	0.3922 (6)	0.4655 (8)	0.041 (2)
H23A	−0.1298	0.3800	0.4626	0.062*
H23B	0.0122	0.4240	0.4080	0.062*
H23C	0.0553	0.4227	0.5253	0.062*
O1W	−0.3165 (10)	0.0749 (4)	0.4468 (6)	0.0462 (16)
HW11	−0.270 (17)	0.050 (7)	0.403 (6)	0.069*
HW12	−0.269 (17)	0.050 (7)	0.501 (4)	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0212 (3)	0.0460 (4)	0.0564 (5)	0.0001 (3)	0.0129 (3)	−0.0038 (3)
Cl1	0.0224 (9)	0.0321 (10)	0.0620 (14)	−0.0046 (8)	0.0131 (9)	0.0019 (9)
S1	0.0296 (9)	0.0151 (8)	0.0387 (10)	0.0003 (7)	0.0136 (8)	−0.0007 (7)
Cl2	0.0326 (10)	0.0222 (9)	0.0519 (12)	−0.0081 (7)	0.0128 (9)	−0.0044 (8)
C7	0.027 (4)	0.025 (4)	0.025 (3)	0.003 (3)	0.008 (3)	−0.002 (3)
C8	0.017 (3)	0.026 (4)	0.028 (4)	−0.002 (3)	0.006 (3)	−0.001 (3)
O1	0.049 (4)	0.025 (3)	0.049 (4)	0.005 (3)	0.023 (3)	0.010 (3)
O3	0.044 (4)	0.017 (3)	0.085 (5)	0.004 (3)	0.029 (4)	0.004 (3)
C6	0.021 (3)	0.028 (4)	0.031 (4)	−0.007 (3)	0.009 (3)	0.002 (3)
C4	0.029 (4)	0.022 (4)	0.027 (4)	0.000 (3)	0.007 (3)	0.000 (3)
O2	0.082 (6)	0.029 (3)	0.050 (4)	0.005 (3)	0.001 (4)	−0.015 (3)
N2	0.014 (3)	0.030 (3)	0.029 (3)	0.003 (2)	0.007 (2)	−0.004 (3)
C1	0.017 (3)	0.019 (3)	0.036 (4)	−0.003 (3)	0.010 (3)	−0.001 (3)
N3	0.034 (4)	0.020 (3)	0.062 (5)	0.005 (3)	0.013 (4)	−0.005 (3)
C3	0.023 (4)	0.019 (3)	0.029 (4)	−0.001 (3)	0.006 (3)	−0.001 (3)
N1	0.029 (3)	0.032 (4)	0.037 (4)	0.005 (3)	0.009 (3)	−0.008 (3)
C2	0.029 (4)	0.020 (4)	0.038 (4)	0.002 (3)	0.010 (3)	0.000 (3)
C19	0.032 (4)	0.032 (5)	0.062 (6)	−0.011 (4)	0.019 (4)	−0.006 (4)
C10	0.042 (5)	0.026 (4)	0.036 (4)	−0.002 (3)	0.010 (4)	−0.005 (3)
C5	0.026 (4)	0.026 (4)	0.042 (5)	0.007 (3)	0.009 (3)	0.000 (3)
C9	0.025 (4)	0.034 (4)	0.045 (5)	−0.002 (3)	0.007 (3)	−0.007 (4)
C23	0.040 (5)	0.031 (5)	0.054 (6)	0.010 (4)	0.014 (4)	0.000 (4)
O1W	0.047 (4)	0.044 (4)	0.049 (4)	0.010 (3)	0.014 (3)	0.000 (3)

Geometric parameters (Å, °)

Ag1—N1	2.184 (7)	N2—Ag1^{ii}	2.216 (6)
Ag1—N2^{i}	2.216 (6)	C1—C2	1.385 (10)
Ag1—O1W	2.542 (8)	N3—HN2	0.85 (7)
Cl1—C6	1.745 (8)	N3—HN1	0.85 (9)
S1—O3	1.424 (7)	C3—C2	1.375 (10)
S1—O1	1.435 (6)	N1—C9	1.329 (11)
S1—O2	1.455 (7)	C2—H2	0.9300
S1—C1	1.782 (7)	C19—H19A	0.9600
Cl2—C3	1.726 (8)	C19—H19B	0.9600
C7—C8	1.371 (10)	C19—H19C	0.9600
C7—N1	1.373 (11)	C10—C9	1.369 (12)
C7—C23	1.516 (11)	C10—H10	0.9300
C8—N2	1.350 (10)	C5—H5	0.9300
C8—C19	1.496 (11)	C9—H9	0.9300
C6—C5	1.376 (11)	C23—H23A	0.9600
C6—C1	1.388 (10)	C23—H23B	0.9600
C4—N3	1.333 (10)	C23—H23C	0.9600
C4—C5	1.402 (11)	O1W—HW11	0.85 (10)
C4—C3	1.417 (10)	O1W—HW12	0.85 (7)
N2—C10	1.338 (11)		
N1—Ag1—N2^{i}	170.7 (2)	C4—C3—Cl2	118.5 (6)
N1—Ag1—O1W	97.3 (3)	C9—N1—C7	115.7 (7)
N2^{i}—Ag1—O1W	92.0 (2)	C9—N1—Ag1	117.5 (6)
O3—S1—O1	114.5 (4)	C7—N1—Ag1	126.8 (5)
O3—S1—O2	112.5 (5)	C3—C2—C1	121.9 (7)
O1—S1—O2	111.5 (5)	C3—C2—H2	119.0
O3—S1—C1	104.2 (3)	C1—C2—H2	119.0
O1—S1—C1	108.0 (4)	C8—C19—H19A	109.5
O2—S1—C1	105.3 (4)	C8—C19—H19B	109.5
C8—C7—N1	121.5 (7)	H19A—C19—H19B	109.5
C8—C7—C23	121.9 (7)	C8—C19—H19C	109.5
N1—C7—C23	116.6 (7)	H19A—C19—H19C	109.5
N2—C8—C7	120.7 (7)	H19B—C19—H19C	109.5
N2—C8—C19	116.7 (7)	N2—C10—C9	120.3 (8)
C7—C8—C19	122.5 (7)	N2—C10—H10	119.8
C5—C6—C1	122.0 (7)	C9—C10—H10	119.8
C5—C6—Cl1	117.1 (6)	C6—C5—C4	122.3 (7)
C1—C6—Cl1	120.9 (6)	C6—C5—H5	118.8
N3—C4—C5	123.0 (7)	C4—C5—H5	118.8
N3—C4—C3	122.1 (7)	N1—C9—C10	123.5 (8)
C5—C4—C3	114.9 (7)	N1—C9—H9	118.3
C10—N2—C8	118.1 (7)	C10—C9—H9	118.3
C10—N2—Ag1^{ii}	117.0 (5)	C7—C23—H23A	109.5
C8—N2—Ag1^{ii}	124.7 (5)	C7—C23—H23B	109.5
C2—C1—C6	116.7 (7)	H23A—C23—H23B	109.5

C2—C1—S1	118.6 (6)	C7—C23—H23C	109.5
C6—C1—S1	124.7 (5)	H23A—C23—H23C	109.5
C4—N3—HN2	102 (9)	H23B—C23—H23C	109.5
C4—N3—HN1	102 (9)	Ag1—O1W—HW11	120 (9)
HN2—N3—HN1	123 (10)	Ag1—O1W—HW12	113 (9)
C2—C3—C4	122.2 (7)	HW11—O1W—HW12	104 (10)
C2—C3—Cl2	119.3 (6)		
N1—C7—C8—N2	2.3 (12)	C5—C4—C3—Cl2	176.7 (6)
C23—C7—C8—N2	−177.5 (7)	C8—C7—N1—C9	−1.1 (11)
N1—C7—C8—C19	−175.8 (8)	C23—C7—N1—C9	178.7 (8)
C23—C7—C8—C19	4.4 (13)	C8—C7—N1—Ag1	176.8 (6)
C7—C8—N2—C10	−1.2 (11)	C23—C7—N1—Ag1	−3.4 (10)
C19—C8—N2—C10	177.1 (8)	O1W—Ag1—N1—C9	−4.0 (7)
C7—C8—N2—Ag1^{ii}	175.1 (5)	O1W—Ag1—N1—C7	178.1 (7)
C19—C8—N2—Ag1^{ii}	−6.6 (10)	C4—C3—C2—C1	1.4 (13)
C5—C6—C1—C2	1.5 (12)	Cl2—C3—C2—C1	−176.6 (6)
Cl1—C6—C1—C2	−179.2 (6)	C6—C1—C2—C3	−1.4 (12)
C5—C6—C1—S1	−177.3 (7)	S1—C1—C2—C3	177.5 (6)
Cl1—C6—C1—S1	2.0 (10)	C8—N2—C10—C9	−1.1 (12)
O3—S1—C1—C2	−1.3 (8)	Ag1^{ii}—N2—C10—C9	−177.6 (7)
O1—S1—C1—C2	120.9 (7)	C1—C6—C5—C4	−1.6 (13)
O2—S1—C1—C2	−119.9 (7)	Cl1—C6—C5—C4	179.1 (6)
O3—S1—C1—C6	177.5 (7)	N3—C4—C5—C6	179.5 (9)
O1—S1—C1—C6	−60.3 (8)	C3—C4—C5—C6	1.4 (12)
O2—S1—C1—C6	58.9 (8)	C7—N1—C9—C10	−1.2 (13)
N3—C4—C3—C2	−179.5 (8)	Ag1—N1—C9—C10	−179.3 (7)
C5—C4—C3—C2	−1.3 (12)	N2—C10—C9—N1	2.4 (14)
N3—C4—C3—Cl2	−1.5 (11)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—HW11···O3^{iii}	0.85 (10)	2.15 (10)	2.977 (10)	164 (13)
N3—HN2···O1^{iv}	0.85 (7)	2.34 (8)	3.040 (10)	140 (11)
O1W—HW12···O2	0.85 (7)	1.90 (4)	2.725 (11)	162 (12)

Symmetry codes: (iii) −*x*, −*y*, −*z*+1; (iv) −*x*−1/2, *y*+1/2, −*z*+3/2.

Fig. 1

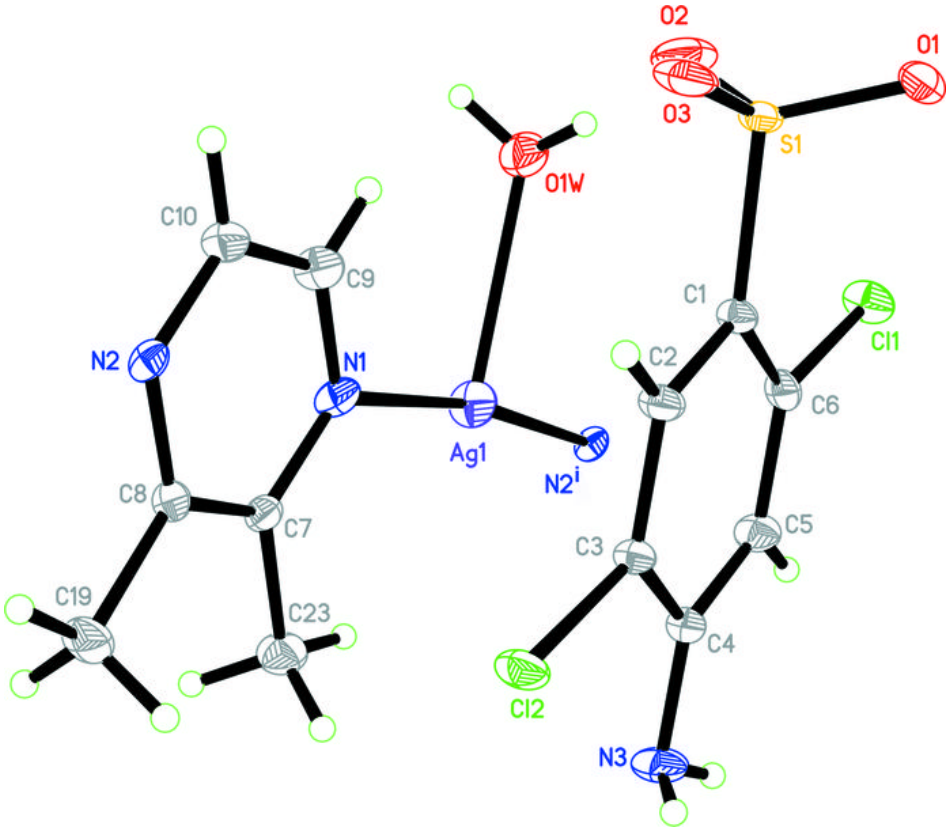
O2
O1
O3
S1
O1W
C10
C9
C1
Cl1
N2
N1
C2
C6
Ag1
N2i
C8
C7
C5
C3
C19
C23
C4
Cl2
N3

Fig. 2