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Aquapyridinesilver(I) 4-amino-2,5-dichlorobenzenesulfonate dihydrate

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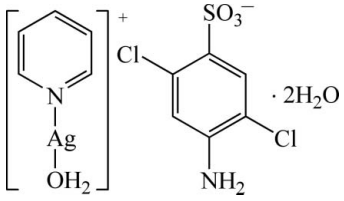
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.010 Å; R factor = 0.048; wR factor = 0.093; data-to-parameter ratio = 17.1.

The title compound, $[Ag(C_5H_5N)(H_2O)](C_6H_4Cl_2NO_3S)\cdot 2H_2O$, has a mononuclear structure in which the Ag^+ cation is two-coordinated by one N atom from a pyridine molecule and one O atom from a water molecule. The 4-amino-2,5-dichlorobenzenesulfonate anion does not coordinate to the Ag atom, but acts as a counterion. Intermolecular O—H···O hydrogen bonds link the ions and water molecules.

Related literature

The related compound, $[Ag(HL3)(Pic)_2]$ (HL3 = *p*-hydroxybenzenesulfonic acid, Pic = *β*-picoline), has a dimeric structure and each Ag^+ cation is coordinated by two N atoms from two different *β*-picoline ligands and two O atoms from two HL3 anions with Ag—N distances of 2.168 (3) and 2.163 (3) Å (Li *et al.*, 2006).



Experimental

Crystal data

$[Ag(C_5H_5N)(H_2O)](C_6H_4Cl_2NO_3S)\cdot 2H_2O$
M_r = 482.08
Monoclinic, $P2_1$
a = 9.325 (2) Å
b = 7.6101 (13) Å
c = 12.3466 (19) Å
β = 95.365 (13)°
V = 872.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 294 (2) K
0.21 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.705, T_{max} = 0.75
6338 measured reflections
3963 independent reflections
2001 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.093
S = 0.80
3963 reflections
232 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Absolute structure: Flack (1983), with 1632 Friedel pairs
Flack parameter: −0.06 (4)

Table 1
Selected geometric parameters (Å, °).

Ag1—N2	2.148 (6)	Ag1—O1*W*	2.162 (5)
N2—Ag1—O1*W*	172.1 (3)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H2*B*···O2	0.79 (4)	2.53 (10)	2.855 (8)	106 (8)
O2*W*—H2*A*···O3*W*^{i}	0.85 (4)	2.00 (6)	2.753 (8)	147 (8)
O3*W*—H3*B*···O1	0.76 (4)	2.14 (5)	2.842 (8)	155 (9)
O3*W*—H3*A*···O2*W*^{ii}	0.84 (4)	1.92 (4)	2.744 (7)	171 (8)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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: AT2291).

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supplementary materials

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Aquapyridinesilver(I) 4-amino-2,5-dichlorobenzenesulfonate dihydrate

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Comment

The structure of the title compound, (I) (Fig. 1), containing a pyridine molecule, three water molecules and 2,5-dichloro-4-amino-benzenesulfonate (*L*) anion is described. In (I), pyridine and water molecule are coordinated to the metal, resulting in a slightly distorted linear coordination geometry for Ag (Table 1). Atoms Ag1, N1 and O1W are almost linear and the angle of N1—Ag1—O1W is 172.07°. The Ag—$N_{pyrindine}$ and Ag—O1W distances are 2.148 (6)Å and 2.162 (5) Å, respectively; the Ag—$N_{pyrindine}$ distance is similar to the equivalent value in related compound (Li *et al.*, 2006). 2,5-Dichloro-4-amino-benzenesulfonate anion does not coordinate with Ag atom, but acts as counterions..

In (I), the coordination ability of the oxygen atom of guest water molecule is evidently stronger than that of sulfonate group and the latter group does not coordinate to the Ag ion. Adjacent molecules of *L* are interconnected by strong O—H···O hydrogen-bonding interactions between uncoordinated sulfonate O atoms and uncoordinated water molecules (Table 2). Thus, the compound forms a one-dimensional anions chain through extensive intermolecular hydrogen bonding (Fig. 2).

Experimental

An aqueous solution (10 ml) of 2,5-dichloro-4-amino-benzenesulfonic acid (0.121 g, 0.5 mmol) was added to solid Ag_2CO_3 (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO_2 was given off; pyridine (0.0395 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_3 (14 *M*). Crystals of (I) were obtained by evaporation of the solution for several days at room temperature.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 ° A and U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C). The amino H atoms were located in a difference Fourier map and refined isotropically. The water H atoms were located in a difference Fourier map and refined with U_{iso}(H) = 1.5U_{eq}(O).

Figures

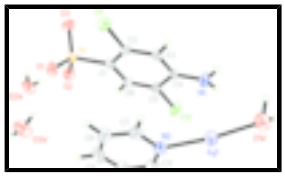

Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

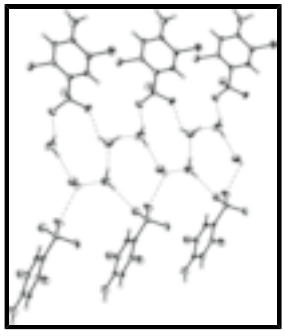

Fig. 2. One-dimensional chain of (I), formed through hydrogen-bonding (dashed lines) interactions·The atoms not involved in hydrogen bonding have been omitted.

Aquapyridinesilver(I) 4-amino-2,5-dichlorobenzenesulfonate dihydrate

Crystal data

$[Ag(C_5H_5N)(H_2O)](C_6H_4Cl_2NO_3S)\cdot 2H_2O$	$F_{000} = 480$
$M_r = 482.08$	$D_x = 1.835$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 3963 reflections
$a = 9.325$ (2) Å	$\theta = 1.7$–28.3º
$b = 7.6101$ (13) Å	$\mu = 1.61$ mm^{-1}
$c = 12.3466$ (19) Å	$T = 294$ (2) K
$\beta = 95.365$ (13)º	Block, white
$V = 872.3$ (3) Å^3	0.21 × 0.20 × 0.18 mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD diffractometer	3963 independent reflections
Radiation source: fine-focus sealed tube	2001 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.066$
$T = 292$(2) K	$\theta_{max} = 28.3$º
phi and ω scans	$\theta_{min} = 1.7$º
Absorption correction: empirical (using intensity measurements) SADABS (Sheldrick, 1996)	$h = -12\rightarrow7$
$T_{min} = 0.705$, $T_{max} = 0.75$	$k = -10\rightarrow8$
6338 measured reflections	$l = -16\rightarrow15$

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
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.093$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.80$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
3963 reflections	$\Delta\rho_{min} = -0.38$ e Å^{-3}
232 parameters	Extinction correction: none
13 restraints	Absolute structure: Flack (1983), 1632 Freidel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.06 (4)
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 $F^2 > 2\text{sigma}(F^2)$ 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	0.14273 (6)	0.76552 (8)	0.76877 (5)	0.0596 (2)
C1	0.6240 (7)	0.2943 (9)	0.8378 (4)	0.0313 (15)
C2	0.5928 (7)	0.4023 (8)	0.9251 (5)	0.0312 (16)
C3	0.4540 (8)	0.4444 (8)	0.9427 (5)	0.0338 (16)
H3	0.4378	0.5136	1.0025	0.041*
C4	0.3366 (7)	0.3871 (8)	0.8744 (5)	0.0311 (16)
C5	0.3702 (6)	0.2774 (10)	0.7844 (4)	0.0354 (15)
C6	0.5080 (6)	0.2342 (9)	0.7697 (5)	0.0319 (16)
H6	0.5253	0.1615	0.7118	0.038*
C7	0.4620 (8)	0.7543 (13)	0.7271 (5)	0.0561 (18)
H7	0.4749	0.8099	0.7944	0.067*
C8	0.5811 (9)	0.7031 (12)	0.6767 (8)	0.075 (3)
H8	0.6731	0.7213	0.7108	0.090*
C9	0.5637 (11)	0.6263 (13)	0.5774 (8)	0.077 (3)
H9	0.6433	0.5953	0.5414	0.092*
C10	0.4290 (11)	0.5955 (13)	0.5315 (7)	0.075 (3)
H10	0.4143	0.5386	0.4647	0.090*
C11	0.3146 (10)	0.6493 (12)	0.5847 (6)	0.069 (3)
H11	0.2222	0.6313	0.5513	0.083*
N1	0.1990 (7)	0.4291 (8)	0.8898 (6)	0.0493 (17)
N2	0.3290 (6)	0.7260 (8)	0.6816 (4)	0.0474 (16)
O1	0.8803 (5)	0.3887 (6)	0.7913 (4)	0.0484 (13)
O2	0.7831 (5)	0.1100 (6)	0.7236 (4)	0.0512 (14)
O3	0.8638 (5)	0.1433 (6)	0.9135 (4)	0.0504 (14)

O1W	−0.0366 (6)	0.7715 (10)	0.8677 (4)	0.0765 (15)
O2W	0.9509 (9)	−0.0802 (8)	0.5812 (5)	0.0661 (19)
O3W	0.9266 (11)	0.5599 (7)	0.5930 (6)	0.076 (2)
S1	0.80197 (17)	0.2296 (2)	0.81471 (13)	0.0344 (4)
Cl1	0.7303 (2)	0.4896 (2)	1.01407 (15)	0.0508 (5)
Cl2	0.2283 (2)	0.1997 (2)	0.69835 (16)	0.0566 (6)
H1A	−0.010 (7)	0.759 (12)	0.945 (3)	0.085*
H1B	−0.107 (7)	0.680 (9)	0.867 (6)	0.085*
H2A	0.909 (8)	−0.178 (7)	0.586 (5)	0.085*
H2B	0.981 (10)	−0.055 (10)	0.641 (4)	0.085*
H1N	0.123 (7)	0.383 (10)	0.858 (6)	0.085*
H3A	0.963 (10)	0.506 (10)	0.543 (5)	0.085*
H3B	0.902 (10)	0.494 (9)	0.633 (5)	0.085*
H2N	0.173 (8)	0.472 (11)	0.943 (5)	0.085*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0553 (4)	0.0648 (4)	0.0599 (4)	0.0080 (4)	0.0108 (3)	0.0016 (4)
C1	0.041 (4)	0.027 (4)	0.027 (3)	−0.005 (3)	0.006 (3)	0.005 (3)
C2	0.031 (4)	0.029 (4)	0.033 (4)	0.002 (3)	−0.001 (3)	0.001 (3)
C3	0.046 (5)	0.028 (4)	0.028 (4)	0.005 (3)	0.005 (3)	−0.005 (3)
C4	0.029 (4)	0.029 (4)	0.038 (4)	0.003 (3)	0.014 (3)	0.011 (3)
C5	0.034 (4)	0.032 (3)	0.039 (3)	0.008 (4)	0.000 (3)	−0.002 (4)
C6	0.035 (4)	0.032 (4)	0.030 (3)	−0.002 (4)	0.007 (3)	0.001 (3)
C7	0.052 (5)	0.062 (5)	0.052 (4)	−0.003 (6)	−0.002 (4)	0.002 (6)
C8	0.049 (6)	0.089 (9)	0.086 (7)	−0.004 (6)	−0.004 (5)	0.014 (6)
C9	0.066 (7)	0.095 (7)	0.074 (7)	−0.002 (6)	0.033 (6)	0.000 (6)
C10	0.079 (8)	0.093 (7)	0.057 (6)	−0.014 (6)	0.024 (6)	−0.015 (5)
C11	0.059 (6)	0.100 (7)	0.046 (5)	−0.003 (5)	−0.002 (5)	−0.007 (5)
N1	0.038 (4)	0.048 (4)	0.062 (5)	0.012 (3)	0.004 (3)	−0.005 (3)
N2	0.051 (4)	0.048 (4)	0.043 (3)	0.001 (3)	0.003 (3)	0.001 (3)
O1	0.040 (3)	0.045 (3)	0.061 (3)	−0.011 (3)	0.011 (3)	0.004 (3)
O2	0.042 (3)	0.058 (3)	0.054 (3)	0.008 (3)	0.008 (3)	−0.030 (3)
O3	0.053 (3)	0.046 (3)	0.051 (3)	0.025 (3)	−0.001 (3)	0.011 (2)
O1W	0.078 (4)	0.073 (4)	0.080 (3)	−0.002 (5)	0.020 (3)	0.001 (5)
O2W	0.083 (5)	0.063 (4)	0.057 (4)	0.002 (4)	0.026 (4)	0.000 (3)
O3W	0.114 (7)	0.054 (4)	0.064 (5)	0.014 (4)	0.037 (4)	0.004 (3)
S1	0.0331 (9)	0.0353 (11)	0.0355 (9)	0.0011 (8)	0.0070 (7)	−0.0034 (8)
Cl1	0.0497 (13)	0.0557 (12)	0.0460 (11)	0.0030 (10)	−0.0013 (9)	−0.0191 (9)
Cl2	0.0391 (11)	0.0650 (14)	0.0631 (12)	−0.0029 (10)	−0.0087 (10)	−0.0129 (10)

Geometric parameters (Å, °)

Ag1—N2	2.148 (6)	C8—H8	0.9300
Ag1—O1W	2.162 (5)	C9—C10	1.349 (12)
C1—C6	1.384 (8)	C9—H9	0.9300
C1—C2	1.408 (8)	C10—C11	1.367 (11)
C1—S1	1.779 (6)	C10—H10	0.9300

C2—C3	1.371 (9)	C11—N2	1.327 (9)
C2—Cl1	1.740 (7)	C11—H11	0.9300
C3—C4	1.388 (9)	N1—H1N	0.85 (4)
C3—H3	0.9300	N1—H2N	0.79 (4)
C4—N1	1.353 (8)	O1—S1	1.457 (5)
C4—C5	1.447 (9)	O2—S1	1.445 (4)
C5—C6	1.355 (8)	O3—S1	1.456 (4)
C5—Cl2	1.722 (6)	O1W—H1A	0.97 (4)
C6—H6	0.9300	O1W—H1B	0.96 (4)
C7—N2	1.330 (8)	O2W—H2A	0.85 (4)
C7—C8	1.380 (10)	O2W—H2B	0.79 (4)
C7—H7	0.9300	O3W—H3A	0.84 (4)
C8—C9	1.355 (11)	O3W—H3B	0.76 (4)
N2—Ag1—O1W	172.1 (3)	C10—C9—H9	120.5
C6—C1—C2	116.9 (6)	C8—C9—H9	120.5
C6—C1—S1	119.9 (5)	C9—C10—C11	118.9 (9)
C2—C1—S1	123.1 (5)	C9—C10—H10	120.5
C3—C2—C1	121.6 (6)	C11—C10—H10	120.5
C3—C2—Cl1	117.5 (5)	N2—C11—C10	123.2 (8)
C1—C2—Cl1	120.9 (5)	N2—C11—H11	118.4
C2—C3—C4	122.2 (6)	C10—C11—H11	118.4
C2—C3—H3	118.9	C4—N1—H1N	126 (5)
C4—C3—H3	118.9	C4—N1—H2N	125 (6)
N1—C4—C3	123.0 (6)	H1N—N1—H2N	105 (5)
N1—C4—C5	121.4 (6)	C11—N2—C7	117.6 (7)
C3—C4—C5	115.7 (6)	C11—N2—Ag1	119.7 (6)
C6—C5—C4	121.3 (6)	C7—N2—Ag1	122.1 (5)
C6—C5—Cl2	121.1 (5)	Ag1—O1W—H1A	115 (4)
C4—C5—Cl2	117.6 (5)	Ag1—O1W—H1B	123 (5)
C5—C6—C1	122.4 (6)	H1A—O1W—H1B	93 (4)
C5—C6—H6	118.8	H2A—O2W—H2B	106 (5)
C1—C6—H6	118.8	H3A—O3W—H3B	109 (5)
N2—C7—C8	121.5 (8)	O2—S1—O3	112.2 (3)
N2—C7—H7	119.3	O2—S1—O1	113.3 (3)
C8—C7—H7	119.3	O3—S1—O1	112.0 (3)
C9—C8—C7	119.8 (8)	O2—S1—C1	104.5 (3)
C9—C8—H8	120.1	O3—S1—C1	107.0 (3)
C7—C8—H8	120.1	O1—S1—C1	107.1 (3)
C10—C9—C8	118.9 (9)		
C6—C1—C2—C3	0.8 (9)	S1—C1—C6—C5	179.1 (6)
S1—C1—C2—C3	−177.6 (5)	N2—C7—C8—C9	1.8 (14)
C6—C1—C2—Cl1	−178.5 (5)	C7—C8—C9—C10	−2.5 (14)
S1—C1—C2—Cl1	3.2 (8)	C8—C9—C10—C11	2.7 (14)
C1—C2—C3—C4	−1.7 (10)	C9—C10—C11—N2	−2.2 (14)
Cl1—C2—C3—C4	177.6 (5)	C10—C11—N2—C7	1.5 (13)
C2—C3—C4—N1	−179.1 (7)	C10—C11—N2—Ag1	−169.8 (7)
C2—C3—C4—C5	1.1 (9)	C8—C7—N2—C11	−1.2 (12)
N1—C4—C5—C6	−179.4 (7)	C8—C7—N2—Ag1	169.8 (7)

C3—C4—C5—C6	0.3 (10)	C6—C1—S1—O2	−2.8 (6)
N1—C4—C5—Cl2	−0.8 (9)	C2—C1—S1—O2	175.5 (5)
C3—C4—C5—Cl2	179.0 (5)	C6—C1—S1—O3	−122.0 (5)
C4—C5—C6—C1	−1.2 (11)	C2—C1—S1—O3	56.3 (6)
Cl2—C5—C6—C1	−179.8 (5)	C6—C1—S1—O1	117.7 (5)
C2—C1—C6—C5	0.7 (9)	C2—C1—S1—O1	−64.0 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2W—H2B···O2	0.79 (4)	2.53 (10)	2.855 (8)	106 (8)
O2W—H2A···O3W^{i}	0.85 (4)	2.00 (6)	2.753 (8)	147 (8)
O3W—H3B···O1	0.76 (4)	2.14 (5)	2.842 (8)	155 (9)
O3W—H3A···O2W^{ii}	0.84 (4)	1.92 (4)	2.744 (7)	171 (8)

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

Fig. 1

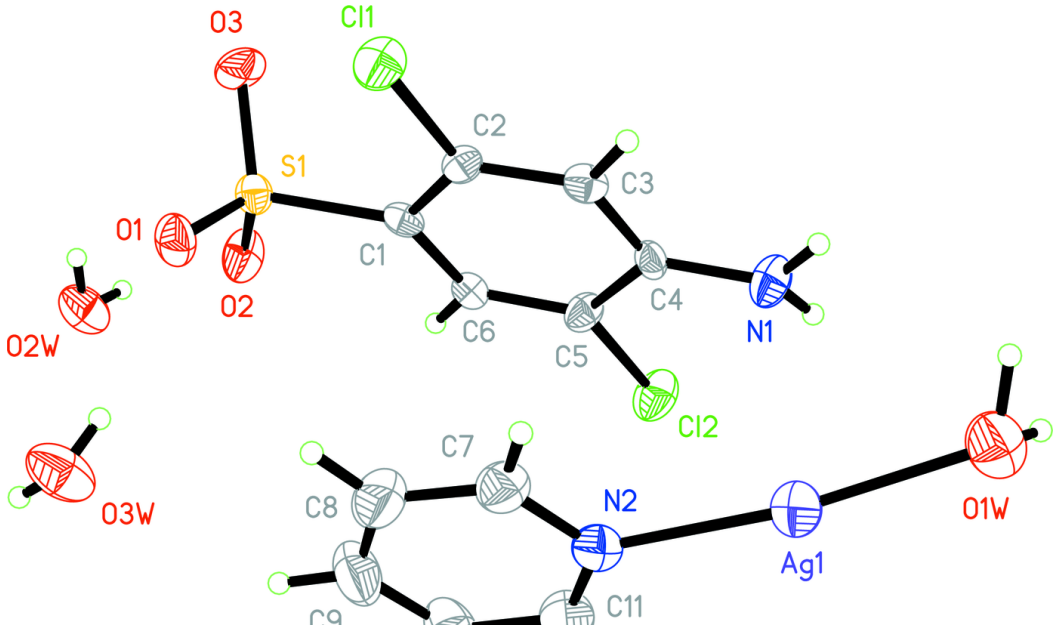

Fig. 2