Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquasilver(I) 6-aminonaphthalene-1-sulfonate monohydrate

Yu-Jie Li,[a] Xian-Wu Dong[a]* and Hua Wu[b]

[a]JiLin Agriculture, Science and Technology College, People's Republic of China, and [b]School of Heilongjiang Agricultural College of Vocational Technology, People's Republic of China
Correspondence e-mail: hljwuhua@163.com

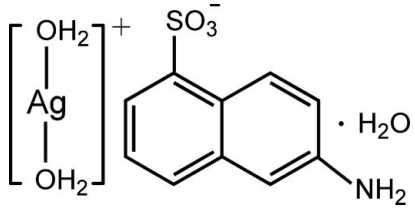
Received 24 June 2007; accepted 25 July 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.010 Å; R factor = 0.033; wR factor = 0.140; data-to-parameter ratio = 11.1.

The title compound, $[Ag(H_2O)_2](C_{10}H_8NO_3S)\cdot H_2O$, has a mononuclear structure in which the Ag^+ cation is coordinated by two O atoms from two water molecules. The 6-aminonaphthalene-1-sulfonate anion does not coordinate to the Ag^+ ion, but acts as a counter-ion. Intermolecular O—H···O and N—H···O hydrogen bonds link the ions and water molecules.

Related literature

The related 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 coordinated by one N atom from a pyridine molecule and one O atom from a water molecule, and the 2,5-dichloro-4-aminobenzenesulfonate anion is not coordinated to Ag (Shangguan *et al.*, 2007).



Experimental

Crystal data

$[Ag(H_2O)_2](C_{10}H_8NO_3S)\cdot H_2O$
M_r = 384.15
Monoclinic, $P2_1$
a = 8.8780 (11) Å
b = 9.0141 (11) Å
c = 9.5576 (12) Å
β = 116.989 (2)°
V = 681.57 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.65 mm^{-1}
T = 292 (2) K
0.25 × 0.23 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.652, T_{max} = 0.718
4251 measured reflections
2177 independent reflections
1740 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.141
S = 1.01
2177 reflections
196 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Absolute structure: Flack (1983), with 482 Friedel pairs
Flack parameter: −0.08 (6)

Table 1
Selected geometric parameters (Å, °).

Ag1—O1*W*	2.132 (7)	Ag1—O2*W*	2.139 (7)
O1*W*—Ag1—O2*W*	176.0 (6)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3*W*^{i}	0.87 (5)	2.12 (5)	2.980 (11)	170 (8)
O3*W*—H5*W*···O1	0.87 (5)	1.94 (5)	2.746 (12)	155 (8)
O3*W*—H6*W*···O2^{ii}	0.93 (4)	1.89 (5)	2.789 (9)	160 (7)
O2*W*—H3*W*···O1	0.83 (4)	2.43 (5)	3.169 (8)	150 (8)
O2*W*—H3*W*···O3	0.83 (4)	2.54 (7)	3.272 (13)	149 (9)
O2*W*—H4*W*···O3*W*^{iii}	0.87 (4)	2.35 (6)	3.177 (14)	159 (9)
O1*W*—H2*W*···O2^{iv}	0.86 (4)	2.48 (6)	3.286 (12)	155 (9)

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

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*.

The authors thank the JiLin Agriculture, Science and Technology College (China) for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2112).

References

Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Shangguan, S.-P., Li, Y.-J. & Wu, H. (2007). *Acta Cryst.* E**63**, m1680.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807036495

supplementary materials

Acta Cryst. (2007). E**63**, m2230 [**doi:10.1107/S1600536807036495**]

Diaquasilver(I) 6-aminonaphthalene-1-sulfonate monohydrate

Y.-J. Li, X.-W. Dong and H. Wu

Comment

The structure of the title compound, (I) (Fig. 1), containing three water molecules and a 6-amino-1-naphthalenesulfonate (*L*) anion, is described. In (I), two water molecules are coordinated to the metal, resulting in a slightly distorted linear coordination geometry for Ag (Table 1). Atoms Ag1, O1W, O2W are almost collinear; the angle O1W—Ag1—O2W is 176.0 (6)°. The Ag1—O1W and Ag1—O2W distances are 2.132 (7)Å and 2.139 (7) Å; the Ag—O_{water} distance is similar to the corresponding value in a related compound (Shangguan *et al.*, 2007). The 6-amino-1-naphthalenesulfonate anion does not coordinate to the Ag^+ ion, but acts as a counterion.

In (I), the coordination ability of the oxygen atoms of the water molecules is evidently stronger than that of the sulfonate group and the latter group does not coordinate to the Ag^+ ion. Adjacent ions and water molecules are interconnected by strong O—H···O and N—H···O hydrogen-bonding interactions (Table 2). Thus, the compound forms a three-dimensional supramolecular framework through extensive intermolecular hydrogen bonding (Fig. 2).

Experimental

An aqueous solution (10 ml) of 6-amino-1-naphthalenesulfonic acid (0.112 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. 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 over several days at room temperature.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H)= 1.2U_{eq}(C). The water H atoms were located in a difference Fourier map and refined isotropically [O—H = 0.83 (4)–0.93 (4) Å and U_{iso}(H) = 0.06 $Å^2$. The amino H atoms were located in a difference Fourier map and refined isotropically with the N—H distance restrained to 0.9 (5) Å and U_{iso}(H) = 0.06 $Å^2$.

Figures

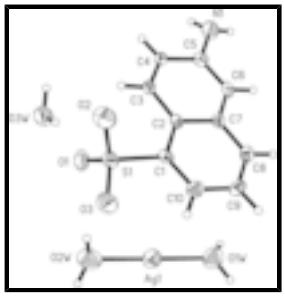


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

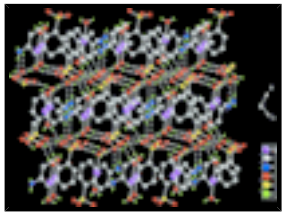


Fig. 2. Three-dimensional supramolecular framework of (I), formed through hydrogen-bonding (dashed lines) interactions. H atoms not involved in hydrogen bonding have been omitted.

Diaquasilver(I) 6-aminonaphthalene-1-sulfonate monohydrate

Crystal data

$[Ag(H_2O)_2](C_{10}H_8NO_3S)\cdot H_2O$	$F_{000} = 384$
$M_r = 384.15$	$D_x = 1.872$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 2177 reflections
$a = 8.8780$ (11) Å	$\theta = 2.4$–$28.3°$
$b = 9.0141$ (11) Å	$\mu = 1.65$ mm^{-1}
$c = 9.5576$ (12) Å	$T = 292$ (2) K
$\beta = 116.989$ (2)°	Block, white
$V = 681.57$ (15) Å^3	0.25 × 0.23 × 0.20 mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD diffractometer	2177 independent reflections
Radiation source: fine-focus sealed tube	1740 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$
$T = 292(2)$ K	$\theta_{max} = 28.3°$
φ and ω scans	$\theta_{min} = 2.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.652$, $T_{max} = 0.718$	$k = -11 \rightarrow 6$
4251 measured reflections	$l = -12 \rightarrow 12$

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
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0984P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.141$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
2177 reflections	$\Delta\rho_{min} = -0.44$ e Å^{-3}
196 parameters	Extinction correction: none
14 restraints	Absolute structure: Flack (1983), with 482 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.08 (6)
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 $F^2 > 2$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	0.80067 (8)	0.46498 (10)	0.74795 (7)	0.0652 (3)
C1	0.5086 (7)	0.3207 (8)	0.3324 (7)	0.0294 (12)
C2	0.3669 (7)	0.4157 (7)	0.2499 (7)	0.0281 (12)
C3	0.3425 (7)	0.5079 (7)	0.1217 (7)	0.0313 (14)
H3	0.4227	0.5065	0.0844	0.038*
C4	0.2089 (7)	0.5968 (8)	0.0524 (7)	0.0327 (13)
H4	0.2003	0.6571	−0.0299	0.039*
C5	0.0779 (8)	0.6023 (8)	0.1009 (8)	0.0358 (14)
C6	0.0952 (8)	0.5125 (8)	0.2234 (7)	0.0366 (14)
H6	0.0127	0.5150	0.2579	0.044*
C7	0.2355 (8)	0.4159 (8)	0.2989 (7)	0.0325 (13)
C8	0.2550 (8)	0.3263 (9)	0.4263 (8)	0.0395 (15)
H8	0.1729	0.3289	0.4613	0.047*
C9	0.3937 (10)	0.2342 (9)	0.5009 (9)	0.0461 (18)

H9	0.4022	0.1719	0.5817	0.055*
C10	0.5212 (11)	0.2362 (9)	0.4525 (9)	0.0454 (17)
H10	0.6167	0.1774	0.5051	0.055*
N1	−0.0621 (9)	0.6922 (10)	0.0216 (10)	0.063 (2)
O1	0.7407 (6)	0.4647 (11)	0.2927 (7)	0.0617 (14)
O2	0.5950 (8)	0.2620 (10)	0.1133 (7)	0.075 (2)
O1W	0.6141 (10)	0.4549 (14)	0.8300 (9)	0.0801 (18)
O3	0.8013 (7)	0.2118 (8)	0.3828 (8)	0.0615 (16)
O2W	0.9824 (9)	0.4600 (17)	0.6590 (8)	0.086 (2)
O3W	0.7058 (8)	0.7430 (8)	0.1647 (9)	0.0691 (18)
S1	0.6754 (2)	0.3129 (2)	0.2756 (2)	0.0403 (4)
H1A	−0.137 (9)	0.713 (10)	0.053 (10)	0.060*
H1W	0.543 (9)	0.530 (8)	0.825 (9)	0.060*
H2A	−0.050 (11)	0.783 (7)	−0.014 (12)	0.060*
H2W	0.632 (12)	0.426 (9)	0.922 (7)	0.060*
H3W	0.935 (9)	0.428 (10)	0.568 (6)	0.060*
H4W	1.082 (7)	0.423 (10)	0.718 (8)	0.060*
H5W	0.696 (11)	0.649 (6)	0.176 (10)	0.060*
H6W	0.616 (8)	0.770 (9)	0.069 (7)	0.060*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0660 (4)	0.0669 (4)	0.0606 (4)	−0.0042 (4)	0.0267 (3)	0.0046 (4)
C1	0.025 (3)	0.028 (3)	0.031 (3)	0.006 (3)	0.010 (2)	−0.004 (3)
C2	0.025 (3)	0.025 (3)	0.033 (3)	−0.006 (2)	0.012 (2)	−0.006 (2)
C3	0.028 (3)	0.036 (4)	0.031 (3)	−0.006 (2)	0.014 (2)	−0.004 (2)
C4	0.032 (3)	0.035 (3)	0.031 (3)	−0.004 (3)	0.014 (2)	0.000 (3)
C5	0.034 (3)	0.034 (3)	0.038 (3)	0.005 (3)	0.016 (3)	−0.005 (3)
C6	0.029 (3)	0.039 (4)	0.047 (3)	−0.008 (2)	0.021 (3)	−0.005 (3)
C7	0.032 (3)	0.034 (3)	0.032 (3)	−0.004 (2)	0.015 (2)	−0.005 (2)
C8	0.039 (3)	0.042 (4)	0.043 (3)	−0.002 (3)	0.024 (3)	−0.002 (3)
C9	0.053 (4)	0.039 (4)	0.043 (4)	0.001 (3)	0.020 (4)	0.016 (3)
C10	0.050 (4)	0.041 (4)	0.040 (4)	−0.004 (3)	0.015 (3)	0.004 (3)
N1	0.046 (4)	0.069 (5)	0.074 (5)	0.020 (4)	0.028 (4)	0.026 (4)
O1	0.049 (3)	0.072 (4)	0.077 (3)	−0.001 (5)	0.039 (2)	0.016 (5)
O2	0.055 (3)	0.123 (7)	0.054 (3)	0.019 (4)	0.032 (3)	−0.027 (4)
O1W	0.087 (4)	0.070 (5)	0.086 (4)	0.004 (6)	0.042 (4)	0.014 (6)
O3	0.049 (3)	0.067 (4)	0.070 (4)	0.021 (3)	0.028 (3)	0.007 (3)
O2W	0.075 (4)	0.112 (6)	0.057 (3)	0.004 (7)	0.017 (3)	−0.018 (7)
O3W	0.059 (4)	0.063 (4)	0.082 (5)	0.011 (3)	0.028 (3)	0.023 (4)
S1	0.0333 (7)	0.0476 (10)	0.0434 (8)	0.0096 (7)	0.0204 (7)	−0.0016 (8)

Geometric parameters (Å, °)

Ag1—O1W	2.132 (7)	C8—C9	1.384 (11)
Ag1—O2W	2.139 (7)	C8—H8	0.930
C1—C10	1.340 (10)	C9—C10	1.404 (11)
C1—C2	1.427 (8)	C9—H9	0.930

C1—S1	1.795 (6)	C10—H10	0.930
C2—C3	1.413 (8)	N1—H1A	0.87 (5)
C2—C7	1.442 (8)	N1—H2A	0.92 (5)
C3—C4	1.332 (9)	O1—S1	1.466 (10)
C3—H3	0.930	O2—S1	1.456 (6)
C4—C5	1.436 (9)	O1W—H1W	0.91 (4)
C4—H4	0.930	O1W—H2W	0.86 (4)
C5—C6	1.373 (10)	O3—S1	1.446 (6)
C5—N1	1.386 (10)	O2W—H3W	0.83 (4)
C6—C7	1.419 (10)	O2W—H4W	0.87 (4)
C6—H6	0.930	O3W—H5W	0.87 (5)
C7—C8	1.404 (10)	O3W—H6W	0.93 (4)
O1W—Ag1—O2W	176.0 (6)	C7—C8—H8	119.3
C10—C1—C2	121.6 (6)	C8—C9—C10	119.0 (7)
C10—C1—S1	118.5 (5)	C8—C9—H9	120.5
C2—C1—S1	119.8 (5)	C10—C9—H9	120.5
C3—C2—C1	125.6 (5)	C1—C10—C9	121.5 (8)
C3—C2—C7	116.9 (5)	C1—C10—H10	119.2
C1—C2—C7	117.5 (5)	C9—C10—H10	119.2
C4—C3—C2	122.5 (5)	C5—N1—H1A	125 (6)
C4—C3—H3	118.7	C5—N1—H2A	120 (6)
C2—C3—H3	118.7	H1A—N1—H2A	100 (6)
C3—C4—C5	121.9 (6)	Ag1—O1W—H1W	126 (4)
C3—C4—H4	119.1	Ag1—O1W—H2W	125 (6)
C5—C4—H4	119.1	H1W—O1W—H2W	95 (5)
C6—C5—N1	122.5 (6)	Ag1—O2W—H3W	108 (6)
C6—C5—C4	117.5 (6)	Ag1—O2W—H4W	119 (6)
N1—C5—C4	120.0 (7)	H3W—O2W—H4W	116 (7)
C5—C6—C7	121.9 (6)	H5W—O3W—H6W	107 (6)
C5—C6—H6	119.1	O3—S1—O2	113.8 (4)
C7—C6—H6	119.1	O3—S1—O1	111.7 (4)
C8—C7—C6	121.9 (6)	O2—S1—O1	113.0 (4)
C8—C7—C2	118.8 (6)	O3—S1—C1	106.8 (3)
C6—C7—C2	119.2 (6)	O2—S1—C1	105.1 (3)
C9—C8—C7	121.5 (6)	O1—S1—C1	105.6 (3)
C9—C8—H8	119.3		
C10—C1—C2—C3	−179.7 (6)	C3—C2—C7—C6	−3.3 (8)
S1—C1—C2—C3	0.4 (8)	C1—C2—C7—C6	177.9 (6)
C10—C1—C2—C7	−1.0 (9)	C6—C7—C8—C9	−178.9 (7)
S1—C1—C2—C7	179.1 (4)	C2—C7—C8—C9	−2.6 (10)
C1—C2—C3—C4	−178.3 (6)	C7—C8—C9—C10	3.1 (11)
C7—C2—C3—C4	3.0 (8)	C2—C1—C10—C9	1.5 (11)
C2—C3—C4—C5	−1.6 (10)	S1—C1—C10—C9	−178.5 (6)
C3—C4—C5—C6	0.4 (10)	C8—C9—C10—C1	−2.6 (12)
C3—C4—C5—N1	−177.5 (7)	C10—C1—S1—O3	−1.7 (7)
N1—C5—C6—C7	177.1 (8)	C2—C1—S1—O3	178.3 (5)
C4—C5—C6—C7	−0.8 (10)	C10—C1—S1—O2	119.6 (6)
C5—C6—C7—C8	178.7 (6)	C2—C1—S1—O2	−60.5 (6)

C5—C6—C7—C2	2.3 (10)	C10—C1—S1—O1	−120.7 (6)
C3—C2—C7—C8	−179.7 (6)	C2—C1—S1—O1	59.3 (6)
C1—C2—C7—C8	1.5 (9)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O3W^{i}	0.87 (5)	2.12 (5)	2.980 (11)	170 (8)
O3W—H5W···O1	0.87 (5)	1.94 (5)	2.746 (12)	155 (8)
O3W—H6W···O2^{ii}	0.93 (4)	1.89 (5)	2.789 (9)	160 (7)
O2W—H3W···O1	0.83 (4)	2.43 (5)	3.169 (8)	150 (8)
O2W—H3W···O3	0.83 (4)	2.54 (7)	3.272 (13)	149 (9)
O2W—H4W···O3W^{iii}	0.87 (4)	2.35 (6)	3.177 (14)	159 (9)
O1W—H2W···O2^{iv}	0.86 (4)	2.48 (6)	3.286 (12)	155 (9)

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

Fig. 1

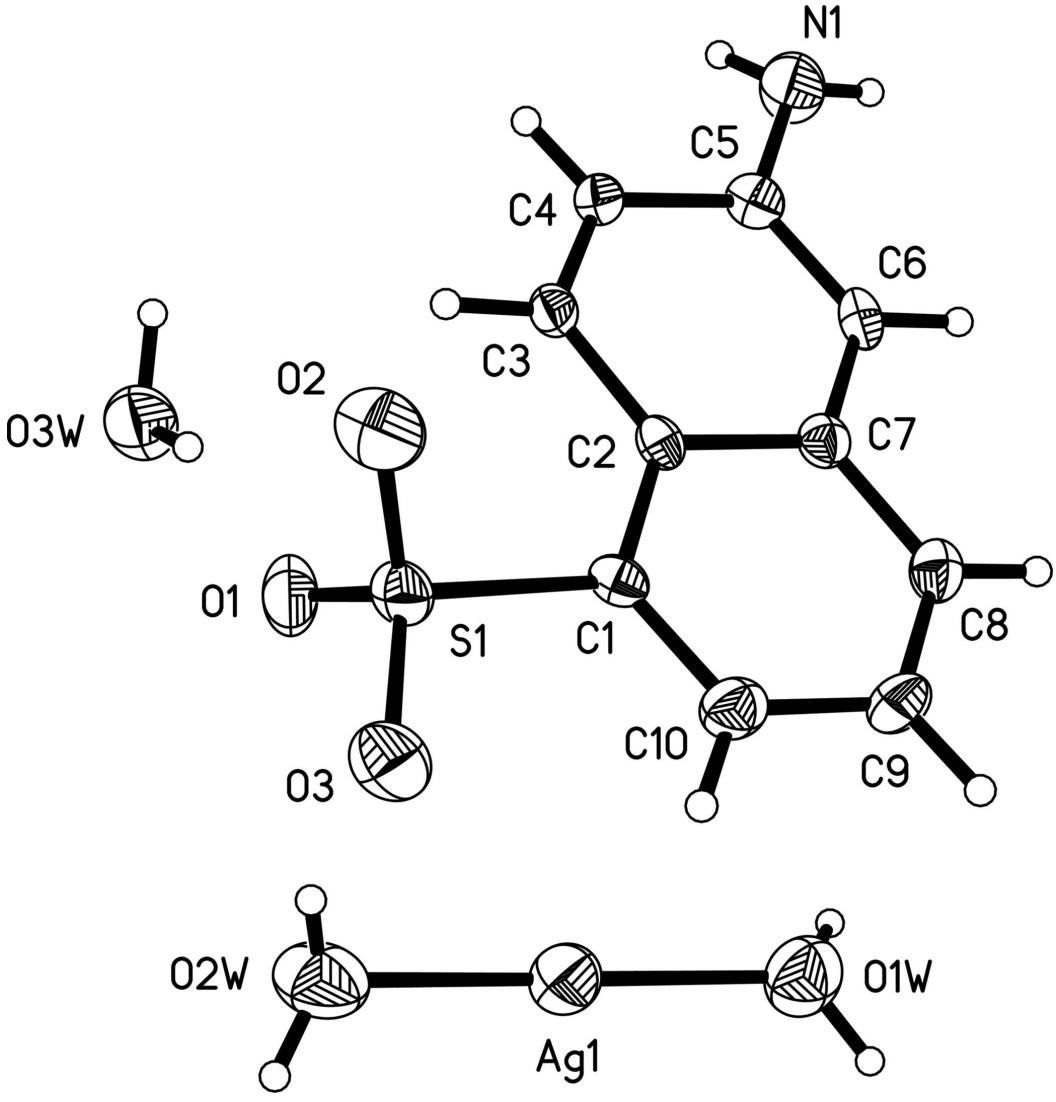


Fig. 2