Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2-Amino-4,5-dimethylbenzenesulfonato-κ*N*)aquasilver(I) monohydrate

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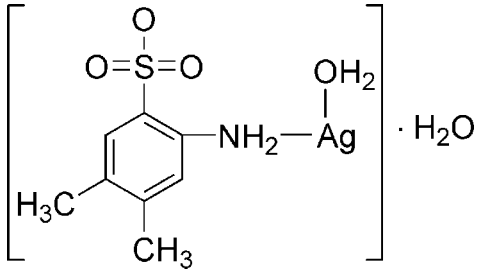
Received 25 September 2007; accepted 29 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.087; data-to-parameter ratio = 15.3.

The title compound, $[Ag(C_8H_{10}NO_3S)(H_2O)]\cdot H_2O$, has a mononuclear structure in which the Ag^+ cation is two-coordinated by one N atom from a 2-amino-4,5-dimethylbenzenesulfonate anion and one water O atom in a nearly linear arrangement. A network of O—H···O and N—H···O hydrogen bonds helps to consolidate the crystal packing.

Related literature

For a related structure, see: Han & Li (2007).



Experimental

Crystal data

$[Ag(C_8H_{10}NO_3S)(H_2O)]\cdot H_2O$
M_r = 344.13
Triclinic, $P\overline{1}$
a = 6.555 (5) Å
b = 7.626 (6) Å
c = 12.1290 (11) Å
α = 78.889 (4)°
β = 85.746 (7)°
γ = 87.754 (4)°
V = 593.1 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.88 mm^{-1}
T = 293 (2) K
0.25 × 0.23 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.625, T_{max} = 0.677
4856 measured reflections
2584 independent reflections
2277 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.087
S = 1.14
2584 reflections
169 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—O1*W*	2.139 (3)	Ag1—N1	2.176 (3)
O1*W*—Ag1—N1	166.73 (10)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*A*···O1^{i}	0.95 (4)	2.11 (4)	3.038 (4)	165 (4)
O1*W*—H1*B*···O3^{ii}	1.00 (4)	2.11 (4)	3.091 (4)	167 (4)
O2*W*—H2*A*···O2^{iii}	0.94 (4)	2.12 (6)	2.901 (5)	140 (6)
N1—H3*A*···O3	0.86 (7)	2.15 (7)	2.843 (3)	138 (7)
N1—H3*A*···O3^{iv}	0.86 (7)	2.38 (8)	3.073 (3)	138 (7)
N1—H3*B*···O2^{v}	0.80 (3)	2.18 (3)	2.961 (4)	165 (4)

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

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*.

The authors thank JiLin Agricultural Science and Technology College, China, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2561).

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supplementary materials

Acta Cryst. (2007). E**63**, m2695 [**doi:10.1107/S1600536807047897**]

(2-Amino-4,5-dimethylbenzenesulfonato-*κN*)aquasilver(I) monohydrate

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

Comment

In the title compound, (I), one water molecule and one 2-amino-4,5-dimethylbenzenesulfonate (*L*) anion are coordinated to the metal, restulting in slightly distorted linear geometry for Ag (Table 1). The Ag—O_{water} distance is simiar to the equivalent value in a related compound (Han & Li, 2007).

Here, the coordination ability of the amine group of *L* is evidently stronger than that of sulfonate group and the latter group does not coordinate to the Ag ion. In the crystal of (I), adjacent ions and water molecules are interconnected by strong O—H···O and N—H···O hydrogen bonds (Table 2) to form a two-dimensional supramolecular network (Fig. 2).

Experimental

An aqueous solution (10 ml) of 2-amino-4,5-dimethylbenzenesulfonic acid (0.5 mmol) was added to solid Ag_2CO_3 (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*). Then a methanolic solution of pyridine was added and the mixture stirred for 30 minutes. Crystals of (I) were obtained by evaporation of the solution for several days at room temperature, but the pyridine did not react with silver sulfonate.

Refinement

The H atoms bonded to O were located in a difference map and were freely refined. The H atoms bonded to N were located in a difference map and their positions refined freely, with U_{iso}(H) = 1.5U_{eq}(N). The H atoms bonded to C atom were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

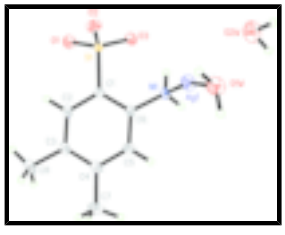

Fig. 1. The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

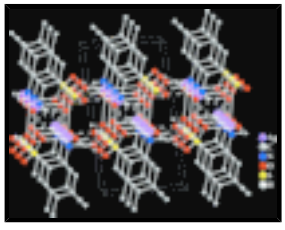

Fig. 2. Two-dimensional supramolecular framework of (I), formed through hydrogen-bonding (dashed lines) interactions. The H atoms not involved in hydrogen bonding have been omitted for clarity.

(2-Amino-4,5-dimethylbenzenesulfonato-κ*N*)aquasilver(I) monohydrate

Crystal data

$[Ag(C_8H_{10}NO_3S)(H_2O)]\cdot H_2O$	$Z = 2$
$M_r = 344.13$	$F_{000} = 344$
Triclinic, $P\overline{1}$	$D_x = 1.927$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.555$ (5) Å	Cell parameters from 2584 reflections
$b = 7.626$ (6) Å	$\theta = 1.7$–27.5º
$c = 12.1290$ (11) Å	$\mu = 1.88$ mm^{-1}
$\alpha = 78.889$ (4)º	$T = 293$ (2) K
$\beta = 85.746$ (7)º	Block, colourless
$\gamma = 87.754$ (4)º	0.25 × 0.23 × 0.21 mm
$V = 593.1$ (7) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	2584 independent reflections
Radiation source: fine-focus sealed tube	2277 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 292(2)$ K	$\theta_{min} = 1.7$º
ω scans	$h = -8\rightarrow8$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -9\rightarrow8$
$T_{min} = 0.625$, $T_{max} = 0.677$	$l = -15\rightarrow15$
4856 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.087$	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.0536P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{max} = 0.001$
2584 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
169 parameters	$\Delta\rho_{min} = -0.72$ e Å^{-3}
7 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	0.33890 (4)	0.48750 (3)	0.39012 (2)	0.04069 (11)
C1	0.6290 (4)	0.1518 (3)	0.2095 (2)	0.0240 (5)
C2	0.7019 (4)	0.1533 (4)	0.0981 (2)	0.0295 (5)
H2	0.8337	0.1096	0.0841	0.035*
C3	0.5843 (5)	0.2179 (4)	0.0075 (2)	0.0303 (6)
C4	0.3854 (5)	0.2816 (4)	0.0293 (2)	0.0310 (6)
C5	0.3130 (4)	0.2813 (4)	0.1399 (2)	0.0287 (5)
H5	0.1810	0.3248	0.1538	0.034*
C6	0.4314 (4)	0.2180 (3)	0.2310 (2)	0.0230 (5)
C7	0.2479 (6)	0.3485 (5)	−0.0654 (3)	0.0456 (8)
H7A	0.3104	0.4471	−0.1163	0.068*
H7B	0.1182	0.3869	−0.0350	0.068*
H7C	0.2279	0.2539	−0.1052	0.068*
C8	0.6710 (6)	0.2165 (5)	−0.1103 (3)	0.0431 (7)
H8A	0.5863	0.1468	−0.1457	0.065*
H8B	0.8070	0.1651	−0.1083	0.065*
H8C	0.6751	0.3367	−0.1525	0.065*
N1	0.3465 (4)	0.2264 (3)	0.3425 (2)	0.0255 (4)
O1	0.9374 (4)	−0.0551 (3)	0.2715 (2)	0.0460 (6)
O2	0.8951 (3)	0.2202 (3)	0.3429 (2)	0.0406 (5)
O3	0.6674 (3)	−0.0227 (3)	0.41254 (19)	0.0393 (5)
O1W	0.2817 (5)	0.7591 (4)	0.4077 (3)	0.0538 (6)
O2W	0.2412 (6)	0.4253 (4)	0.6255 (3)	0.0702 (9)
S1	0.79500 (9)	0.06607 (9)	0.31726 (6)	0.02624 (15)
H1A	0.194 (7)	0.829 (6)	0.357 (4)	0.078 (16)*
H2A	0.210 (10)	0.511 (8)	0.671 (5)	0.12 (2)*
H1B	0.405 (6)	0.836 (6)	0.396 (4)	0.071 (15)*
H2B	0.106 (6)	0.420 (8)	0.621 (5)	0.078 (17)*
H3A	0.407 (11)	0.159 (10)	0.396 (6)	0.039*
H3B	0.227 (5)	0.205 (5)	0.348 (3)	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.05284 (18)	0.03144 (15)	0.04011 (16)	0.00482 (10)	−0.00194 (11)	−0.01421 (10)
C1	0.0262 (12)	0.0232 (12)	0.0226 (12)	−0.0011 (9)	0.0000 (9)	−0.0046 (9)
C2	0.0320 (13)	0.0297 (14)	0.0270 (14)	−0.0025 (11)	0.0060 (10)	−0.0089 (11)
C3	0.0414 (14)	0.0280 (13)	0.0216 (13)	−0.0058 (11)	0.0030 (10)	−0.0059 (10)
C4	0.0409 (14)	0.0280 (14)	0.0248 (14)	−0.0040 (11)	−0.0044 (11)	−0.0050 (11)
C5	0.0302 (12)	0.0260 (13)	0.0309 (14)	0.0009 (10)	−0.0028 (10)	−0.0079 (11)
C6	0.0268 (12)	0.0207 (11)	0.0222 (12)	−0.0027 (9)	0.0014 (9)	−0.0062 (9)
C7	0.057 (2)	0.0457 (19)	0.0351 (17)	0.0030 (15)	−0.0166 (14)	−0.0061 (14)
C8	0.0564 (19)	0.0478 (19)	0.0258 (15)	−0.0063 (15)	0.0060 (13)	−0.0110 (13)
N1	0.0254 (11)	0.0266 (11)	0.0241 (11)	0.0005 (9)	0.0039 (8)	−0.0063 (9)
O1	0.0447 (12)	0.0547 (14)	0.0387 (13)	0.0253 (11)	−0.0037 (10)	−0.0145 (11)
O2	0.0352 (10)	0.0441 (13)	0.0458 (13)	−0.0060 (9)	−0.0077 (9)	−0.0136 (10)
O3	0.0368 (11)	0.0471 (13)	0.0278 (11)	−0.0036 (9)	0.0009 (8)	0.0076 (9)
O1W	0.0664 (17)	0.0416 (14)	0.0564 (17)	0.0055 (13)	−0.0097 (13)	−0.0164 (12)
O2W	0.081 (2)	0.0529 (18)	0.072 (2)	0.0036 (16)	0.0116 (17)	−0.0081 (16)
S1	0.0232 (3)	0.0301 (3)	0.0250 (3)	0.0029 (2)	0.0003 (2)	−0.0057 (3)

Geometric parameters (Å, °)

Ag1—O1W	2.139 (3)	C7—H7B	0.9600
Ag1—N1	2.176 (3)	C7—H7C	0.9600
C1—C2	1.397 (4)	C8—H8A	0.9600
C1—C6	1.397 (4)	C8—H8B	0.9600
C1—S1	1.774 (3)	C8—H8C	0.9600
C2—C3	1.390 (4)	N1—H3B	0.80 (3)
C2—H2	0.9300	N1—H3A	0.86 (7)
C3—C4	1.398 (4)	O1—S1	1.445 (2)
C3—C8	1.500 (4)	O2—S1	1.462 (2)
C4—C5	1.390 (4)	O3—S1	1.447 (2)
C4—C7	1.511 (4)	O1W—H1B	1.00 (4)
C5—C6	1.395 (4)	O1W—H1A	0.95 (4)
C5—H5	0.9300	O2W—H2B	0.89 (4)
C6—N1	1.436 (3)	O2W—H2A	0.94 (4)
C7—H7A	0.9600		
O1W—Ag1—N1	166.73 (10)	H7B—C7—H7C	109.5
C2—C1—C6	119.1 (2)	C3—C8—H8A	109.5
C2—C1—S1	117.8 (2)	C3—C8—H8B	109.5
C6—C1—S1	123.1 (2)	H8A—C8—H8B	109.5
C3—C2—C1	122.4 (3)	C3—C8—H8C	109.5
C3—C2—H2	118.8	H8A—C8—H8C	109.5
C1—C2—H2	118.8	H8B—C8—H8C	109.5
C2—C3—C4	118.5 (3)	C6—N1—Ag1	116.43 (17)
C2—C3—C8	120.0 (3)	C6—N1—H3B	110 (3)
C4—C3—C8	121.5 (3)	Ag1—N1—H3B	101 (3)

C5—C4—C3	119.2 (3)	C6—N1—H3A	115 (5)
C5—C4—C7	119.8 (3)	Ag1—N1—H3A	103 (5)
C3—C4—C7	121.0 (3)	H3B—N1—H3A	110 (6)
C4—C5—C6	122.3 (3)	Ag1—O1W—H1B	115 (3)
C4—C5—H5	118.8	Ag1—O1W—H1A	117 (3)
C6—C5—H5	118.8	H1B—O1W—H1A	101 (4)
C5—C6—C1	118.5 (2)	H2B—O2W—H2A	86 (4)
C5—C6—N1	118.7 (2)	O1—S1—O3	112.80 (15)
C1—C6—N1	122.8 (2)	O1—S1—O2	112.65 (16)
C4—C7—H7A	109.5	O3—S1—O2	111.73 (14)
C4—C7—H7B	109.5	O1—S1—C1	106.17 (13)
H7A—C7—H7B	109.5	O3—S1—C1	106.57 (13)
C4—C7—H7C	109.5	O2—S1—C1	106.35 (14)
H7A—C7—H7C	109.5		
C6—C1—C2—C3	−0.2 (4)	S1—C1—C6—C5	−179.6 (2)
S1—C1—C2—C3	−179.9 (2)	C2—C1—C6—N1	−178.1 (2)
C1—C2—C3—C4	−0.7 (4)	S1—C1—C6—N1	1.5 (4)
C1—C2—C3—C8	179.9 (3)	C5—C6—N1—Ag1	−76.6 (3)
C2—C3—C4—C5	1.1 (4)	C1—C6—N1—Ag1	102.3 (3)
C8—C3—C4—C5	−179.5 (3)	O1W—Ag1—N1—C6	66.5 (5)
C2—C3—C4—C7	−178.2 (3)	C2—C1—S1—O1	−24.8 (3)
C8—C3—C4—C7	1.2 (4)	C6—C1—S1—O1	155.5 (2)
C3—C4—C5—C6	−0.6 (4)	C2—C1—S1—O3	−145.3 (2)
C7—C4—C5—C6	178.7 (3)	C6—C1—S1—O3	35.1 (3)
C4—C5—C6—C1	−0.4 (4)	C2—C1—S1—O2	95.4 (2)
C4—C5—C6—N1	178.5 (2)	C6—C1—S1—O2	−84.3 (2)
C2—C1—C6—C5	0.8 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O1^{i}	0.95 (4)	2.11 (4)	3.038 (4)	165 (4)
O1W—H1B···O3^{ii}	1.00 (4)	2.11 (4)	3.091 (4)	167 (4)
O2W—H2A···O2^{iii}	0.94 (4)	2.12 (6)	2.901 (5)	140 (6)
N1—H3A···O3	0.86 (7)	2.15 (7)	2.843 (3)	138 (7)
N1—H3A···O3^{iv}	0.86 (7)	2.38 (8)	3.073 (3)	138 (7)
N1—H3B···O2^{v}	0.80 (3)	2.18 (3)	2.961 (4)	165 (4)

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

Fig. 1

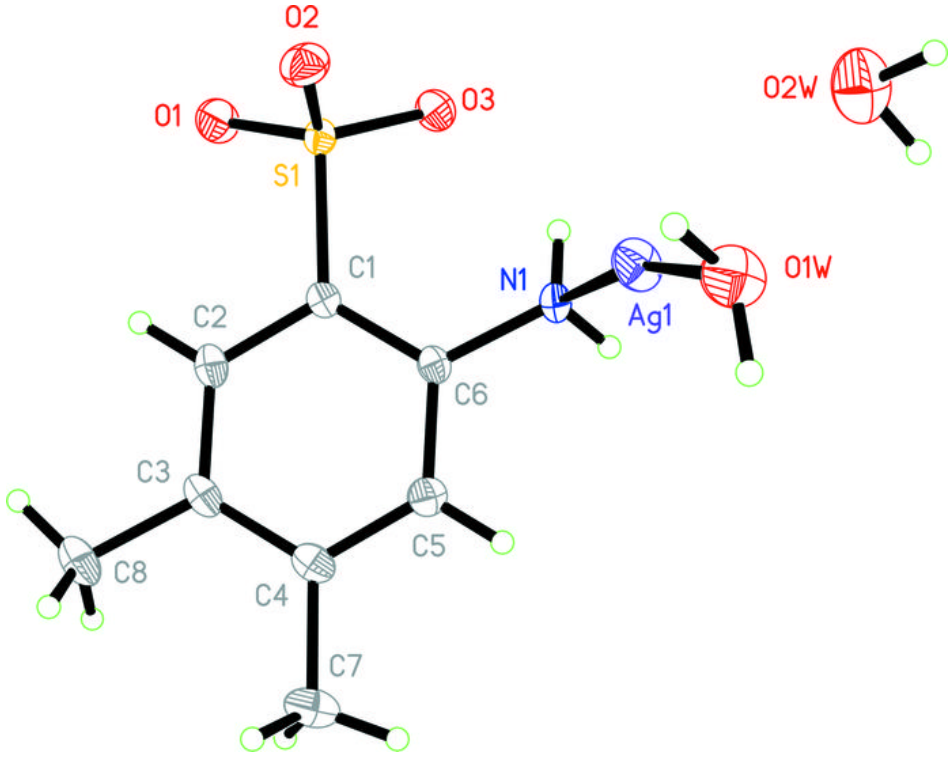

Fig. 2