Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Di-μ-aqua-bis[(2-amino-4,5-dimethylbenzenesulfonato-κN)aquasilver(I)]

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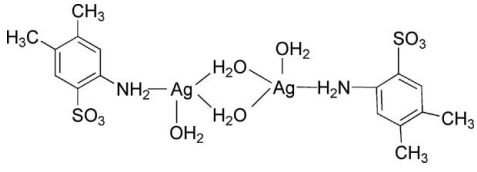
Received 23 October 2007; accepted 29 October 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.074; data-to-parameter ratio = 16.6.

In the title compound, $[Ag_2(C_8H_{10}NO_3S)_2(H_2O)_4]$, each Ag^I atom is coordinated by three water molecules and one N atom from a 2-amino-4,5-dimethylbenzenesulfonate ligand in a severely distorted tetrahedral geometry. The two Ag^I atoms are bridged by two water molecules, forming a centrosymmetric binuclear complex. The distance of 3.615 (9) Å between the two Ag^I atoms suggests that there are no Ag···Ag interaction within the binuclear molecule.

Related literature

The related compound, $[Ag(C_8H_{10}NO_3S)(H_2O)_2]$, has a mononuclear structure (Li *et al.*, 2007).



Experimental

Crystal data

$[Ag_2(C_8H_{10}NO_3S)_2(H_2O)_4]$
M_r = 688.26
Monoclinic, $P2_1/c$
a = 12.5391 (11) Å
b = 8.7406 (7) Å
c = 11.3861 (10) Å
β = 106.319 (1)°
V = 1197.63 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 292 (2) K
0.35 × 0.25 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.515, T_{max} = 0.715
7202 measured reflections
2822 independent reflections
2077 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.074
S = 0.92
2822 reflections
170 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—O2*W*	2.186 (3)	Ag1—O1*W*	2.645 (3)
Ag1—N1	2.273 (2)	Ag1—O1*W*^{i}	2.651 (4)
O2*W*—Ag1—N1	160.00 (9)	O1*W*—Ag1—N1	88.69 (8)
O1*W*—Ag1—O1*W*^{i}	93.92 (8)	O2*W*—Ag1—O1*W*^{i}	92.74 (8)
O1*W*—Ag1—O2*W*	110.79 (9)	N1—Ag1—O1*W*^{i}	90.30 (8)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*A*···O2^{ii}	0.84 (3)	2.02 (3)	2.830 (3)	161 (3)
O1*W*—H1*B*···O3^{iii}	0.76 (3)	2.12 (3)	2.874 (3)	169 (4)
O2*W*—H2*A*···O1^{iii}	0.98 (4)	2.14 (4)	3.022 (3)	148 (4)
O2*W*—H2*B*···O3^{iv}	0.92 (3)	2.28 (3)	3.154 (3)	159 (3)
N1—H1*N*···O2^{ii}	0.81 (3)	2.40 (3)	3.154 (3)	156 (4)
N1—H2*N*···O1^{v}	0.95 (3)	2.12 (3)	3.065 (3)	172 (2)

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

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*.

We 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: HY2095).

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.
Li, Y.-J., Li, S.-H. & Dong, X.-W. (2007). *Acta Cryst.* E**63**, m2695.
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/S1600536807053950

supplementary materials

Acta Cryst. (2007). E**63**, m2910 [**doi:10.1107/S1600536807053950**]

Di-μ-aqua-bis[(2-amino-4,5-dimethylbenzenesulfonato-κN)aquasilver(I)]

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

Comment

The title compound shows a binuclear structure (Fig. 1). Each Ag^{I} atom is coordinated by three water molecules with Ag—O_{bridge} distance larger than that of Ag—$O_{terminal}$ (Table 1), but both in the range of normal Ag—O distance. The Ag^{I} atom has a seriously distorted tetrahedral coodination geometry. The two Ag^{I} atoms are bridged by two water molecules, forming a binuclear structure. The Ag···Ag distance is 3.615 (9) Å, indicating no metal–metal interaction within the binuclear molecule. The molecular geometry of the title compound has been changed largely when compared with a related compound (Li *et al.*, 2007). Adjacent molecules are connected by O—H···O and N—H···O hydrogen bonds (Table2), forming a two-dimensional supramolecular structure (Fig.2).

Experimental

An aqueous solution (10 ml) of 2-amino-4,5-dimethylbenzenesulfonic acid (0.101 g, 0.5 mmol) was added to solid Ag_2CO_3 (0.069 g, 0.25 mmol) with stirring 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 solution of β-picoline (0.039 g, 0.5 mmol) in CH_3OH (8 ml) was added with stirring for 30 min. Crystals of the title compound were obtained by evaporation of the solution for several days at room temperature. β-Picoline did not react with the silversulfonate.

Refinement

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, and C—H = 0.96Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl groups. H atoms bonded to N atom and water molecules were located in a difference map and refined isotropically.

Figures

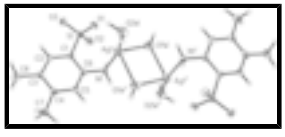


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) −*x*, 1 − *y*, 1 − *z*.]

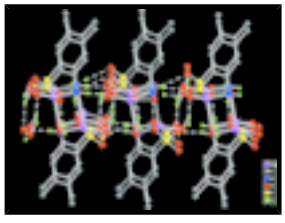


Fig. 2. Two-dimensional supramolecular structure of the title compound, formed through hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonds have been omitted.

Di-μ-aqua-bis[(2-amino-4,5-dimethylbenzenesulfonato-κ*N*)aquasilver(I)]

Crystal data

$[Ag_2(C_8H_{10}NO_3S)_2(H_2O)_4]$	$F_{000} = 688$
$M_r = 688.26$	$D_x = 1.909$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2822 reflections
$a = 12.5391$ (11) Å	$\theta = 1.7$–28.3º
$b = 8.7406$ (7) Å	$\mu = 1.86$ mm^{-1}
$c = 11.3861$ (10) Å	$T = 292$ (2) K
$\beta = 106.319$ (1)º	Plate, colorless
$V = 1197.63$ (18) Å^3	0.35 × 0.25 × 0.18 mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD diffractometer	2822 independent reflections
Radiation source: fine-focus sealed tube	2077 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.063$
$T = 292$(2) K	$\theta_{max} = 28.3$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan SADABS (Sheldrick, 1996)	$h = -14 \rightarrow 16$
$T_{min} = 0.515$, $T_{max} = 0.715$	$k = -10 \rightarrow 11$
7202 measured reflections	$l = -13 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.074$	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.92$	$(\Delta/\sigma)_{max} < 0.001$
2822 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
170 parameters	$\Delta\rho_{min} = -0.55$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.09929 (2)	0.40908 (3)	0.62723 (2)	0.05391 (11)
C1	0.27697 (19)	0.0783 (3)	0.6403 (2)	0.0286 (5)
C2	0.3878 (2)	0.0391 (3)	0.6914 (2)	0.0336 (6)
H2	0.4056	−0.0315	0.7551	0.040*
C3	0.4731 (2)	0.1015 (3)	0.6508 (3)	0.0358 (6)
C4	0.4451 (2)	0.2062 (3)	0.5542 (2)	0.0345 (6)
C5	0.3339 (2)	0.2459 (3)	0.5042 (2)	0.0341 (6)
H5	0.3158	0.3166	0.4406	0.041*
C6	0.24956 (19)	0.1846 (3)	0.5454 (2)	0.0285 (5)
C7	0.5317 (2)	0.2733 (4)	0.5006 (3)	0.0453 (7)
H7A	0.4973	0.3451	0.4375	0.068*
H7B	0.5659	0.1930	0.4665	0.068*
H7C	0.5872	0.3247	0.5637	0.068*
C8	0.5921 (2)	0.0541 (4)	0.7108 (3)	0.0501 (8)
H8A	0.6243	0.0148	0.6497	0.075*
H8B	0.5935	−0.0236	0.7707	0.075*
H8C	0.6339	0.1412	0.7498	0.075*
N1	0.13838 (19)	0.2376 (3)	0.4950 (2)	0.0345 (5)
O1	0.12030 (16)	0.1204 (2)	0.74406 (18)	0.0406 (4)
O2	0.09741 (15)	−0.0815 (2)	0.59466 (19)	0.0458 (5)
O3	0.22979 (15)	−0.1105 (2)	0.79442 (19)	0.0477 (5)
O1W	−0.1147 (2)	0.3633 (3)	0.5210 (2)	0.0572 (6)
O2W	0.1232 (2)	0.5614 (3)	0.7848 (2)	0.0672 (7)
S1	0.17342 (5)	−0.00523 (7)	0.69825 (6)	0.02996 (15)
H1N	0.088 (3)	0.177 (4)	0.486 (3)	0.076 (13)*
H1A	−0.125 (2)	0.278 (3)	0.486 (3)	0.047 (9)*
H1B	−0.152 (3)	0.364 (4)	0.564 (3)	0.063 (12)*
H2N	0.128 (2)	0.287 (3)	0.419 (3)	0.038 (7)*
H2B	0.159 (3)	0.648 (4)	0.770 (3)	0.057 (10)*
H2A	0.052 (3)	0.559 (6)	0.805 (4)	0.120 (18)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.06478 (19)	0.04141 (16)	0.06053 (19)	0.00582 (11)	0.02579 (14)	−0.00630 (11)
C1	0.0268 (13)	0.0302 (13)	0.0298 (13)	−0.0002 (10)	0.0095 (10)	−0.0024 (10)
C2	0.0321 (14)	0.0371 (14)	0.0321 (14)	0.0013 (11)	0.0096 (11)	0.0015 (11)
C3	0.0269 (13)	0.0420 (15)	0.0390 (15)	−0.0012 (11)	0.0100 (11)	−0.0081 (12)
C4	0.0339 (13)	0.0384 (14)	0.0337 (14)	−0.0094 (11)	0.0138 (11)	−0.0067 (12)
C5	0.0385 (14)	0.0358 (14)	0.0287 (13)	−0.0044 (11)	0.0103 (11)	0.0009 (11)
C6	0.0290 (12)	0.0296 (13)	0.0271 (12)	−0.0013 (10)	0.0078 (10)	−0.0047 (10)
C7	0.0377 (15)	0.0569 (19)	0.0459 (17)	−0.0137 (13)	0.0190 (13)	−0.0043 (14)
C8	0.0289 (14)	0.063 (2)	0.058 (2)	0.0013 (14)	0.0118 (14)	0.0009 (16)
N1	0.0323 (12)	0.0355 (13)	0.0355 (13)	0.0021 (10)	0.0091 (10)	0.0045 (10)

O1	0.0416 (11)	0.0412 (11)	0.0460 (11)	0.0032 (8)	0.0237 (9)	−0.0013 (9)
O2	0.0371 (11)	0.0474 (13)	0.0513 (12)	−0.0114 (8)	0.0097 (9)	−0.0092 (9)
O3	0.0358 (11)	0.0527 (13)	0.0562 (13)	0.0038 (8)	0.0153 (10)	0.0243 (10)
O1W	0.0778 (17)	0.0461 (14)	0.0578 (15)	−0.0058 (12)	0.0354 (14)	−0.0052 (12)
O2W	0.0702 (17)	0.0601 (15)	0.0814 (19)	−0.0123 (13)	0.0378 (14)	−0.0108 (13)
S1	0.0259 (3)	0.0309 (3)	0.0338 (3)	−0.0009 (2)	0.0096 (3)	0.0024 (3)

Geometric parameters (Å, °)

Ag1—O2W	2.186 (3)	C7—H7A	0.9600
Ag1—N1	2.273 (2)	C7—H7B	0.9600
Ag1—O1W	2.645 (3)	C7—H7C	0.9600
Ag1—O1W^{i}	2.651 (4)	C8—H8A	0.9600
C1—C2	1.391 (3)	C8—H8B	0.9600
C1—C6	1.394 (3)	C8—H8C	0.9600
C1—S1	1.771 (2)	N1—H1N	0.81 (3)
C2—C3	1.390 (4)	N1—H2N	0.95 (3)
C2—H2	0.9300	O1—S1	1.4551 (19)
C3—C4	1.398 (4)	O2—S1	1.453 (2)
C3—C8	1.513 (4)	O3—S1	1.4524 (19)
C4—C5	1.394 (4)	O1W—H1A	0.84 (3)
C4—C7	1.506 (3)	O1W—H1B	0.76 (3)
C5—C6	1.380 (3)	O2W—H2B	0.92 (3)
C5—H5	0.9300	O2W—H2A	0.98 (4)
C6—N1	1.427 (3)		
O2W—Ag1—N1	160.00 (9)	H7A—C7—H7B	109.5
O1W—Ag1—O1W^{i}	93.92 (8)	C4—C7—H7C	109.5
O1W—Ag1—O2W	110.79 (9)	H7A—C7—H7C	109.5
O1W—Ag1—N1	88.69 (8)	H7B—C7—H7C	109.5
O2W—Ag1—O1W^{i}	92.74 (8)	C3—C8—H8A	109.5
N1—Ag1—O1W^{i}	90.30 (8)	C3—C8—H8B	109.5
C2—C1—C6	119.3 (2)	H8A—C8—H8B	109.5
C2—C1—S1	119.59 (19)	C3—C8—H8C	109.5
C6—C1—S1	121.14 (18)	H8A—C8—H8C	109.5
C3—C2—C1	122.4 (2)	H8B—C8—H8C	109.5
C3—C2—H2	118.8	C6—N1—Ag1	108.40 (16)
C1—C2—H2	118.8	C6—N1—H1N	118 (3)
C2—C3—C4	118.1 (2)	Ag1—N1—H1N	102 (3)
C2—C3—C8	119.7 (3)	C6—N1—H2N	112.8 (15)
C4—C3—C8	122.1 (2)	Ag1—N1—H2N	107.7 (16)
C5—C4—C3	119.1 (2)	H1N—N1—H2N	106 (3)
C5—C4—C7	119.4 (2)	H1A—O1W—H1B	106 (3)
C3—C4—C7	121.5 (2)	Ag1—O2W—H2B	108 (2)
C6—C5—C4	122.6 (2)	Ag1—O2W—H2A	105 (3)
C6—C5—H5	118.7	H2B—O2W—H2A	125 (4)
C4—C5—H5	118.7	O3—S1—O2	112.99 (12)
C5—C6—C1	118.5 (2)	O3—S1—O1	112.48 (12)
C5—C6—N1	119.5 (2)	O2—S1—O1	112.04 (12)

C1—C6—N1	121.9 (2)	O3—S1—C1	106.83 (11)
C4—C7—H7A	109.5	O2—S1—C1	105.61 (12)
C4—C7—H7B	109.5	O1—S1—C1	106.26 (11)
C6—C1—C2—C3	−0.4 (4)	S1—C1—C6—C5	179.91 (18)
S1—C1—C2—C3	−179.4 (2)	C2—C1—C6—N1	−175.5 (2)
C1—C2—C3—C4	−0.7 (4)	S1—C1—C6—N1	3.5 (3)
C1—C2—C3—C8	179.8 (2)	C5—C6—N1—Ag1	−99.9 (2)
C2—C3—C4—C5	1.2 (4)	C1—C6—N1—Ag1	76.5 (2)
C8—C3—C4—C5	−179.3 (2)	O2W—Ag1—N1—C6	7.0 (4)
C2—C3—C4—C7	−177.0 (2)	C2—C1—S1—O3	−1.5 (2)
C8—C3—C4—C7	2.5 (4)	C6—C1—S1—O3	179.50 (19)
C3—C4—C5—C6	−0.8 (4)	C2—C1—S1—O2	−122.0 (2)
C7—C4—C5—C6	177.5 (2)	C6—C1—S1—O2	59.0 (2)
C4—C5—C6—C1	−0.3 (4)	C2—C1—S1—O1	118.8 (2)
C4—C5—C6—N1	176.2 (2)	C6—C1—S1—O1	−60.2 (2)
C2—C1—C6—C5	0.9 (4)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O2^{ii}	0.84 (3)	2.02 (3)	2.830 (3)	161 (3)
O1W—H1B···O3^{iii}	0.76 (3)	2.12 (3)	2.874 (3)	169 (4)
O2W—H2A···O1^{iii}	0.98 (4)	2.14 (4)	3.022 (3)	148 (4)
O2W—H2B···O3^{iv}	0.92 (3)	2.28 (3)	3.154 (3)	159 (3)
N1—H1N···O2^{ii}	0.81 (3)	2.40 (3)	3.154 (3)	156 (4)
N1—H2N···O1^{v}	0.95 (3)	2.12 (3)	3.065 (3)	172 (2)

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

Fig. 1

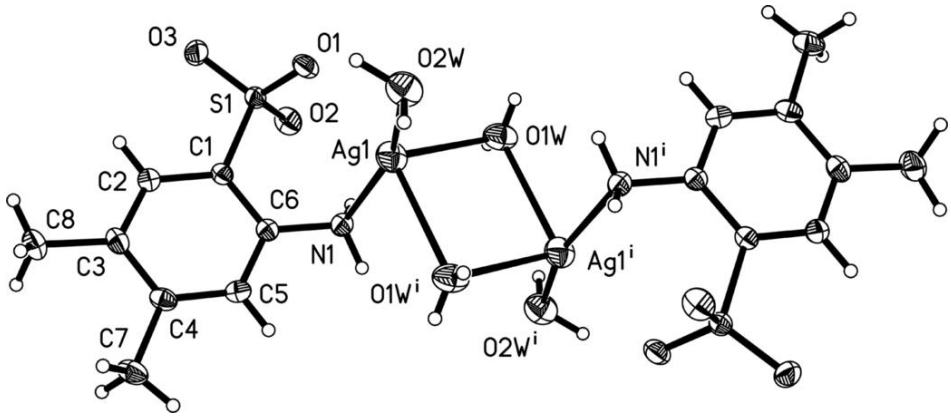

O3
O1
O2W
S1
O2
C1
Ag1
O1W
N1i
C2
C6
C8
N1
C3
Ag1i
C5
O1Wi
C7
C4
O2Wi

Fig. 2