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

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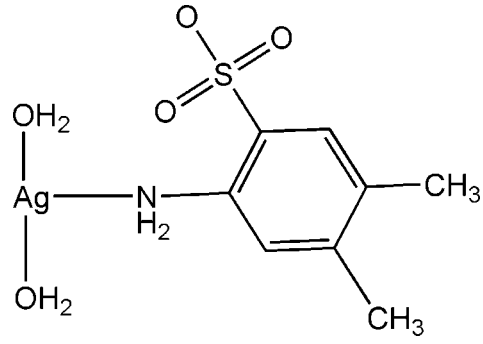
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 17.4.

The title compound, $[Ag(C_8H_{10}NO_3S)(H_2O)_2]$, shows a T-shaped coordination; the 2-amino-4,5-dimethylbenzenesulfonate monoanion binds through the amino group. The molecules are linked together through O—H···O and N—H···O hydrogen bonds into a layer structure.

Related literature

For studies on metal sulfonates, see: May & Shimizu (2005); Gao *et al.* (2005); Liu *et al.* (2006).



Experimental

Crystal data

$[Ag(C_8H_{10}NO_3S)(H_2O)_2]$
M_r = 344.13
Monoclinic, $P2_1/c$
a = 12.0636 (6) Å
b = 9.8642 (5) Å
c = 10.3509 (6) Å
β = 93.263 (1)°
V = 1229.74 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.81 mm^{-1}
T = 293 (2) K
0.33 × 0.27 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SAINT*; Bruker, 1998)
T_{min} = 0.542, T_{max} = 0.637
7355 measured reflections
2881 independent reflections
2381 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.04
2881 reflections
166 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—O1*W*	2.130 (3)	Ag1—N1	2.930 (3)
Ag1—O2*W*	2.136 (3)		
O1*W*—Ag1—O2*W*	171.50 (10)	O2*W*—Ag1—N1	92.22 (9)
O1*W*—Ag1—N1	96.09 (9)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H*W*12···O3^{i}	0.866 (10)	2.210 (12)	3.067 (3)	170 (4)
O1*W*—H*W*11···O2^{ii}	0.87 (3)	2.294 (19)	3.119 (3)	159 (4)
O2*W*—H*W*21···O1^{iii}	0.866 (10)	2.151 (12)	3.013 (3)	174 (4)
O2*W*—H*W*22···O3^{iv}	0.864 (10)	2.32 (2)	3.131 (3)	157 (4)
N1—H2*A*···O3^{iv}	0.85 (4)	2.29 (4)	3.095 (3)	158 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2266).

References

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supplementary materials

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

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Comment

Metal sulfonates are a class of compounds showing interesting structures and properties (May & Shimizu, 2005; Gao *et al.*, 2005); however, the sulfonate unit itself typically exists as a non-coordinating anion (Liu *et al.*, 2006). Indeed, in a majority of metal complexes with sulfonate counterions, the sulfonate group cannot displace water from the coordination sphere of the metal ion. This feature is also found in the present silver derivative of 2-amino-4,5-dimethylbenzenesulfonic acid.

The silvera tom in (I) is coordinated by the amino group instead; it is also linked to two water molecules in a T–shaped environment (Fig. 1). The molecules are linked through O—H···O and N—H···O hydrogen bonds (Table 2) to form a two-dimensional supramolecular structure (Fig. 2).

Experimental

To a mixture of 2-amino-4,5-dimethylbenzenesulfonic acid (0.5 mmol) and sodium hydroxide 0.5 mmol) in water was added silver nitrate (0.5 mmol). The precipitate that formed was dissolved by ammonium hydroxide. Colorless crystals were obtained from the filtrate after being set aside, away from light, after a week (33% yield).

Refinement

H atoms bonded to N atom were located in a difference map and refined freely, and with U_{iso}(H) = 1.2U_{eq}(N). 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}(carrier). The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H = 0.85 Å; their temperature factors were tied to those of parent atoms by a factor of 1.2.

Figures

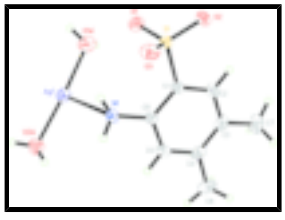

Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. (arbitrary spheres for the H atoms).

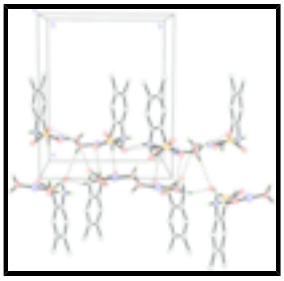

Fig. 2. View of the two-dimensional H-bonding structure of (I). H atoms bonded to C atoms have been omitted.

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

Crystal data

$[Ag(C_8H_{10}NO_3S)(H_2O_1)_2]$	F_{000} = 688
M_r = 344.13	D_x = 1.859 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2881 reflections
a = 12.0636 (6) Å	θ = 1.7–28.2º
b = 9.8642 (5) Å	μ = 1.81 mm^{-1}
c = 10.3509 (6) Å	T = 293 (2) K
β = 93.2630 (10)º	Block, colorless
V = 1229.74 (11) Å^3	0.33 × 0.27 × 0.25 mm
Z = 4	

Data collection

Bruker APEX CCD area-detector diffractometer	2881 independent reflections
Radiation source: fine-focus sealed tube	2381 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.074
T = 293(2) K	θ_{max} = 28.2º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SAINT; Bruker, 1998)	h = −12→16
T_{min} = 0.542, T_{max} = 0.637	k = −12→10
7355 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.097	$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001

2881 reflections	$\Delta\rho_{max}$ = 0.81 e Å^{-3}
166 parameters	$\Delta\rho_{min}$ = −0.67 e Å^{-3}
7 restraints	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0241 (14)

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}
C1	0.7014 (2)	0.5742 (2)	0.2547 (2)	0.0302 (5)
C2	0.5932 (2)	0.5483 (3)	0.2888 (3)	0.0378 (6)
H2	0.5821	0.5069	0.3677	0.045*
C3	0.5019 (2)	0.5827 (3)	0.2082 (3)	0.0414 (7)
C4	0.5188 (2)	0.6492 (3)	0.0924 (3)	0.0408 (6)
C5	0.6275 (2)	0.6730 (3)	0.0580 (3)	0.0386 (6)
H5	0.6386	0.7167	−0.0199	0.046*
C6	0.7194 (2)	0.6339 (3)	0.1355 (2)	0.0311 (5)
C7	0.3854 (3)	0.5482 (5)	0.2461 (4)	0.0643 (10)
H7A	0.3445	0.6304	0.2580	0.096*
H7B	0.3895	0.4974	0.3253	0.096*
H7C	0.3484	0.4951	0.1789	0.096*
C8	0.4235 (3)	0.6948 (4)	0.0021 (4)	0.0580 (9)
H8A	0.4520	0.7349	−0.0738	0.087*
H8B	0.3797	0.7604	0.0450	0.087*
H8C	0.3780	0.6181	−0.0225	0.087*
N1	0.8264 (2)	0.6491 (3)	0.0889 (2)	0.0391 (5)
H2A	0.829 (3)	0.717 (4)	0.040 (4)	0.059*
H1A	0.8871 (19)	0.639 (4)	0.126 (3)	0.059*
O1	0.86923 (19)	0.4162 (2)	0.3114 (2)	0.0460 (5)
O2	0.76622 (16)	0.5008 (2)	0.48734 (17)	0.0433 (5)
O3	0.88482 (17)	0.6513 (2)	0.3724 (2)	0.0467 (5)
S1	0.81314 (5)	0.53146 (7)	0.36498 (6)	0.02929 (17)
Ag1	0.887415 (18)	0.42546 (3)	−0.07922 (2)	0.04829 (14)
O1W	0.8839 (2)	0.2714 (3)	0.0647 (3)	0.0591 (6)
HW11	0.836 (2)	0.210 (3)	0.039 (4)	0.089*

HW12	0.9488 (15)	0.234 (4)	0.073 (4)	0.089*
O2W	0.8922 (2)	0.5559 (3)	−0.2436 (3)	0.0587 (6)
HW21	0.9604 (15)	0.558 (4)	−0.266 (5)	0.088*
HW22	0.872 (3)	0.6373 (18)	−0.226 (4)	0.088*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0332 (12)	0.0315 (13)	0.0256 (11)	−0.0003 (10)	0.0005 (9)	−0.0019 (9)
C2	0.0360 (14)	0.0489 (17)	0.0288 (13)	−0.0049 (12)	0.0041 (10)	−0.0018 (11)
C3	0.0324 (13)	0.0505 (18)	0.0413 (15)	−0.0021 (12)	0.0004 (11)	−0.0114 (13)
C4	0.0403 (15)	0.0389 (16)	0.0418 (15)	0.0055 (12)	−0.0088 (11)	−0.0053 (12)
C5	0.0478 (15)	0.0347 (14)	0.0325 (13)	−0.0012 (11)	−0.0036 (11)	0.0061 (11)
C6	0.0348 (12)	0.0298 (13)	0.0287 (12)	−0.0014 (10)	0.0023 (9)	−0.0006 (10)
C7	0.0345 (16)	0.099 (3)	0.059 (2)	−0.0115 (17)	0.0026 (14)	−0.016 (2)
C8	0.0491 (17)	0.053 (2)	0.069 (2)	0.0071 (15)	−0.0193 (15)	0.0019 (17)
N1	0.0382 (12)	0.0436 (15)	0.0363 (12)	−0.0022 (11)	0.0089 (10)	0.0063 (10)
O1	0.0530 (13)	0.0471 (13)	0.0378 (11)	0.0164 (9)	0.0015 (9)	−0.0060 (9)
O2	0.0433 (10)	0.0616 (14)	0.0251 (9)	0.0013 (10)	0.0040 (8)	0.0036 (9)
O3	0.0452 (11)	0.0460 (13)	0.0472 (11)	−0.0137 (9)	−0.0125 (8)	0.0066 (10)
S1	0.0311 (3)	0.0332 (3)	0.0235 (3)	−0.0006 (2)	0.0007 (2)	−0.0003 (2)
Ag1	0.04155 (18)	0.0547 (2)	0.04816 (19)	0.00171 (9)	−0.00134 (11)	0.00677 (10)
O1W	0.0624 (14)	0.0517 (14)	0.0621 (14)	0.0034 (12)	−0.0073 (12)	−0.0065 (12)
O2W	0.0590 (15)	0.0646 (16)	0.0526 (14)	−0.0003 (12)	0.0043 (11)	−0.0009 (12)

Geometric parameters (Å, °)

C1—C2	1.395 (4)	C8—H8A	0.9600
C1—C6	1.396 (4)	C8—H8B	0.9600
C1—S1	1.767 (3)	C8—H8C	0.9600
C2—C3	1.386 (4)	N1—H2A	0.85 (4)
C2—H2	0.9300	N1—H1A	0.814 (19)
C3—C4	1.392 (4)	O1—S1	1.450 (2)
C3—C7	1.519 (4)	O2—S1	1.4484 (18)
C4—C5	1.398 (4)	O3—S1	1.464 (2)
C4—C8	1.509 (4)	Ag1—O1W	2.130 (3)
C5—C6	1.386 (4)	Ag1—O2W	2.136 (3)
C5—H5	0.9300	Ag1—N1	2.930 (3)
C6—N1	1.411 (3)	O1W—HW11	0.87 (3)
C7—H7A	0.9600	O1W—HW12	0.866 (10)
C7—H7B	0.9600	O2W—HW21	0.866 (10)
C7—H7C	0.9600	O2W—HW22	0.864 (10)
C2—C1—C6	119.7 (2)	C4—C8—H8A	109.5
C2—C1—S1	118.9 (2)	C4—C8—H8B	109.5
C6—C1—S1	121.4 (2)	H8A—C8—H8B	109.5
C3—C2—C1	121.8 (3)	C4—C8—H8C	109.5
C3—C2—H2	119.1	H8A—C8—H8C	109.5
C1—C2—H2	119.1	H8B—C8—H8C	109.5

C2—C3—C4	118.9 (3)	C6—N1—H2A	111 (3)
C2—C3—C7	120.4 (3)	C6—N1—H1A	130 (3)
C4—C3—C7	120.7 (3)	H2A—N1—H1A	109 (4)
C3—C4—C5	119.0 (2)	O2—S1—O1	112.63 (13)
C3—C4—C8	122.0 (3)	O2—S1—O3	112.46 (13)
C5—C4—C8	119.0 (3)	O1—S1—O3	111.48 (14)
C6—C5—C4	122.5 (3)	O2—S1—C1	107.04 (12)
C6—C5—H5	118.8	O1—S1—C1	107.20 (12)
C4—C5—H5	118.8	O3—S1—C1	105.53 (12)
C5—C6—C1	118.0 (2)	O1W—Ag1—O2W	171.50 (10)
C5—C6—N1	119.4 (2)	O1W—Ag1—N1	96.09 (9)
C1—C6—N1	122.5 (2)	O2W—Ag1—N1	92.22 (9)
C3—C7—H7A	109.5	Ag1—O1W—HW11	109 (3)
C3—C7—H7B	109.5	Ag1—O1W—HW12	109 (3)
H7A—C7—H7B	109.5	HW11—O1W—HW12	108 (2)
C3—C7—H7C	109.5	Ag1—O2W—HW21	107 (3)
H7A—C7—H7C	109.5	Ag1—O2W—HW22	112 (3)
H7B—C7—H7C	109.5	HW21—O2W—HW22	109 (2)
C6—C1—C2—C3	−1.3 (4)	C4—C5—C6—N1	173.8 (3)
S1—C1—C2—C3	178.3 (2)	C2—C1—C6—C5	3.9 (4)
C1—C2—C3—C4	−2.4 (4)	S1—C1—C6—C5	−175.7 (2)
C1—C2—C3—C7	177.7 (3)	C2—C1—C6—N1	−172.8 (3)
C2—C3—C4—C5	3.3 (4)	S1—C1—C6—N1	7.7 (4)
C7—C3—C4—C5	−176.8 (3)	C2—C1—S1—O2	−11.9 (3)
C2—C3—C4—C8	−177.6 (3)	C6—C1—S1—O2	167.6 (2)
C7—C3—C4—C8	2.4 (5)	C2—C1—S1—O1	109.1 (2)
C3—C4—C5—C6	−0.6 (4)	C6—C1—S1—O1	−71.3 (2)
C8—C4—C5—C6	−179.8 (3)	C2—C1—S1—O3	−131.9 (2)
C4—C5—C6—C1	−3.0 (4)	C6—C1—S1—O3	47.6 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—HW12···O3^{i}	0.866 (10)	2.210 (12)	3.067 (3)	170 (4)
O1W—HW11···O2^{ii}	0.87 (3)	2.294 (19)	3.119 (3)	159 (4)
O2W—HW21···O1^{iii}	0.866 (10)	2.151 (12)	3.013 (3)	174 (4)
O2W—HW22···O3^{iv}	0.864 (10)	2.32 (2)	3.131 (3)	157 (4)
N1—H2A···O3^{iv}	0.85 (4)	2.29 (4)	3.095 (3)	158 (3)

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

Fig. 1

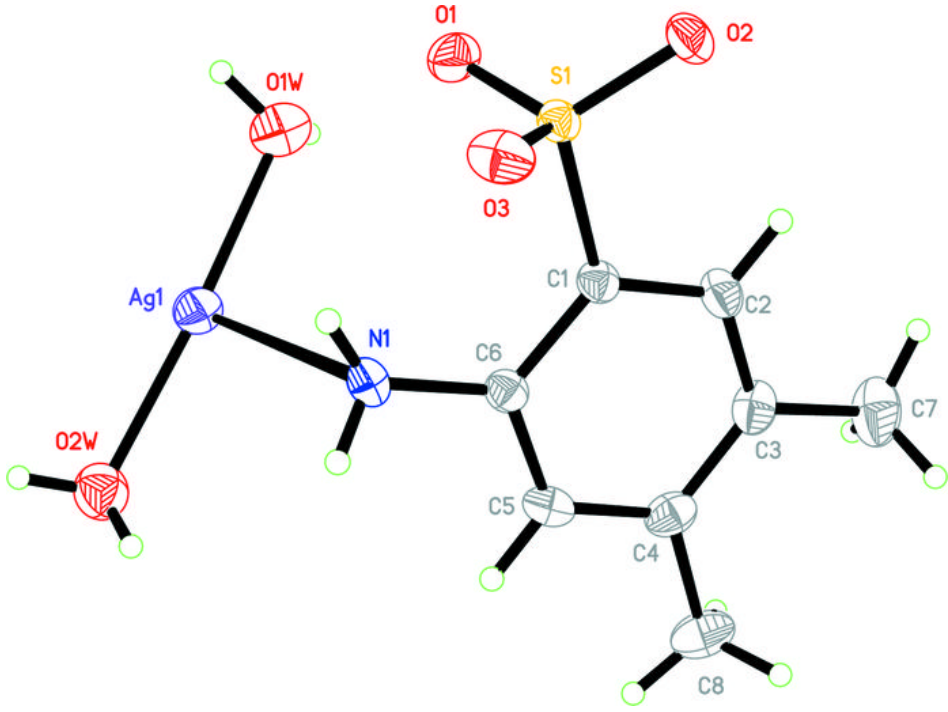

Fig. 2