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# Aqua(3-methylisoquinoline- $\kappa$ N)silver(I) 4-aminobenzenesulfonate

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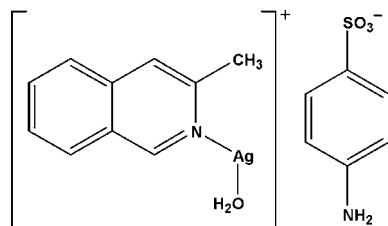
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å; H-atom completeness 95%;  $R$  factor = 0.046;  $wR$  factor = 0.117; data-to-parameter ratio = 17.7.

In the title compound,  $[\text{Ag}(\text{C}_{10}\text{H}_9\text{N})(\text{H}_2\text{O})](\text{C}_6\text{H}_6\text{NO}_3\text{S})$ , the  $\text{Ag}^{\text{I}}$  atom is two-coordinated by one N atom from a 3-methylisoquinoline ligand and one water molecule. The 4-aminobenzenesulfonate counter-anion does not show any bonding interactions with the  $\text{Ag}^{\text{I}}$  atom. The compound exhibits a three-dimensional supramolecular structure constructed by hydrogen bonds. Adjacent isoquinoline groups form  $\pi$ - $\pi$  interactions, with a centroid-centroid distance of 3.54 (1) Å. The crystal studied was an inversion twin.

## Related literature

For related literature, see: Atria *et al.* (1994); Cai *et al.* (2003); Li *et al.* (2006).



## Experimental

### Crystal data

$[\text{Ag}(\text{C}_{10}\text{H}_9\text{N})(\text{H}_2\text{O})](\text{C}_6\text{H}_6\text{NO}_3\text{S})$   
 $M_r = 441.25$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 6.779$  (1) Å  
 $b = 13.997$  (3) Å  
 $c = 18.076$  (4) Å

$V = 1715.2$  (6) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.32$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.47 \times 0.09 \times 0.06$  mm

### Data collection

Rigaku R-AXIS RAPID  
 diffractometer  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{\text{min}} = 0.529$ ,  $T_{\text{max}} = 0.911$

7289 measured reflections  
 3904 independent reflections  
 2458 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.069$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.117$   
 $S = 0.97$   
 3904 reflections  
 221 parameters  
 1 restraint

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.35$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.49$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 1646 Friedel pairs  
 Flack parameter: 0.46 (6)

Table 1

Selected geometric parameters (Å, °).

Ag1—N1	2.137 (4)	Ag1—O1W	2.138 (5)
N1—Ag1—O1W	178.7 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A $\cdots$ O1 <sup>i</sup>	0.86	2.37	3.092 (6)	142
N2—H2B $\cdots$ O3 <sup>ii</sup>	0.86	2.18	3.005 (7)	160
O1W—H36 $\cdots$ O2 <sup>i</sup>	0.86 (4)	2.25 (3)	3.027 (8)	150 (6)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Siemens, 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: HY2101).

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**supplementary materials**

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## Aqua(3-methylisoquinoline- $\kappa$ N)silver(I) 4-aminobenzenesulfonate

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### Comment

Sulfonate group can adopt various bridging coordination modes. Silver, a  $d^{10}$  metal, has no crystal field stabilization energy and hence no dominant geometrical preferences (Li *et al.*, 2006). In this paper, we report the synthesis and crystal structure of a new silver(I) complex with a 4-aminobenzenesulfonate as a counter anion.

As shown in Fig. 1, the sulfonate group in the title compound does not show any bonding interactions with  $\text{Ag}^{\text{I}}$  atom.  $\text{Ag}^{\text{I}}$  atom is two-coordinated by one N atom from a neutral 3-methylisoquinoline ligand and one water molecule.  $\text{Ag1}$ , N1 and O1W are almost co-linear and the N1—Ag1—O1W angle is  $179.2(2)^\circ$ . The bond distances and angles are normal (Atria *et al.*, 1994; Cai *et al.*, 2003). Furthermore, the compound shows a three-dimensional supramolecular structure constructed by hydrogen bonds. Adjacent isoquinoline groups form  $\pi$ – $\pi$  interactions with a centroid-to-centroid distance of  $3.54(1)\text{ \AA}$ .

### Experimental

A mixture of  $\text{AgNO}_3$  (0.170 g, 1 mmol), NaOH (0.040 g, 1 mmol) and 4-aminobenzenesulfonic acid (0.173 g, 1 mmol) in water (15 ml) was stirring for 10 min at room temperature. Then 3-methylisoquinoline (0.143 g, 1 mmol) was added to the solution with stirring for 30 min and a white precipitate was obtained. The precipitate was dissolved by dropwise addition of ammonia (5 M). Green single crystals were obtained by slow evaporation of the solution at room temperature.

### Refinement

H atoms on C and N atoms were positioned geometrically and refined as riding atoms, with C—H =  $0.93\text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic ring, C—H =  $0.96\text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl group, and N—H =  $0.86\text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$  for amino group. One of H atoms of the water molecule was located in a difference Fourier map and refined with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ , and the other one was not located.

### Figures

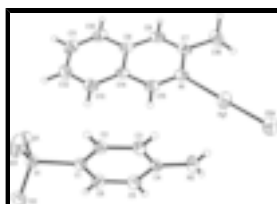


Fig. 1. The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms of the water molecule are not shown.

## Aqua(3-methylisoquinoline- $\kappa$ N)silver(I) 4-aminobenzenesulfonate

### Crystal data

$[\text{Ag}(\text{C}_{10}\text{H}_9\text{N})(\text{H}_2\text{O})](\text{C}_6\text{H}_6\text{NO}_3\text{S})$	$F_{000} = 888$
$M_r = 441.25$	$D_x = 1.709 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
Hall symbol: P 2ac 2ab	$\lambda = 0.71073 \text{ \AA}$
$a = 6.779 (1) \text{ \AA}$	Cell parameters from 3904 reflections
$b = 13.997 (3) \text{ \AA}$	$\theta = 2.5\text{--}27.5^\circ$
$c = 18.076 (4) \text{ \AA}$	$\mu = 1.32 \text{ mm}^{-1}$
$V = 1715.2 (6) \text{ \AA}^3$	$T = 293 (2) \text{ K}$
$Z = 4$	Prism, colorless
	$0.47 \times 0.09 \times 0.06 \text{ mm}$

### Data collection

Rigaku R-Axis RAPID diffractometer	3904 independent reflections
Radiation source: rotation anode	2458 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.069$
$T = 293(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
$\omega$ scan	$\theta_{\text{min}} = 1.8^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = 0 \rightarrow 8$
$T_{\text{min}} = 0.529$ , $T_{\text{max}} = 0.911$	$k = -18 \rightarrow 18$
7289 measured reflections	$l = -23 \rightarrow 23$

### 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
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2]$
$wR(F^2) = 0.117$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3904 reflections	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
221 parameters	$\Delta\rho_{\text{min}} = -0.49 \text{ e \AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1646 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.46 (6)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.70457 (8)	0.50911 (3)	1.00258 (3)	0.06244 (18)
C1	0.7687 (8)	0.2835 (3)	0.7059 (3)	0.0348 (12)
C2	0.9238 (9)	0.3384 (4)	0.7295 (4)	0.0427 (14)
H2	1.0520	0.3204	0.7176	0.051*
C3	0.8914 (10)	0.4213 (4)	0.7712 (4)	0.0460 (15)
H3	0.9976	0.4579	0.7872	0.055*
C4	0.6990 (10)	0.4487 (3)	0.7887 (3)	0.0399 (12)
C5	0.5426 (8)	0.3942 (4)	0.7618 (4)	0.0448 (15)
H5	0.4134	0.4130	0.7711	0.054*
C6	0.5789 (8)	0.3121 (4)	0.7212 (4)	0.0442 (15)
H6	0.4734	0.2759	0.7040	0.053*
C7	0.7119 (9)	0.3173 (4)	1.0899 (3)	0.0461 (13)
C8	0.7113 (9)	0.2190 (4)	1.0960 (3)	0.0491 (14)
H8	0.7116	0.1919	1.1430	0.059*
C9	0.7104 (9)	0.1581 (4)	1.0341 (3)	0.0434 (13)
C10	0.7105 (10)	0.0559 (4)	1.0380 (4)	0.0566 (16)
H10	0.7098	0.0257	1.0838	0.068*
C11	0.7118 (10)	0.0041 (4)	0.9762 (4)	0.0633 (17)
H11	0.7126	-0.0622	0.9796	0.076*
C12	0.7120 (11)	0.0471 (4)	0.9061 (4)	0.0596 (16)
H12	0.7111	0.0091	0.8639	0.072*
C13	0.7136 (9)	0.1444 (4)	0.8992 (4)	0.0515 (14)
H13	0.7153	0.1729	0.8528	0.062*
C14	0.7124 (8)	0.2006 (4)	0.9637 (3)	0.0400 (12)
C15	0.7111 (9)	0.3032 (4)	0.9614 (3)	0.0443 (13)
H15	0.7102	0.3326	0.9153	0.053*
C16	0.7102 (11)	0.3833 (5)	1.1546 (4)	0.0719 (19)
H16A	0.7096	0.4482	1.1374	0.108*
H16B	0.8256	0.3725	1.1842	0.108*
H16C	0.5944	0.3718	1.1838	0.108*
N1	0.7112 (7)	0.3582 (3)	1.0203 (3)	0.0427 (11)
N2	0.6671 (7)	0.5272 (3)	0.8343 (3)	0.0530 (13)
H2A	0.5489	0.5431	0.8465	0.064*
H2B	0.7656	0.5599	0.8504	0.064*
O1	0.7523 (6)	0.0984 (2)	0.7042 (3)	0.0573 (13)
O2	0.6892 (9)	0.1821 (3)	0.5914 (2)	0.0673 (13)
O3	1.0187 (7)	0.1748 (3)	0.6393 (3)	0.0701 (15)
O1W	0.7047 (8)	0.6603 (3)	0.9857 (3)	0.0828 (15)
S1	0.8103 (2)	0.17638 (8)	0.65704 (8)	0.0415 (3)
H36	0.593 (5)	0.685 (4)	0.974 (4)	0.099*

Atomic displacement parameters ( $\text{\AA}^2$ )

$U^{11}$        $U^{22}$        $U^{33}$        $U^{12}$        $U^{13}$        $U^{23}$

## supplementary materials

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Ag1	0.0663 (3)	0.0474 (2)	0.0736 (4)	-0.0021 (2)	0.0064 (3)	-0.0002 (3)
C1	0.040 (3)	0.030 (2)	0.035 (3)	0.000 (2)	-0.001 (2)	0.0032 (19)
C2	0.039 (3)	0.048 (3)	0.041 (4)	0.004 (3)	-0.001 (3)	0.000 (3)
C3	0.049 (3)	0.038 (3)	0.051 (4)	-0.005 (3)	-0.010 (3)	-0.005 (3)
C4	0.053 (3)	0.038 (2)	0.029 (3)	0.003 (3)	0.001 (3)	0.000 (2)
C5	0.037 (3)	0.048 (3)	0.050 (4)	0.002 (3)	0.006 (3)	0.001 (3)
C6	0.040 (3)	0.039 (3)	0.053 (4)	-0.005 (3)	-0.003 (3)	-0.003 (3)
C7	0.033 (3)	0.072 (3)	0.034 (3)	0.000 (3)	-0.001 (3)	0.002 (3)
C8	0.044 (3)	0.069 (3)	0.034 (3)	0.003 (3)	0.001 (3)	0.015 (3)
C9	0.033 (2)	0.048 (3)	0.049 (4)	0.003 (3)	-0.002 (3)	0.015 (2)
C10	0.053 (3)	0.052 (3)	0.065 (5)	0.000 (4)	-0.002 (4)	0.022 (3)
C11	0.058 (3)	0.046 (3)	0.086 (5)	0.000 (4)	-0.001 (4)	0.005 (3)
C12	0.059 (4)	0.061 (3)	0.059 (5)	0.002 (4)	-0.004 (4)	-0.015 (3)
C13	0.042 (3)	0.065 (3)	0.048 (4)	0.000 (3)	-0.003 (4)	0.001 (3)
C14	0.028 (2)	0.050 (3)	0.041 (3)	-0.002 (3)	-0.005 (3)	0.007 (2)
C15	0.041 (3)	0.048 (3)	0.043 (4)	-0.005 (3)	0.000 (3)	0.014 (3)
C16	0.066 (4)	0.094 (4)	0.056 (5)	0.001 (4)	0.007 (5)	-0.030 (4)
N1	0.033 (2)	0.053 (2)	0.041 (3)	-0.003 (2)	-0.002 (3)	0.0053 (19)
N2	0.061 (3)	0.047 (2)	0.051 (3)	-0.001 (2)	0.009 (3)	-0.015 (2)
O1	0.082 (4)	0.0380 (17)	0.052 (3)	-0.0009 (19)	0.004 (2)	0.0096 (16)
O2	0.108 (4)	0.051 (2)	0.043 (3)	0.007 (3)	-0.021 (3)	-0.0049 (18)
O3	0.057 (3)	0.054 (2)	0.099 (5)	0.002 (2)	0.030 (3)	-0.018 (2)
O1W	0.104 (4)	0.065 (2)	0.080 (4)	0.010 (3)	-0.009 (4)	-0.014 (3)
S1	0.0534 (8)	0.0328 (6)	0.0383 (8)	0.0019 (7)	0.0015 (8)	-0.0011 (5)

### *Geometric parameters (Å, °)*

Ag1—N1	2.137 (4)	C10—C11	1.331 (9)
Ag1—O1W	2.138 (5)	C10—H10	0.9300
C1—C2	1.370 (7)	C11—C12	1.403 (9)
C1—C6	1.376 (8)	C11—H11	0.9300
C1—S1	1.762 (5)	C12—C13	1.367 (8)
C2—C3	1.402 (8)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.406 (8)
C3—C4	1.396 (9)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.437 (7)
C4—N2	1.390 (6)	C15—N1	1.312 (7)
C4—C5	1.393 (8)	C15—H15	0.9300
C5—C6	1.386 (8)	C16—H16A	0.9600
C5—H5	0.9300	C16—H16B	0.9600
C6—H6	0.9300	C16—H16C	0.9600
C7—C8	1.380 (7)	N2—H2A	0.8600
C7—N1	1.383 (7)	N2—H2B	0.8600
C7—C16	1.490 (8)	O1—S1	1.440 (4)
C8—C9	1.406 (8)	O2—S1	1.445 (5)
C8—H8	0.9300	O3—S1	1.449 (5)
C9—C14	1.405 (8)	O1W—H36	0.86 (4)
C9—C10	1.431 (7)		
N1—Ag1—O1W	178.7 (2)	C12—C11—H11	119.2

C2—C1—C6	119.4 (5)	C13—C12—C11	120.7 (6)
C2—C1—S1	120.7 (4)	C13—C12—H12	119.7
C6—C1—S1	119.9 (4)	C11—C12—H12	119.7
C1—C2—C3	120.8 (5)	C12—C13—C14	118.8 (6)
C1—C2—H2	119.6	C12—C13—H13	120.6
C3—C2—H2	119.6	C14—C13—H13	120.6
C4—C3—C2	119.7 (5)	C9—C14—C13	120.9 (5)
C4—C3—H3	120.1	C9—C14—C15	116.7 (5)
C2—C3—H3	120.1	C13—C14—C15	122.4 (5)
N2—C4—C5	121.4 (6)	N1—C15—C14	124.2 (5)
N2—C4—C3	119.8 (5)	N1—C15—H15	117.9
C5—C4—C3	118.7 (5)	C14—C15—H15	117.9
C6—C5—C4	120.3 (5)	C7—C16—H16A	109.5
C6—C5—H5	119.9	C7—C16—H16B	109.5
C4—C5—H5	119.9	H16A—C16—H16B	109.5
C1—C6—C5	120.9 (5)	C7—C16—H16C	109.5
C1—C6—H6	119.5	H16A—C16—H16C	109.5
C5—C6—H6	119.5	H16B—C16—H16C	109.5
C8—C7—N1	119.0 (5)	C15—N1—C7	119.7 (4)
C8—C7—C16	123.8 (6)	C15—N1—Ag1	117.3 (4)
N1—C7—C16	117.2 (5)	C7—N1—Ag1	123.0 (4)
C7—C8—C9	122.8 (5)	C4—N2—H2A	120.0
C7—C8—H8	118.6	C4—N2—H2B	120.0
C9—C8—H8	118.6	H2A—N2—H2B	120.0
C14—C9—C8	117.6 (4)	Ag1—O1W—H36	116 (4)
C14—C9—C10	117.8 (6)	O1—S1—O2	111.9 (3)
C8—C9—C10	124.6 (6)	O1—S1—O3	112.7 (3)
C11—C10—C9	120.2 (6)	O2—S1—O3	111.9 (4)
C11—C10—H10	119.9	O1—S1—C1	107.7 (2)
C9—C10—H10	119.9	O2—S1—C1	105.9 (2)
C10—C11—C12	121.5 (5)	O3—S1—C1	106.3 (2)
C10—C11—H11	119.2		
C6—C1—C2—C3	2.4 (9)	C10—C9—C14—C13	0.3 (9)
S1—C1—C2—C3	-177.1 (5)	C8—C9—C14—C15	-1.3 (9)
C1—C2—C3—C4	-0.4 (9)	C10—C9—C14—C15	179.7 (6)
C2—C3—C4—N2	175.7 (5)	C12—C13—C14—C9	0.2 (10)
C2—C3—C4—C5	-2.3 (9)	C12—C13—C14—C15	-179.1 (6)
N2—C4—C5—C6	-175.1 (6)	C9—C14—C15—N1	1.1 (10)
C3—C4—C5—C6	2.8 (9)	C13—C14—C15—N1	-179.6 (6)
C2—C1—C6—C5	-1.9 (9)	C14—C15—N1—C7	-0.2 (9)
S1—C1—C6—C5	177.7 (5)	C14—C15—N1—Ag1	-179.1 (5)
C4—C5—C6—C1	-0.8 (9)	C8—C7—N1—C15	-0.4 (9)
N1—C7—C8—C9	0.1 (10)	C16—C7—N1—C15	-179.5 (7)
C16—C7—C8—C9	179.1 (6)	C8—C7—N1—Ag1	178.4 (4)
C7—C8—C9—C14	0.8 (10)	C16—C7—N1—Ag1	-0.7 (8)
C7—C8—C9—C10	179.7 (7)	C2—C1—S1—O1	111.1 (5)
C14—C9—C10—C11	-0.3 (10)	C6—C1—S1—O1	-68.4 (5)
C8—C9—C10—C11	-179.2 (7)	C2—C1—S1—O2	-129.0 (5)
C9—C10—C11—C12	-0.3 (11)	C6—C1—S1—O2	51.5 (6)

## supplementary materials

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C10—C11—C12—C13	0.9 (11)	C2—C1—S1—O3	-9.8 (6)
C11—C12—C13—C14	-0.8 (11)	C6—C1—S1—O3	170.7 (5)
C8—C9—C14—C13	179.4 (6)		

### *Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2A $\cdots$ O1 <sup>i</sup>	0.86	2.37	3.092 (6)	142
N2—H2B $\cdots$ O3 <sup>ii</sup>	0.86	2.18	3.005 (7)	160
O1W—H36 $\cdots$ O2 <sup>i</sup>	0.86 (4)	2.25 (3)	3.027 (8)	150 (6)

Symmetry codes: (i)  $-x+1, y+1/2, -z+3/2$ ; (ii)  $-x+2, y+1/2, -z+3/2$ .

Fig. 1

