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Aqua(3-methylisoquinoline-κN)silver(I) 4-aminobenzenesulfonate

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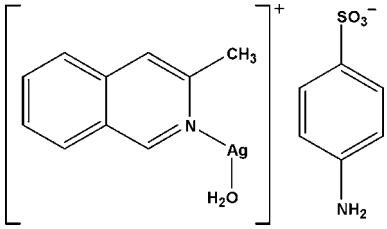
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; H-atom completeness 95%; R factor = 0.046; wR factor = 0.117; data-to-parameter ratio = 17.7.

In the title compound, $[Ag(C_{10}H_9N)(H_2O)](C_6H_6NO_3S)$, the Ag^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 Ag^I atom. The compound exhibits a three-dimensional supramolecular structure constructed by hydrogen bonds. Adjacent isoquinoline groups form π–π 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

$[Ag(C_{10}H_9N)(H_2O)](C_6H_6NO_3S)$
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^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 293 (2) K
0.47 × 0.09 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.529, T_{max} = 0.911
7289 measured reflections
3904 independent reflections
2458 reflections with $I > 2\sigma(I)$
R_{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
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Absolute structure: Flack (1983), 1646 Friedel pairs
Flack parameter: 0.46 (6)

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.137 (4)	Ag1—O1*W*	2.138 (5)
N1—Ag1—O1*W*	178.7 (2)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.86	2.37	3.092 (6)	142
N2—H2*B*···O3^{ii}	0.86	2.18	3.005 (7)	160
O1*W*—H36···O2^{i}	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/MSC, 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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Acta Cryst. (2008). E**64**, m224 [https://doi.org/10.1107/S1600536807061983]

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S1. 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 Ag^{I} atom. Ag^{I} atom is two-coordinated by one N atom from a neutral 3-methylisoquinoline ligand and one water molecule. Ag1, N1 and O1W are almost co-linear and the N1—Ag1—O1W angle is 179.2 (2)°. 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 π–π interactions with a centroid-to-centroid distance of 3.54 (1) Å.

S2. Experimental

A mixture of $AgNO_3$ (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.

S3. Refinement

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

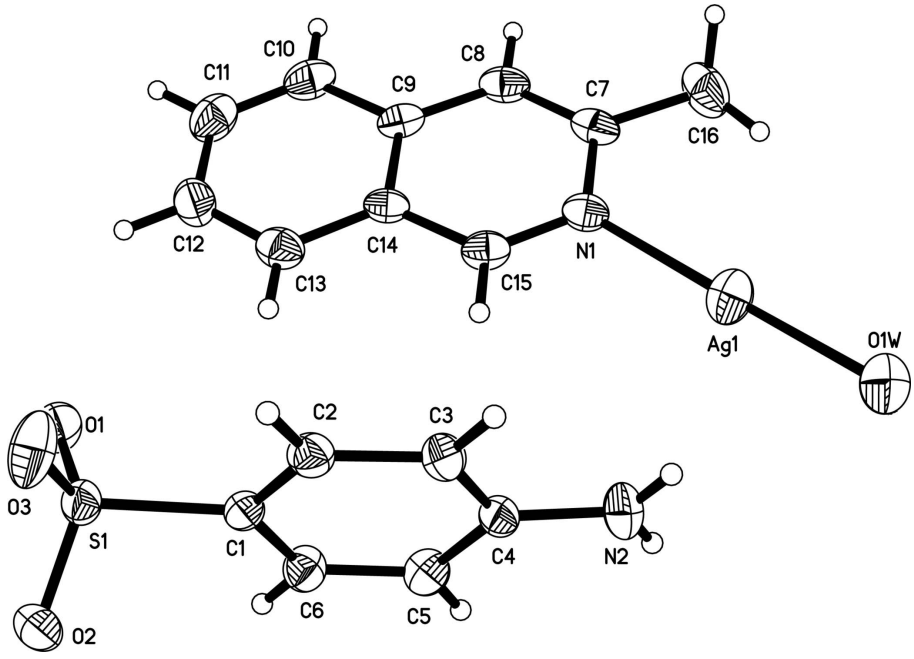

Figure 1

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-κN)silver(I) 4-aminobenzenesulfonate

Crystal data

$[Ag(C_{10}H_9N)(H_2O)](C_6H_6NO_3S)$
$M_r = 441.25$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.779$ (1) Å
$b = 13.997$ (3) Å
$c = 18.076$ (4) Å
$V = 1715.2$ (6) Å^3
$Z = 4$
$F(000) = 888$
$D_x = 1.709$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3904 reflections
$\theta = 2.5$–$27.5°$
$\mu = 1.32$ mm^{-1}
$T = 293$ K
Prism, colorless
0.47 × 0.09 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotation anode
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.529$, $T_{max} = 0.911$
7289 measured reflections
3904 independent reflections
2458 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = 0 \rightarrow 8$
$k = -18 \rightarrow 18$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.117$
$S = 0.97$
3904 reflections
221 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}
Absolute structure: Flack (1983), 1646 Friedel pairs
Absolute structure parameter: 0.46 (6)

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

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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, º)

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)
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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.86	2.37	3.092 (6)	142
N2—H2*B*···O3^{ii}	0.86	2.18	3.005 (7)	160
O1*W*—H36···O2^{i}	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.