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Key indicators

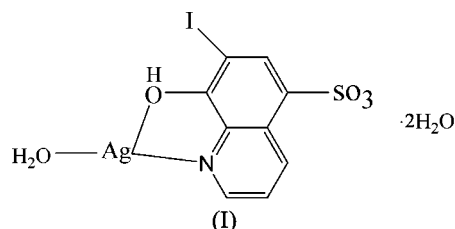
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.029
 wR factor = 0.068
Data-to-parameter ratio = 16.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Aqua(8-hydroxy-7-iodoquinoline-5-sulfonato- $\kappa^2\text{N},\text{O}^8$)silver(I) dihydrate

In the title compound, $[\text{Ag}(\text{C}_9\text{H}_5\text{INO}_4\text{S})(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}$, the Ag^{I} cation has a highly distorted trigonal-planar coordination geometry, with N and O donor atoms from a bidentate 8-hydroxy-7-iodoquinoline-5-sulfonate anion ligand and one O atom from a water molecule. In the crystal structure, the molecules are linked together through extensive intermolecular hydrogen bonding, forming a three-dimensional structure.

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Comment

In recent years, the syntheses and structures of Ag^{I} complexes have been widely explored for the variety of their coordination geometries (Aakeröy & Beatty, 1998; Smith *et al.*, 1996; Dong *et al.*, 2003). In particular, silver-sulfonate complexes have attracted great attention by reason of their ability to form inorganic and organic lamellar structures and to intercalate guest molecules (Shimizu *et al.*, 1998; Cote & Shimizu, 2004; Hoffart *et al.*, 2005). In this paper, the synthesis and crystal structure of a new silver-sulfonate complex, (I), $[\text{Ag}(L)(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}$ (L is the 8-hydroxy-7-iodoquinoline-5-sulfonate anion), is presented.



The molecular structure of (I) is shown in Fig. 1. Selected bond distances and angles are listed in Table 1. The L ligand is chelated to the Ag^{I} ion through its N and O donor sites, forming a five-membered chelate ring. The distorted three-coordinate geometry of Ag^{I} is completed by one coordinated water molecule. Atoms Ag1, N1, O4 and OW1 are almost coplanar and the bond-angle sum about Ag is 359.9° . The Ag1–N1 distance in complex (I) is similar to reported values (Dong *et al.*, 2003), but the Ag1–O4 and Ag1–OW1 distances are significantly shorter than reported values (Ma *et al.*, 2005).

Adjacent molecules of (I) are interconnected by strong O–H...O hydrogen-bonding interactions between uncoordinated sulfonate O atoms, hydroxyl O atoms, and coordinated and uncoordinated water molecules. Thus, the compound forms a three-dimensional supramolecular structure (Fig. 2) through extensive intermolecular hydrogen bonding.

Experimental

To an aqueous solution (10 ml) of 8-hydroxy-7-iodoquinoline-5-sulfonic acid (0.176 g, 0.5 mmol) was added Ag_2CO_3 (0.069 g, 0.25 mmol) and the mixture was stirred for several minutes. A khaki-coloured precipitate formed. The precipitate was dissolved incompletely by dropwise addition of an aqueous solution of NH_3 , then filtered. Yellow crystals of (I) grew out of the filtrate after standing in a dark room for several days at room temperature.

Crystal data

$[\text{Ag}(\text{C}_9\text{H}_5\text{INO}_4\text{S})(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}$
 $M_r = 512.02$
 Monoclinic, $P2_1/n$
 $a = 12.525$ (3) Å
 $b = 7.8707$ (16) Å
 $c = 15.427$ (3) Å
 $\beta = 107.94$ (3)°
 $V = 1446.8$ (5) Å³

$Z = 4$
 $D_x = 2.351$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 3.70$ mm⁻¹
 $T = 293$ (2) K
 Block, yellow
 $0.1 \times 0.1 \times 0.1$ mm

Data collection

Rigaku R-AXIS RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.687$, $T_{\max} = 0.695$

13669 measured reflections
 3298 independent reflections
 2805 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.068$
 $S = 1.05$
 3298 reflections
 206 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 2.8345P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.92$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O4}-\text{H1O}\cdots\text{OW3}$	0.85 (3)	1.93 (4)	2.713 (4)	153 (5)
$\text{OW2}-\text{H2B}\cdots\text{O1}$	0.76 (5)	2.10 (5)	2.855 (4)	175 (5)
$\text{OW3}-\text{H2C}\cdots\text{O2}^i$	0.93 (3)	2.09 (4)	2.971 (5)	158 (5)

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

All H atoms on C atoms were positioned geometrically and refined as riding, with $C-H = 0.93$ Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atoms of the water molecules and the hydroxy group were found in a difference Fourier map and refined freely. The highest residual electron density peak is 0.05 Å from atom H1A(OW1).

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: *SHELXTL-Plus*.

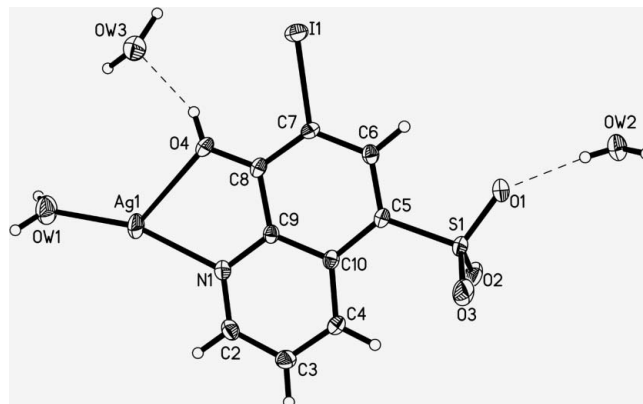


Figure 1

A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The hydrogen bonds are indicated by dashed lines.

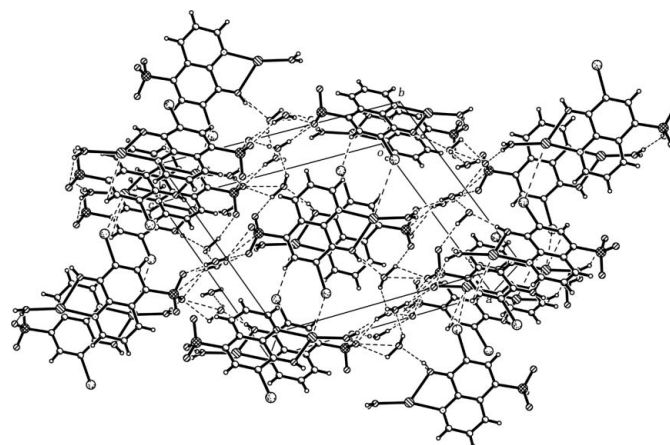


Figure 2

A view of the three-dimensional supramolecular structure formed through extensive intermolecular hydrogen bonds (dashed lines).

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