Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua(8-hydroxyquinoline-5-sulfonato-κ^2N,O^8)-silver(I) monohydrate

Hua Wu, Xian-Wu Dong and Jian-Fang Ma*

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail: jianfangma@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.014 Å
R factor = 0.079
wR factor = 0.169
Data-to-parameter ratio = 15.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

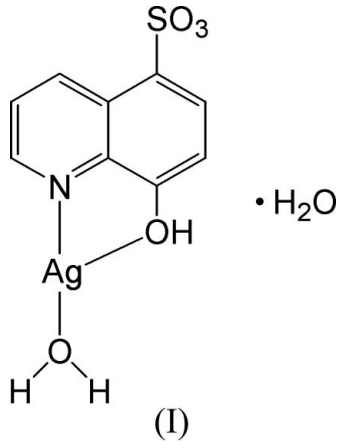
© 2006 International Union of Crystallography
All rights reserved

Received 17 January 2006
Accepted 24 January 2006

In the title compound, $[Ag(C_9H_6NO_4S)(H_2O)]\cdot H_2O$, the Ag^I cation is three-coordinated by one N and one hydroxy O atom from one 8-hydroxyquinoline-5-sulfonate anion and one water molecule in a highly distorted trigonal–planar geometry. The sulfonate group does not coordinate to the Ag^I cation.

Comment

In recent decades, much attention has been focused on the design and synthesis of metal–organic coordination networks (Hagrman *et al.*, 1999; Moulton & Zaworotko, 2001). Compared with carboxylates and phosphonates, the coordination chemistry of sulfonates has been less well studied, due to the perception that sulfonate is a poor ligand (Cote & Shimizu, 2003; Cai, 2004). However, silver sulfonates are an exception, as sulfonate groups can adopt a range of different bridging modes with the Ag^+ cation (Shimizu *et al.*, 1999; Cote & Shimizu, 2004). Here, we report the synthesis and crystal structure of the title compound, (I).



(I)

As shown in Fig. 1, the Ag^+ cation of (I) is three-coordinated by one N and one hydroxy O atom from one 8-hydroxyquinoline-5-sulfonate anion and one water molecule in a highly distorted trigonal–planar coordination geometry for Ag (Table 1). Atoms Ag1, O*W*1, N1 and O4 are almost coplanar and the bond-angle sum about Ag is 359.6°. The Ag—O_w (w = water) distance of 2.127 (9) Å is shorter than the Ag—O_h (h = hydroxy) distance of 2.447 (8) Å. The Ag—N distance of (I) is similar to reported values (Li *et al.*, 2005). However, both the Ag—O_h and Ag—O_w distances of (I) are shorter than reported Ag—O_h distances (Wu *et al.*, 2006; Ma *et al.*, 2005) and Ag—O_w distances (Ma *et al.*, 2005), respectively. In (I), the 8-hydroxyquinoline-5-sulfonate anion coordinates to the Ag^+ cation through the N and hydroxy O atoms in a

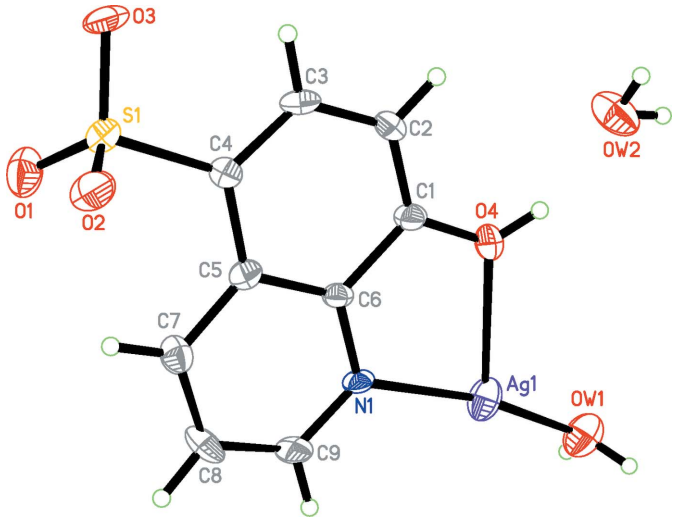


Figure 1
A view of compound (I). Displacement ellipsoids are drawn at the 30% probability level.

chelating mode, and the sulfonate group does not coordinate to the Ag cation.

As shown in Table 2, the coordinated water molecule (*OW*1) is weakly hydrogen-bonded as donor to two sulfonate O atoms. The solvent water molecule (*OW*2) does not coordinate to the Ag^+ cation but is hydrogen-bonded to the hydroxy O atom as an acceptor and to the sulfonate O atom as a donor.

Experimental

An aqueous solution of NaOH (0.1 *M*) was added to a solution of 8-hydroxyquinoline-5-sulfonic acid (0.112 g, 0.5 mmol) in water (5 ml) until the pH reached 7. A solution of $AgNO_3$ (0.085 g, 0.5 mmol) in water (5 ml) was then added, and a yellow precipitate formed immediately. After stirring for 10 min, the precipitate was dissolved by dropwise addition of an aqueous solution of NH_3 (14 *M*, 5 ml). Crystals of (I) were obtained by evaporation of the solution at room temperature over several days.

Crystal data

$[Ag(C_9H_6NO_4S)(H_2O)]\cdot H_2O$
M_r = 368.11
Monoclinic, $C2/c$
a = 20.314 (4) Å
b = 9.2221 (18) Å
c = 13.182 (3) Å
β = 96.34 (3)°
V = 2454.4 (9) Å^3
Z = 8
D_x = 1.992 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8271 reflections
θ = 3.1–27.4°
μ = 1.83 mm^{-1}
T = 292 (2) K
Block, yellow
0.15 × 0.12 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.755, T_{max} = 0.82
11547 measured reflections
2741 independent reflections
2132 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.4°
$h = -26 \rightarrow 26$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 17$

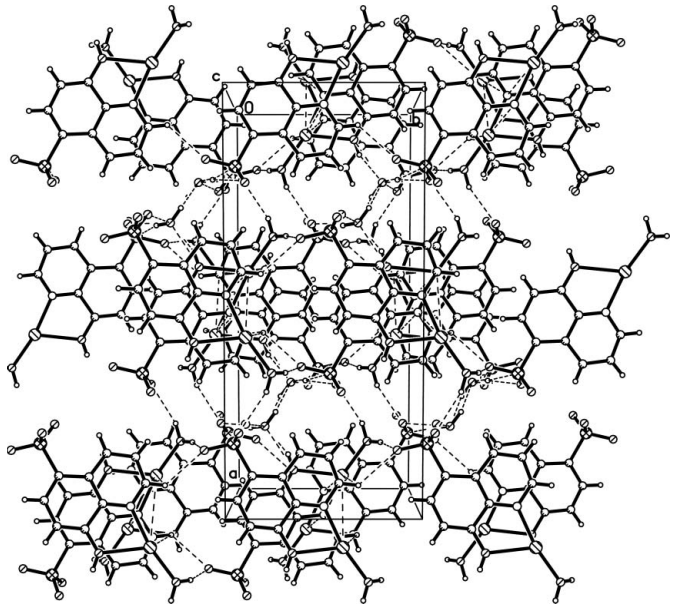


Figure 2
A packing diagram for (I). All H atoms and water molecules have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.169
S = 1.24
2741 reflections
178 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 65.3395P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—*OW*1	2.122 (9)	Ag1—O4	2.446 (8)
Ag1—N1	2.196 (7)		
*OW*1—Ag1—N1	168.8 (3)	N1—Ag1—O4	70.8 (2)
*OW*1—Ag1—O4	120.0 (3)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···*OW*2	0.82 (6)	1.81 (7)	2.595 (11)	160 (13)
*OW*1—H*W*1···O2^{i}	0.92 (6)	2.40 (8)	3.257 (12)	156 (13)
*OW*1—H*W*2···O3^{ii}	0.91 (6)	2.33 (9)	3.180 (12)	154 (13)
*OW*2—H*W*3···O2^{iii}	0.88 (6)	1.96 (7)	2.828 (11)	168 (14)
*OW*2—H*W*4···*OW*2^{iv}	0.91 (6)	2.48 (13)	3.02 (2)	118 (11)

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

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The hydroxy H atom and water H atoms were located in a difference Fourier map and refined with U_{iso}(H) = 1.5U_{eq}(O). The minimum electron-density peak is loacted 0.84 Å from atom Ag1.

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: *SHELXL97*.

The authors thank the National Natural Science Foundation of China (grant No. 20471014), the Programme for New Century Excellent Talents in Chinese Universities, the Fok Ying Tung Education Foundation and the Natural Science Foundation of Jilin Province, China, for support.

References

Cai, J.-W. (2004). *Coord. Chem. Rev.* **248**, 1061–1083.
Cote, A. P. & Shimizu, G. K. H. (2003). *Coord. Chem. Rev.* **245**, 49–64.
Cote, A. P. & Shimizu, G. K. H. (2004). *Inorg. Chem.* **43**, 6663–6673.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Li, F.-F., Ma, J.-F., Song, S.-Y., Yang, J., Liu, Y.-Y. & Su, Z.-M. (2005). *Inorg. Chem.* **44**, 9374–9383.
Ma, J.-F., Yang, J., Li, S.-L., Song, S.-Y., Zhang, H.-J., Wang, H.-S. & Yang, K.-Y. (2005). *Cryst. Growth Des.* **5**, 807–812.
Moulton, B. & Zaworotko, M. (2001). *Chem. Rev.* **101**, 1629–1658.
Hagrman, P. J., Hagrman, D. & Zubieta, J. (1999). *Angew. Chem. Int. Ed.* **38**, 2638–2684.
Rigaku (1998). *PROCESS-AUTO*. Version 1.06. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shimizu, G. K. H., Enright, G. D., Ratcliffe, C. I., Preston, K. F. Reid, J. L. & Ripmeester, J. A. (1999). *Chem. Commun.* pp. 1485–1486.
Wu, H., Dong, X.-W., Ma, J.-F. & Liu, H.-Y. (2006). *Acta Cryst.* E**62**, m281–m282.