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(2-Amino-3,5-dimethylbenzenesulfonato-κ*N*)-(2,2′-bipyridine)silver(I)

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Key indicators

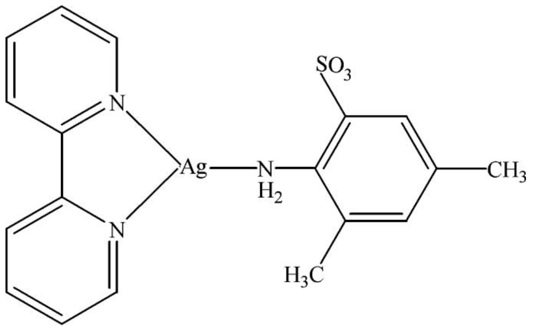
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.060
Data-to-parameter ratio = 16.6

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

The title compound, $[Ag(C_8H_{10}NO_3S)(C_{10}H_8N_2)]$, has a mononuclear structure in which the Ag^+ cation is three-coordinated by two N atoms from one 2,2′-bipyridine molecule and one N atom from a 2-amino-3,5-dimethylbenzenesulfonate anion in highly distorted trigonal–planar geometry. An intramolecular N—H···O hydrogen bond helps to establish the molecular conformation.

Comment

Compared to 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 to this generalization (Shimizu *et al.*, 1999; Mälinen *et al.*, 2001; Cote & Shimizu, 2004). Various silver–sulfonate complexes incorporating neutral ligands have been synthesized (Smith *et al.*, 1998; Li *et al.*, 2005) and these compounds show different silver coordination modes as a result of the presence of the secondary ligand. In this paper, the structure of the title compound, (I) (Fig. 1), containing a chelating 2,2′-bipyridine (bipy) molecule and 2-amino-3,5-dimethylbenzenesulfonate (*L*) anion is described.



(I)

In (I), both the *L* anion and bipy are coordinated to the metal, resulting in a highly distorted trigonal planar coordination geometry for Ag (Table 1). Atoms Ag1, N1, N2 and N3 are almost coplanar and the bond-angle sum about Ag is 359.8°. The $Ag—N_{bipy}$ distances are longer than the $Ag—N_L$ distance; both distances are similar to the equivalent values in related compounds (Wu *et al.*, 1999; Smith *et al.*, 1996). In (I), the coordination ability of the amine group of *L* is evidently stronger than that of sulfonate group and the latter group does not coordinate to the Ag ion. The dihedral angle between the two pyridine rings of the bipy ligand is 26.6 (3)°. There is an intramolecular N—H···O hydrogen bond involving the amino N atom and a sulfonate O atom (Table 2).

Experimental

An aqueous solution (10 ml) of 2-amino-3,5-dimethylbenzenesulfonic acid (0.101 g, 0.5 mmol) was added to solid Ag_2CO_3 (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO_2 was given off; 2,2′-bipyridine (0.096 g, 0.5 mmol) in methanol (5 ml) was then added and a white precipitate formed. The precipitate was dissolved by dropwise addition of an aqueous solution of NH_3 (14 *M*). Crystals of (I) were obtained by evaporation of the solution for several days at room temperature.

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_{10}H_8N_2)]$
$M_r = 464.28$
Monoclinic, $P2_1/n$
$a = 8.8936$ (18) Å
$b = 12.230$ (2) Å
$c = 16.510$ (3) Å
$\beta = 97.32$ (3)°
$V = 1781.1$ (6) Å^3
$Z = 4$
$D_x = 1.731$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10596 reflections
$\theta = 2.1$–27.4°
$\mu = 1.27$ mm^{-1}
$T = 294$ (2) K
Block, colorless
0.41 × 0.22 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.589$, $T_{max} = 0.786$
16745 measured reflections
4060 independent reflections
2708 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.4°$
$h = -11 \rightarrow 11$
$k = -15 \rightarrow 15$
$l = -20 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.060$
$S = 0.90$
4060 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.201 (2)	Ag1—N2	2.3243 (19)
Ag1—N3	2.3072 (19)		
N1—Ag1—N3	156.13 (8)	N3—Ag1—N2	71.85 (7)
N1—Ag1—N2	131.83 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—HN2···O1	0.87 (3)	2.12 (3)	2.862 (3)	144 (2)

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 H atoms of the amino group were located in a difference map and their positions and U_{iso} values were freely refined.

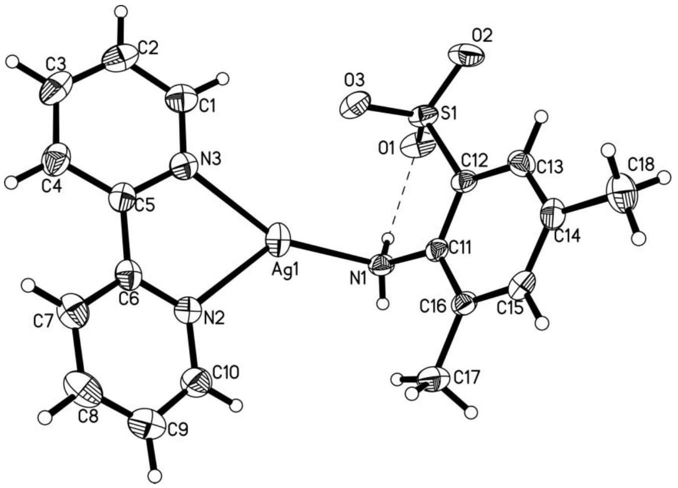


Figure 1
View of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms), with the hydrogen bond indicated by a dashed line.

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*.

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m326 Liu *et al.* • $[Ag(C_8H_{10}NO_3S)(C_{10}H_8N_2)]$ *Acta Cryst.* (2006). E**62**, m325–m326