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Tetrakis(β-picoline)disilver(I)(*Ag*—*Ag*) bis(2-amino-5-chlorobenzenesulfonate) dihydrate

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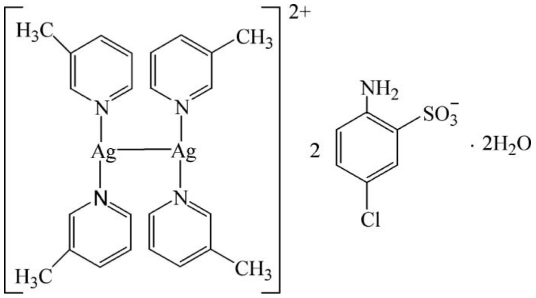
In the title compound $[Ag_2(Pic)_4]L_2\cdot 2H_2O$, where Pic is β-picoline (C_6H_7N) and L is the 2-amino-5-chlorobenzenesulfonate anion ($C_6H_5ClNO_3S$), each Ag^I cation is coordinated by two Pic molecules. Two $[Ag(Pic)_2]$ units are linked by an Ag–Ag interaction to give a centrosymmetric dication.

Key indicators
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.094
Data-to-parameter ratio = 17.8

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

Comment

Silver sulfonates can form inorganic–organic lamellar structures and these have been described recently (Cote & Shimizu, 2003; Shimizu *et al.*, 1998; Shimizu *et al.*, 1999). Silver sulfonate complexes incorporating neutral ligands have also been synthesized (Smith *et al.*, 1998; Li *et al.*, 2005); these compounds show different structural features depending on the secondary ligand. In this paper, the structure of the title compound, (I), is described.



(I)

As shown in Fig. 1, each silver cation is coordinated by two Pic molecules, with selected geometrical parameters in Table 1. The shortest Ag—O distance indicates that the sulfonate group does not coordinate to the Ag cation, but acts as a counter-ion. In the crystal structure, two $[Ag(Pic)_2]$ units (Pic is β-picoline) are linked by an Ag—Ag interaction (Table 1), forming a centrosymmetric dimeric $[Ag_2(Pic)_4]^{2+}$ cation.

In (I), the water molecule does not coordinate to Ag but forms hydrogen bonds to two O atoms from two sulfonate groups as a donor, and to one amino N atom as an acceptor. Each amino group forms hydrogen bonds with one sulfonate O atom and one water O atom.

Experimental

An aqueous solution of NaOH (0.1 M) was added to a solution of 2-amino-5-chlorobenzenesulfonic acid (0.104 g, 0.5 mmol) in water (5 ml) until the pH was 7. A solution of $AgNO_3$ (0.085 g, 0.5 mmol) in water (5 ml) was then added and a white precipitate formed immediately. The precipitate was dissolved by the addition of an aqueous solution of NH_3 (14 M, 5 ml) and a methanol solution (5 ml)

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of β-picoline (0.049 g, 0.5 mmol) was added. Colorless crystals of (I) were obtained by slow evaporation over a period of several days at room temperature.

Crystal data

$[Ag_2(C_6H_7N)_4](C_6H_5ClNO_3)\cdot 2H_2O$
$M_r = 1037.52$
Monoclinic, $P2_1/n$
$a = 12.491\ (3)$ Å
$b = 13.427\ (3)$ Å
$c = 12.984\ (3)$ Å
$\beta = 105.02\ (3)^\circ$
$V = 2103.2\ (9)$ Å^3
$Z = 2$
$D_x = 1.638$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.21$ mm^{-1}
$T = 292\ (2)$ K
Block, colorless
$0.13 \times 0.12 \times 0.10$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.851$, $T_{max} = 0.887$
20293 measured reflections
4797 independent reflections
3642 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.4^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.094$
$S = 1.10$
4797 reflections
269 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.5786P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.030$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.142 (2)	Ag1—Ag1^i	3.1226 (13)
Ag1—N2	2.143 (2)		
N1—Ag1—N2	168.81 (8)	N2—Ag1—Ag1^i	105.24 (6)
N1—Ag1—Ag1^i	83.64 (6)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
OW1—H1$D\cdots$O2	0.85 (1)	2.01 (2)	2.838 (4)	164 (6)
OW1—H1$C\cdots$O3^{ii}	0.85 (1)	2.48 (8)	2.858 (4)	107 (6)
N3—H1$A\cdots$O1	0.85 (1)	2.31 (2)	2.940 (3)	132 (2)
N3—H1$B\cdots$OW1^{iii}	0.84 (1)	2.13 (1)	2.962 (4)	169 (3)

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

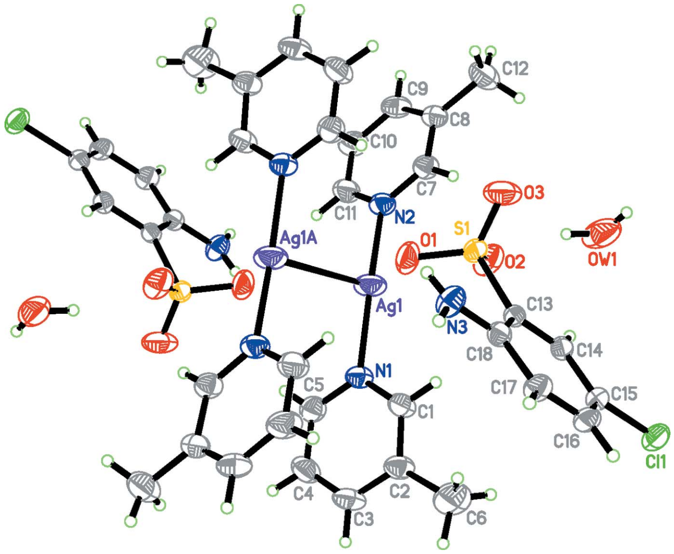

Figure 1
View of the structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H)= 1.2 or 1.5 times U_{eq}(C). The amino H atoms were located in a difference Fourier map and refined isotropically. The water H atoms were located in a difference Fourier map and refined with U_{iso}(H)= 1.5U_{eq}(O).

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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