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Key indicators

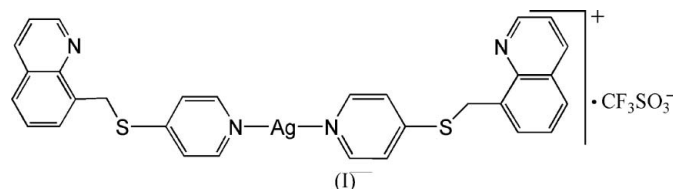
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
Disorder in solvent or counterion
 R factor = 0.048
 wR factor = 0.100
Data-to-parameter ratio = 14.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis[8-(4-pyridylsulfanylmethyl- κ N)quinoline]silver(I) trifluoromethanesulfonate

The title mononuclear complex, $[\text{Ag}(\text{C}_{15}\text{H}_{12}\text{N}_2\text{S}_2)_2]\text{CF}_3\text{SO}_3$, reveals the molecular symmetry C_2 with the Ag atom located on a crystallographic twofold axis. The Ag^{I} centre is coordinated by two pyridine N -donors of two 8-(4-pyridylsulfanylmethyl)quinoline ligands in an almost linear geometry. The $\text{N}-\text{Ag}-\text{N}$ angle is $173.06(18)^\circ$ and the $\text{Ag}-\text{N}$ distance is $2.129(3)$ Å.

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Comment

Heterocyclic flexible thioether ligands containing nitrogen donors are well known ligands in transition metal coordination compounds (Hong *et al.*, 2000*b*; Suenaga *et al.*, 1999; Zou *et al.*, 2004). An increasing number of Ag^{I} complexes with such ligands are being investigated because of their intriguing structural diversity and potential applications as functional materials (Hartshorn & Steel, 1998; Hong *et al.*, 2000*a*; Su *et al.*, 2000; Zheng *et al.*, 2003). Therefore, we prepared the 8-(4-pyridylsulfanylmethyl)quinoline ligand and its title silver complex, (I).



Complex (I) consists of a discrete mononuclear $[\text{Ag}(\text{L})_2]^+$ cation and an uncoordinated trifluoromethanesulfonate anion. The $[\text{Ag}(\text{L})_2]^+$ ion comprises two L ligands and one Ag^{I} ion, and possesses twofold rotation symmetry (Fig. 1). Each Ag atom, located on the twofold axis [special position $4(e)$ of the space group $C2/c$], has a slightly distorted linear geometry, coordinated by two pyridine N atoms of 8-(4-pyridylsulfanylmethyl)quinoline (Table 1, Fig. 1). A weak $\text{Ag} \cdots \text{O}$ interaction with a distance of $3.309(3)$ Å is observed (Fig. 1). The planes of the pyridine and quinoline rings of each L ligand form a dihedral angle of $80.8(1)^\circ$, and the dihedral angle between the two pyridine rings is $65.1(1)^\circ$.

The molecular packing of (I) is influenced by intermolecular $\pi-\pi$ interactions; the pyridine rings are separated by $3.779(4)$ and $3.779(4)$ Å (Fig. 2).

Experimental

The ligand 8-(4-pyridylsulfanylmethyl)quinoline was prepared by the reported procedure (Song *et al.*, 2003). The title complex was prepared by adding slowly a solution of AgCF_3SO_3 (26 mg, 0.1 mmol)

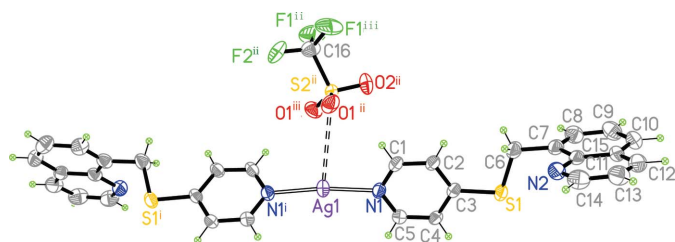


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. The dashed line indicates the weak Ag...O interaction. [Symmetry codes: (i) $-x + 1, y, -z - \frac{1}{2}$; (ii) $x, y, z - 1$; (iii) $1 - x, y, \frac{1}{2} - z$.]

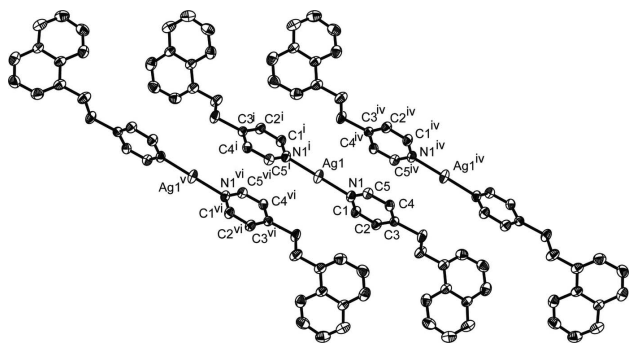


Figure 2
A view of intermolecular π - π interactions between the parallel pyridine rings of neighbouring complex cations [symmetry codes: (i) $-x + 1, y, -z - \frac{1}{2}$; (iv) $1 - x, -y, -z$; (v) $1 - x, -y, -z - 1$; (vi) $x, -y, -\frac{1}{2} + z$].

in CH_3CN (3 ml) to a solution of *L* (25 mg, 0.1 mmol) in CHCl_3 (3 ml). Slow diffusion of acetone into the resulting solution yielded colourless single crystals of (I) suitable for X-ray analysis in 28% yield. Analysis found: C 48.23, H 3.11, N 7.37; calculated for $\text{C}_{31}\text{H}_{24}\text{AgF}_3\text{N}_4\text{O}_3\text{S}_3$: C 48.89, H 3.18, N 7.36%.

Crystal data

$[\text{Ag}(\text{C}_{15}\text{H}_{12}\text{N}_2\text{S})_2]\text{CF}_3\text{SO}_3$	$Z = 4$
$M_r = 761.59$	$D_x = 1.637 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 24.851(8) \text{ \AA}$	$\mu = 0.91 \text{ mm}^{-1}$
$b = 9.276(3) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 14.091(4) \text{ \AA}$	Block, colourless
$\beta = 107.991(6)^\circ$	$0.30 \times 0.22 \times 0.20 \text{ mm}$
$V = 3089.4(17) \text{ \AA}^3$	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	8559 measured reflections
φ and ω scans	3182 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)	1786 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.891, T_{\max} = 1.000$	$R_{\text{int}} = 0.048$
(expected range = 0.742–0.833)	$\theta_{\text{max}} = 26.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.100$
 $S = 1.00$
 3182 reflections
 222 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 2.1514P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Ag1–N1	2.129 (3)	N1–C5	1.338 (5)
N1–C1	1.336 (5)		
N1 ⁱ –Ag1–N1	173.06 (18)	C1–N1–Ag1	120.2 (3)
C1–N1–C5	116.7 (3)	C5–N1–Ag1	123.1 (3)

Symmetry code: (i) $-x + 1, y, -z - \frac{1}{2}$.

H atoms were included in calculated positions and refined in a riding model with C–H distances of 0.93 (aromatic H) and 0.97 \AA (methylene H), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The CF_3SO_3 anion is disordered: S2, O2 and F2 are disordered between two positions, each with occupancy 50%.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1999); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXL97.

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