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## Key indicators

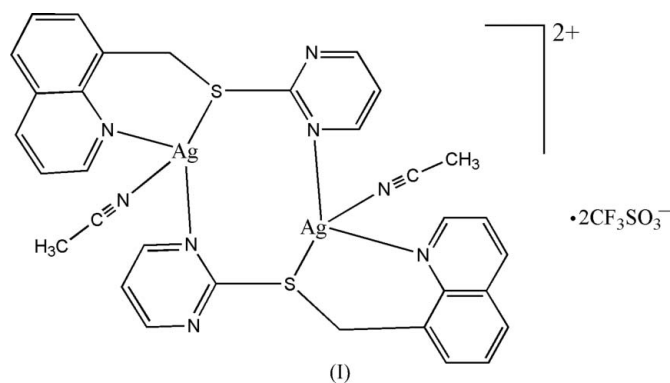
Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$   
Disorder in solvent or counterion  
R factor = 0.038  
wR factor = 0.101  
Data-to-parameter ratio = 14.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis[ $\mu$ -8-(pyrimidin-2-ylsulfanylmethyl)-quinoline- $\kappa^2N,S$ ]bis[(acetonitrile)silver(I)]bis(trifluoromethanesulfonate)

In the twofold-symmetric dinuclear title compound,  $[\text{Ag}_2(\text{C}_{14}\text{H}_{11}\text{N}_3\text{S})_2(\text{CH}_3\text{CN})_2](\text{CF}_3\text{SO}_3)_2$ , each  $\text{Ag}^{\text{I}}$  atom is coordinated by one N atom and one S atom from one 8-(pyrimidin-2-ylsulfanylmethyl)quinoline ligand, one N atom from a second 8-(pyrimidin-2-ylsulfanylmethyl)quinoline ligand, and one N atom of  $\text{CH}_3\text{CN}$ , in a distorted trigonal pyramidal geometry. The *cis* bond angles around the  $\text{Ag}^{\text{I}}$  atom range from  $90.8(2)$  to  $143.48(11)^\circ$ .

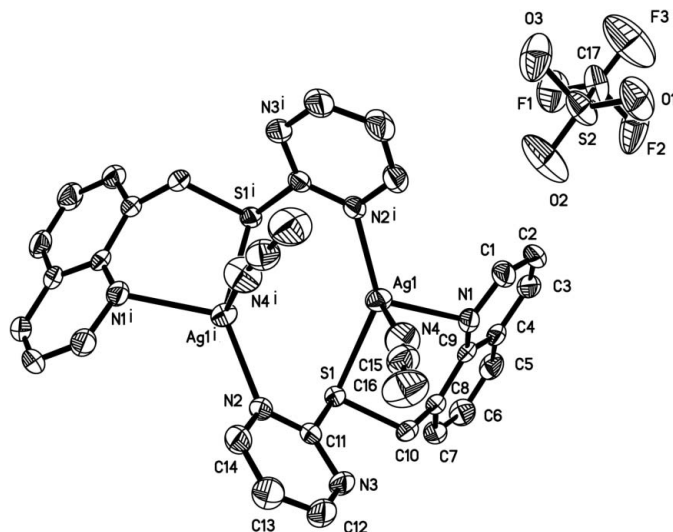
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## Comment

Dinuclear and polynuclear Ag compounds with luminescent properties and varying Ag...Ag interactions have been designed and synthesized by using suitable bridging ligands (Che *et al.*, 2000; Fei *et al.*, 2001; Tong *et al.*, 2000). Heterocyclic flexible thioether ligands containing N-donors exhibit rich structural variety, and reports of  $\text{Ag}^{\text{I}}$  complexes with such ligands have increased in recent years (Hartshorn & Steel, 1998; Su *et al.*, 2000; Suenaga *et al.*, 1999; Zheng *et al.*, 2003). The title compound, (I) is a dinuclear  $\text{Ag}^{\text{I}}$  complex of the flexible thioether ligand 8-(pyrimidin-2-ylsulfanylmethyl)quinoline (L).



Complex (I) consists of twofold-symmetric  $[\text{Ag}_2(\text{L})_2(\text{CH}_3\text{CN})_2]^{2+}$  cations and uncoordinated  $\text{CF}_3\text{SO}_3^-$  anions (Fig. 1). Each  $\text{Ag}^{\text{I}}$  atom is coordinated by a quinoline and a pyrimidine N-donor from two distinct L ligands, an S-donor from one L ligand, and an N-donor from  $\text{CH}_3\text{CN}$ . The coordination geometry of  $\text{Ag}^{\text{I}}$  is best described as trigonal pyramidal, with the basal plane made up of the N- and S-donors from the ligand, and the apical position occupied by the N-donor of  $\text{CH}_3\text{CN}$ . The *cis* bond angles around the  $\text{Ag}^{\text{I}}$  atom range from  $90.8(2)$  to  $143.48(11)^\circ$  (Table 1). All distances around  $\text{Ag}^{\text{I}}$  (Table 1) are within the normal range expected for such coordination bonds (Hartshorn & Steel, 1998; Su *et al.*, 2000; Zheng *et al.*, 2003; Zou *et al.*, 2004). Each



**Figure 1**  
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level. H atoms have been omitted. [Symmetry code: (i)  $1 - x, \frac{1}{2} - y, z$ .]

*L* ligand adopts a chelating coordination mode to  $\text{Ag}^{\text{I}}$  through the S and quinoline N atoms, forming a six-membered ring which has a distorted boat conformation. The pyrimidine N atom of each ligand bridges to another  $\text{Ag}^{\text{I}}$  atom, forming a twofold-symmetric eight-membered dinuclear ring, in which the  $\text{Ag} \cdots \text{Ag}^{\text{i}}$  separation is 3.479 (1) Å [symmetry code: (i)  $1 - x, \frac{1}{2} - y, z$ ].

## Experimental

A solution of  $\text{AgCF}_3\text{SO}_3$  (26 mg, 0.1 mmol) in  $\text{CH}_3\text{CN}$  (3 ml) was slowly added to a solution of 8-(pyrimidin-2-ylsulfanylmethyl)quinoline (25 mg, 0.1 mmol) in  $\text{CHCl}_3$  (3 ml). Slow diffusion of acetone into the resulting solution yielded colourless single crystals of (I) suitable for X-ray crystallographic analysis in 21% yield. Elemental analysis found: C 37.23, H 2.59, N 10.13%; calculated: C 37.04, H 2.56, N 10.16%.

### Crystal data

$[\text{Ag}_2(\text{C}_{14}\text{H}_{11}\text{N}_3\text{S})_2(\text{C}_2\text{H}_3\text{N})_2](\text{CF}_3\text{O}_3\text{S})_2$	$Z = 8$
$M_r = 1102.62$	$D_x = 1.814 \text{ Mg m}^{-3}$
Tetragonal, $I4_1/a$	Mo $K\alpha$ radiation
$a = 21.579$ (3) Å	$\mu = 1.26 \text{ mm}^{-1}$
$c = 17.342$ (5) Å	$T = 293$ (2) K
$V = 8075$ (3) Å <sup>3</sup>	Block, colourless
	$0.30 \times 0.28 \times 0.26 \text{ mm}$

### Data collection

Bruker SMART 1000 CCD diffractometer	22965 measured reflections
$\varphi$ and $\omega$ scans	4145 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2830 reflections with $I > 2\sigma(I)$
$T_{\text{min}} = 0.690, T_{\text{max}} = 0.720$	$R_{\text{int}} = 0.043$
	$\theta_{\text{max}} = 26.5^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.101$   
 $S = 1.03$   
 4145 reflections  
 290 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 13.311P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.51 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.43 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Ag1—S1	2.5347 (10)	Ag1—N2 <sup>i</sup>	2.233 (3)
Ag1—N1	2.377 (3)	Ag1—N4	2.440 (5)
N2 <sup>i</sup> —Ag1—N1	123.33 (11)	N2 <sup>i</sup> —Ag1—S1	143.44 (8)
N2 <sup>i</sup> —Ag1—N4	91.22 (14)	N1—Ag1—S1	90.85 (8)
N1—Ag1—N4	100.75 (15)	N4—Ag1—S1	94.86 (12)

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

H atoms were included in calculated positions and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 (methylene) or 0.96 Å (methyl), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . The trifluoromethanesulfonate anion was modelled as disordered, with atoms F2/F2' and O3/O3' having site-occupancy factors 0.773 (8)/0.227 (8).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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: *SHELXTL*.

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## References

- Bruker (1998). *SMART, SAINT and SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Che, C. M., Tse, M. C., Chan, M. C. W., Cheung, K. K., Phillips, D. L. & Leung, K. H. (2000). *J. Am. Chem. Soc.* **122**, 2464–2468.
- Fei, B. L., Sun, W. Y., Okamura, T., Tang, W. X. & Ueyama, N. (2001). *New J. Chem.* **25**, 210–212.
- Hartshorn, C. M. & Steel, P. J. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3935–3940.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97 and SHELXL97*. University of Göttingen, Germany.
- Su, C. Y., Liao, S., Zhu, H. L., Kang, B. S., Chen, X. M. & Liu, H. Q. (2000). *J. Chem. Soc. Dalton Trans.* pp. 1985–1993.
- Suenaga, Y., Kuroda-Sowa, T., Mackewa, M. & Munakata, M. (1999). *J. Chem. Soc. Dalton Trans.* pp. 2737–2741.
- Tong, M. L., Yu, X. L. & Chen, X. M. (2000). *Inorg. Chem. Commun.* **3**, 694–696.
- Zheng, Y., Du, M., Li, J.-R., Zhang, R. H. & Bu, X.-H. (2003). *Dalton Trans.* pp. 1509–1514.
- Zou, R.-Q., Li, J.-R., Xie, Y.-B., Zhang, R.-H. & Bu, X.-H. (2004). *Cryst. Growth Des.* **4**, 79–84.