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Hexakis(μ_3-pyridine-2-thiolato-κ^3N:S:S)hexasilver(I), [$Ag_6(\mu_3\text{-SPy})_6$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.019 Å
R factor = 0.053
wR factor = 0.120
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.

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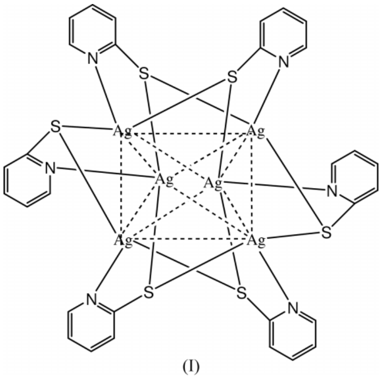
All six Ag^I atoms of the title compound, [$Ag_6(\mu_3\text{-}C_5H_4NS)_6$], are bridged through the six S atoms of the six pyridine-2-thiolate ligands to form an Ag_6 cluster. Each of the six Ag^I atoms exhibits a distorted trigonal coordination geometry, with two thiolate S atoms and an N atom from three pyridine-2-thiolate ligands. The Ag—S distances are in the range 2.459 (3)–2.488 (3) Å and the Ag—N bond distances range from 2.307 (8) to 2.320 (8) Å. Each thiolate S atom bridges two Ag^I atoms. In the hexamer, the six Ag^I atoms are in a nearly perfect octahedral configuration and this hints at a weak $Ag^I\cdots Ag^I$ interaction. The molecule is located on a centre of inversion, with only one half constituting the asymmetric unit.

Comment

There is currently considerable interest in coinage metal compounds, such as silver(I) and copper(I) with thiolate ligands, because of their potential as functional solid materials (Jin *et al.*, 2002; Tang *et al.*, 2002). Thiolates, acting as μ_2-, μ_3- or μ_4-bridging ligands, are used to link metal ions, yielding polynuclear or polymeric complexes as a result of versatile coordination modes (Kitagawa *et al.*, 1990; Su *et al.*, 1998). Recently, several silver(I) thiolate polymers have been synthesized with different architectures, using pyridine-2-thiolate as a ligand (Hong *et al.*, 1999; Su *et al.*, 2000). Herein, we report the crystal structure of a silver complex, [$Ag_6(SPy)_6$], (I), which contains a distorted octahedral Ag_6 cluster located on a centre of inversion.



(I)

The title complex has a hexanuclear structure with the Ag atoms in a distorted octahedral arrangement. The $Ag\cdots Ag$ distances are in the range 2.9950 (11)–3.2830 (12) Å, indicating the existence of weak metal–metal interactions, similar to those (2.882–3.159 Å) observed in the molecule of [{Ag(SR)}$_6$] (R = 6-*tert*-butyldimethylsilyl-2-pyridyl; Perez-

Lourido *et al.*, 1996). Each Ag atom is bonded to a pyridine N atom and two thiolate S atoms from three pyridine-2-thiolate ligands, forming a trigonal geometry. Each pyridine-2-thiolate ligand is bonded to three different Ag^I atoms, defining a face of an octahedron. Each thiolate S atom bridges two Ag^I atoms. The Ag—S distances are in the range 2.459 (3)–2.488 (3) Å and the Ag—N bond distances range from 2.307 (8) to 2.320 (8) Å; these are very similar to those found in other hexanuclear complexes of silver with derivatives of pyridine-2-thiolate (Nomiya *et al.*, 2000; Block *et al.*, 1988; Garcia-Vazquez *et al.*, 2000).

Experimental

To a solution of sodium pyridine-2-thiolate (0.027 g, 0.2 mmol) in dichloromethane (10 ml), a methanol solution (5 ml) of $AgPF_6$ (0.05 g, 0.2 mmol) was added dropwise. After stirring the mixture with exclusion of light for 12 h, it was filtered. Slow diffusion of diethyl ether into the resulting solution yielded, in a few days, well-shaped pale-yellow crystals suitable for X-ray diffraction.

Crystal data

$[Ag_6(C_5H_4NS)_6]$
$M_r = 1308.14$
Monoclinic, $P2_1/n$
$a = 9.9298$ (2) Å
$b = 16.4275$ (5) Å
$c = 12.4812$ (4) Å
$\beta = 108.817$ (1)°
$V = 1927.14$ (9) Å^3
$Z = 2$

$D_x = 2.254$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 217 reflections
$\theta = 2.1$–25.0°
$\mu = 3.35$ mm^{-1}
$T = 293$ (2) K
Block, pale yellow
0.35 × 0.25 × 0.22 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.325$, $T_{\max} = 0.479$
6003 measured reflections

3348 independent reflections
2591 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 25.0°$
$h = -8 \rightarrow 11$
$k = -12 \rightarrow 19$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.120$
$S = 1.26$
3348 reflections
217 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0246P)^2 + 13.1839P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.01$ e Å^{-3}
$\Delta\rho_{\min} = -0.87$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N3	2.307 (8)	Ag2—S2	2.480 (3)
Ag1—S1	2.459 (3)	Ag2—S3	2.480 (3)
Ag1—S2^i	2.488 (3)	Ag2···Ag3	2.9950 (11)
Ag1···Ag2	3.0021 (11)	Ag2···Ag3^i	3.1867 (12)
Ag1···Ag3^i	3.0089 (11)	Ag3—N2	2.320 (8)
Ag1···Ag3	3.1609 (11)	Ag3—S1	2.472 (3)
Ag1···Ag2^i	3.2830 (12)	Ag3—S3^i	2.483 (3)
Ag2—N1	2.311 (8)		
N3—Ag1—S1	121.9 (2)	S2—Ag2—S3	122.07 (9)
N3—Ag1—S2^i	106.4 (2)	N2—Ag3—S1	113.8 (2)
S1—Ag1—S2^i	123.27 (9)	N2—Ag3—S3^i	109.9 (2)
N1—Ag2—S2	108.9 (2)	S1—Ag3—S3^i	126.77 (9)
N1—Ag2—S3	119.8 (2)		

Symmetry code: (i) $3 - x, -y, -z$.

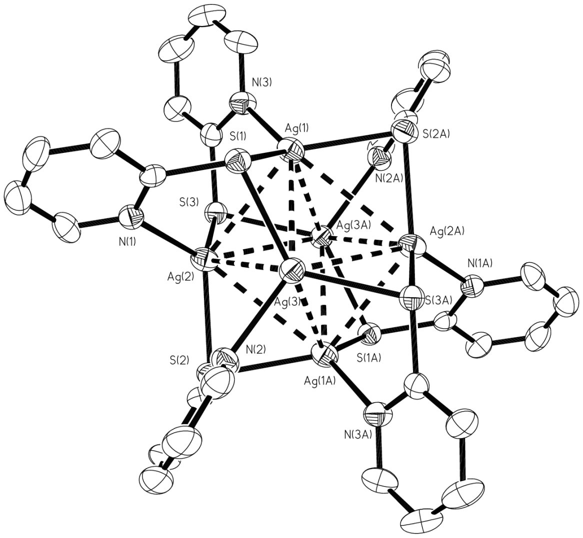


Figure 1
Perspective view of the title complex, with the atom-numbering scheme. Displacement ellipsoids are shown at the 30% probability level. All H atoms have been omitted for clarity.

H-atom positions were generated geometrically and the H atoms were allowed to ride on their respective parent C atoms.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL*97.

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