Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[silver(I)-di-μ-1,5-bis(phenylthio)pentane] hexafluorophosphate]: a two-dimensional molecular-rectangle coordination ploymer

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Received 11 April 2001
Accepted 19 April 2001
Online 10 May 2001

In the title Ag^I complex of 1,5-bis(phenylthio)pentane, $\{[Ag(C_{17}H_{20}S_2)_2]PF_6\}_n$, Ag^I centers coordinate to four S atoms and display a distorted tetrahedral geometry. Ligands link adjacent Ag^I atoms to form an infinite parquet-like framework. The PF_6^- ions are incorporated in the cavities of the network to complete and stabilize the structure.

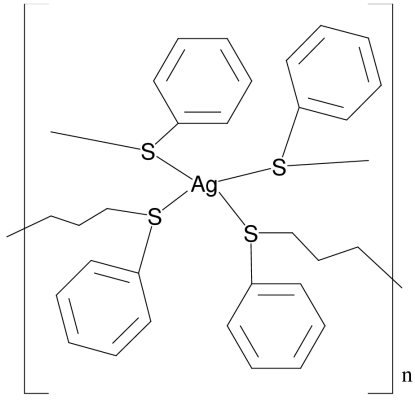
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.034
wR factor = 0.089
Data-to-parameter ratio = 12.4

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

Comment

Crystal engineering and the construction of coordination networks with fascinating structural topologies has attracted much attention in recent years due to their potential as functional materials (Li *et al.*, 1999). Concurrent with this has been the development of multidimensional networks based primarily on linking metal centers with rigid bridging components, such as 4,4′-bipyridine, *etc* (Blake *et al.*, 1999). Far less common has been the use of flexible bridging units in the construction of extended networks (Ma *et al.*, 2000), and because of the flexibility and conformational freedom of such ligands, the construction of unprecedented frameworks with useful properties is possible. We report herein a Ag^I complex forming a unique macrometallocyclic lamellar network by using a flexible dithioether, *viz*. 1,5-bis(phenylthio)pentane (L), as building block, namely poly[[silver(I)-di-μ-1,5-bis(-phenylthio)pentane] hexafluorophosphate], (I).



(I)

In the title complex, (I), each Ag^I center is coordinated by four S atoms from four distinct ligands and displays a distorted tetrahedral geometry, as shown in Fig. 1. Each Ag^I center is connected to four other adjacent Ag^I centers by four ligands in orthogonal directions, forming a 32-membered macrometallocyclic Ag_4L_4 repeating unit with dimensions 10.22 × 9.39 $Å^2$ (Fig. 2). Four Ag^I centers in the unit are coplanar (the

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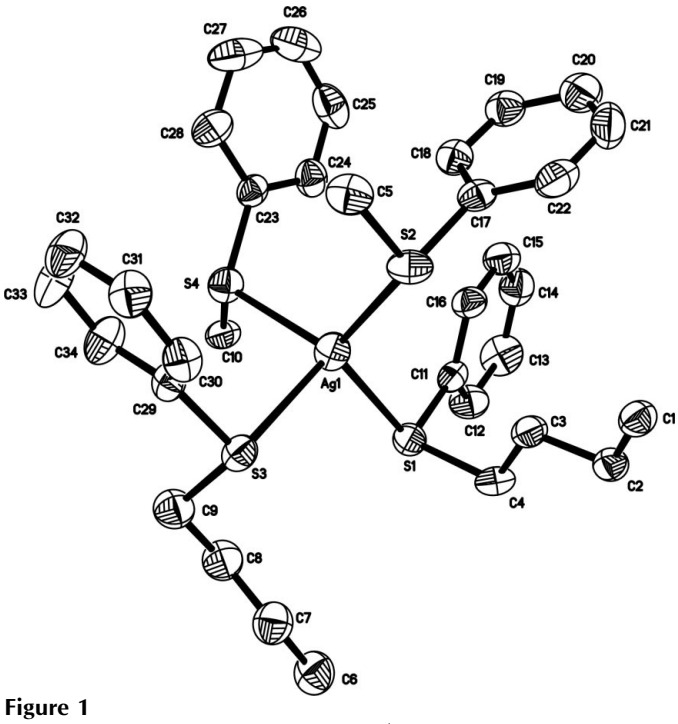

Figure 1
*ORTEP*II (Johnson, 1976) view of $[Ag\mathit{L}]^+$ of the title complex with 30% probability displacement ellipsoids.

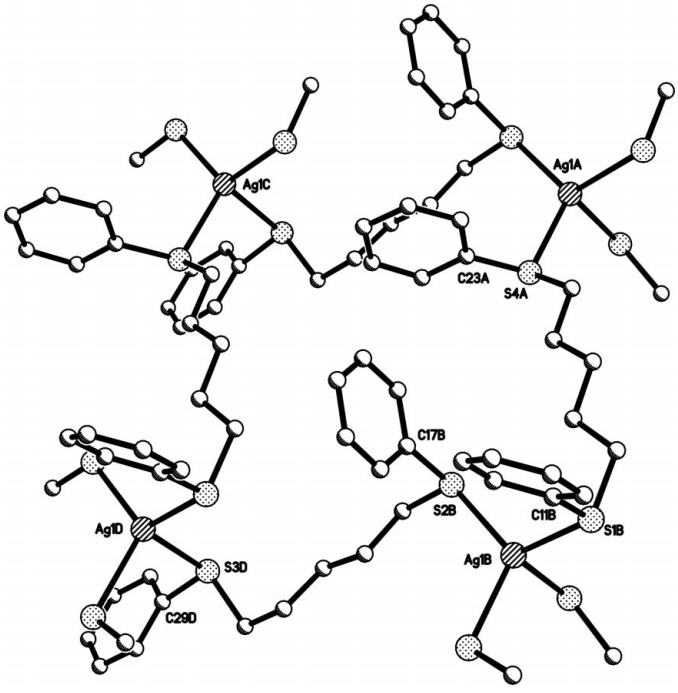

Figure 2
View of the 32-membered $Ag_4\mathit{L}_4$ macrometallocyclic repeat unit of (I).

mean planar derivation is zero). There are two conformations (*A* and *B*) of *L*. In conformtion *A*, *L* joins adjacent Ag^I atoms in a *cis*-mode: two phenyl groups of *L* are located on the same side of the Ag_4 plane, with a C11*b*—S1*b*—S4*a*—C23*a* torsion angle of 29.6°, *i.e.* between two S—C_{Ph} units. The dihedral angle between the phenyl groups is 29.2°. In comparison with

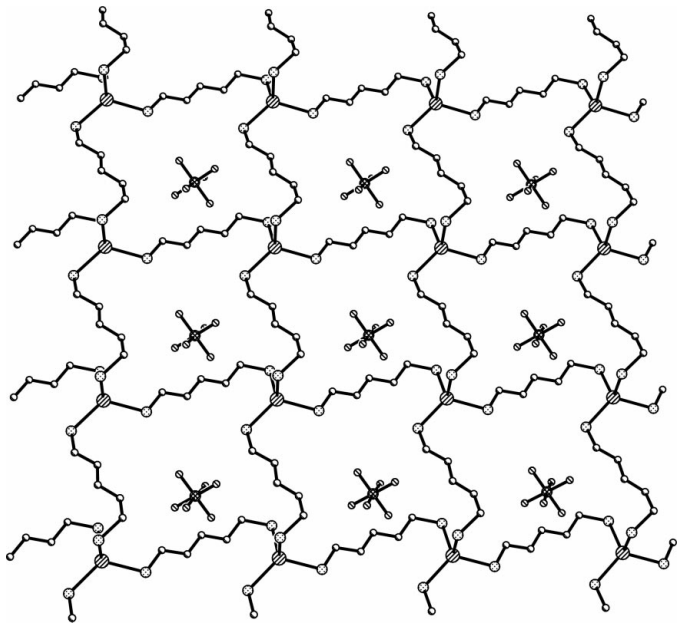

Figure 3
View of the two-dimensional molecular-rectangle network of (I)

conformation *A*, *L* in *B* adopts a *trans*-mode: the phenyl groups of *L* (dihedral angle 85.3°) are located on different sides of the Ag_4 plane and form a C17*b*—S2*b*—S3*d*—C29*d* torsion angle of 170.5°. The two-dimensional molecular-rectangle network of (I) is shown in Fig. 3, which presents an interesting example of an Ag^I complex with dithioether ligands. The PF_6^- ions are incorporated in the cavity of the repeating unit to keep the structure stable. Adjacent rectangle rings are fused in a parquet-like pattern to form an infinite lamellar molecular-rectangle framework.

Experimental

1,5-Bis(phenylthio)pentane (*L*) was prepared by a reported procedure (Shao *et al.*, 1991). The title complex, $\{[Ag(\mathit{L})_2]PF_6\}_n$, was obtained by mixing equimolar amounts of *L* dissolved in $CHCl_3$ and $AgPF_6$ in acetone at room temperature. Colorless single crystals were obtained by slow evaporation of the solvent in the dark (yield 40%). Analysis calculated for the title complex: C 49.21, H 4.86%; found: C 49.17, H 5.01%.

Crystal data

$[Ag(C_{17}H_{20}S_2)_2]PF_6$
M_r = 829.74
Monoclinic, *Pc*
a = 9.3876 (10) Å
b = 10.2213 (11) Å
c = 19.640 (2) Å
β = 103.161 (2)°
V = 1835.0 (3) Å^3
Z = 2
D_x = 1.502 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7412 reflections
θ = 2.0–25.0°
μ = 0.87 mm^{-1}
T = 293 (2) K
Prism, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART1000 diffractometer
ω scans
Absorption correction: multi-scan [*SAINT* (Bruker, 1998) and *SADABS* (Sheldrick, 1997)]
$T_{min} = 0.779$, $T_{max} = 0.845$
7412 measured reflections
5142 independent reflections
4522 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.0°$
$h = -11 \rightarrow 8$
$k = -12 \rightarrow 9$
$l = -22 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.089$
$S = 1.02$
5142 reflections
415 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.1885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.019$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—S4	2.6040 (13)	Ag1—S1	2.6241 (14)
Ag1—S2	2.6059 (15)	Ag1—S3	2.6809 (13)
S4—Ag1—S2	120.18 (5)	S4—Ag1—S3	100.97 (4)
S4—Ag1—S1	105.66 (4)	S2—Ag1—S3	99.81 (5)
S2—Ag1—S1	120.61 (5)	S1—Ag1—S3	106.64 (4)

The C-bound H atoms were placed in geometrically calculated positions and included in the final refinement in the riding model approximation with displacement parameters derived from the atoms to which they were bonded.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *XP* (Bruker, 1998).

We gratefully acknowledge financial support from the National Natural Science Foundation of China (No. 29971019), Tianjin Natural Science Foundation and the Trans-Century Talents Training Program Foundation from the State Education Ministry of China.

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