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The two-dimensional coordination polymer poly[[silver(I)-di-μ-1,5-bis(phenylsulfanyl)pentane] tetrafluoroborate]

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Key indicators

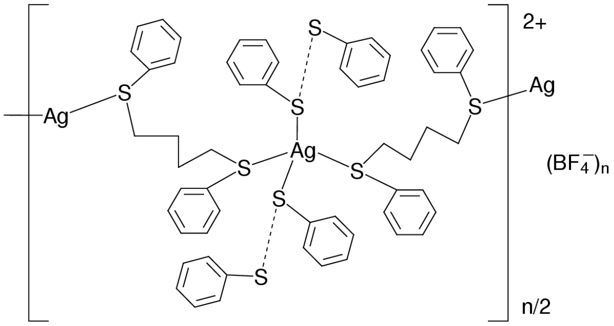
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
Disorder in solvent or counterion
R factor = 0.030
wR factor = 0.064
Data-to-parameter ratio = 11.9

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

A two-dimensional silver(I) coordination polymer, $\{[Ag(L)_2]BF_4\}_n$, has been formed from $AgBF_4$ and 1,5-bis(phenylsulfanyl)pentane (L, $C_{17}H_{20}S_2$), in which each silver(I) center is coordinated by four S atoms from distinct ligands and displays a distorted tetrahedral geometry. Each ligand links two Ag^I atoms to form an infinite two-dimensional (4,4)-grid-like network. The BF_4^- ions are incorporated into the cavities of the coordination framework to complete and stabilize the structure.

Comment

The crystal engineering of one-, two- and three-dimensional coordination polymers is currently attracting considerable attention, not only because of their novel topologies and fascinating structural diversities, but also for their potential applications in optical, electrical, magnetic and microporous materials (Blake *et al.*, 1999; Hagrman *et al.*, 1999; Evans & Lin, 2002). In the past decade, a variety of discrete and a wide range of one- or multi-dimensional infinite solid-state coordination architectures have been achieved by chemists. It is well known that the overall topology of coordination polymers depends mainly on the coordination preferences of metal centers and the backbone of bridging ligands. The rational design of organic building blocks plays a key role in adjusting the coordination frameworks, and the nature of the coordinating donors may lead to the formation of unique networks with desired properties and functions. We report here an Ag^I complex, namely poly[[silver(I)-di-μ-1,5-bis(phenylsulfanyl)-pentane] tetrafluoroborate], (I), which forms a unique macrometallacyclic lamellar network using the flexible dithioether ligand 1,5-bis(phenylsulfanyl)pentane, L, as the building block.



(I)

A two-dimensional silver(I) coordination polymer is found for the $[Ag(L)_2]^+$ cation of (I). As depicted in Fig. 1, each silver(I) center is coordinated by four S donors from four

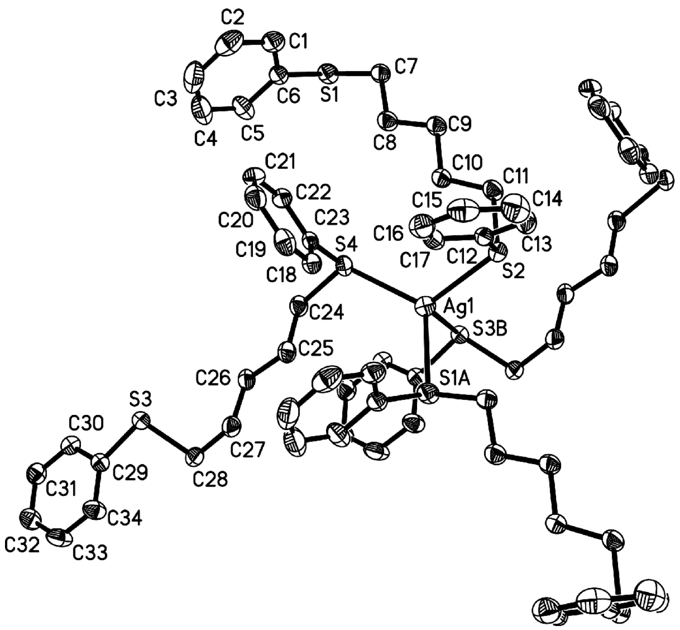


Figure 1
Coordination environment of silver(I) in the structure of (I) (the BF_4^- ion has been omitted for clarity), with displacement ellipsoids drawn at the 30% probability level. Atoms with suffixes *A* and *B* are related to those with no suffixes by the symmetry codes $(x, y - 1, z)$ and $(1 + x, y, z)$, respectively.

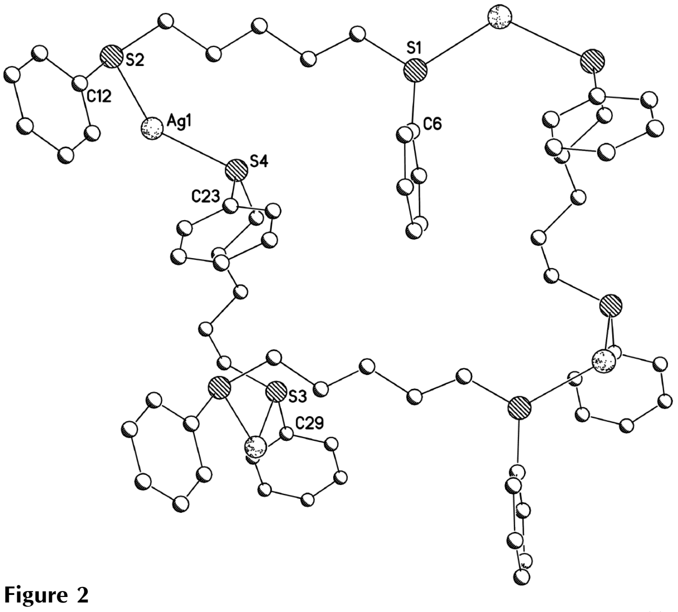


Figure 2
View of the 32-membered Ag_4L_4 macrometallacyclic repeating unit of (I).

distinct ligands, displaying a distorted tetrahedral geometry (see Table 1 for selected geometric parameters), and is thus connected to four other adjacent silver(I) centers by four ligands, forming a 32-membered macrometallocyclic $[Ag_4L_4]$ repeating unit, with dimensions of 10.18 × 9.21 Å^2, in which four Ag^I atoms are coplanar, as shown in Fig. 2. There are two configurations, *A* and *B*, for the ligand molecules. In type *A*, *L* links adjacent Ag^I atoms in a *cis*-mode; the two phenyl groups of *L* are located on the same side of the Ag_4 plane, with a C6—S1—S2—C12 torsion angle (between two S/C_{Ph} units) of 35.3 (4)°, and a dihedral angle between the phenyl groups of 29.2 (4)°. In contrast with conformation *A*, *L* in type *B* adopts a *trans*-mode; the phenyl groups of *L* [dihedral angle: 94.3 (3)°] are located on opposite sides of the Ag_4 plane, forming a C29—S3—S4—C23 torsion angle of −179.5 (4)°. The BF_4^- ions are incorporated in the cavities of the repeating units to balance the charge, and have a special templating effect in building up this coordination polymer. Adjacent rectangular rings are fused in a parquet-like pattern to form an infinite lamellar (4,4) coordination framework parallel to (110), as shown in Fig. 3. Examination of the structure with *PLATON* (Spek, 2003) indicates that there are no solvent-accessible voids or π–π stacking interactions in the crystal structure of (I).

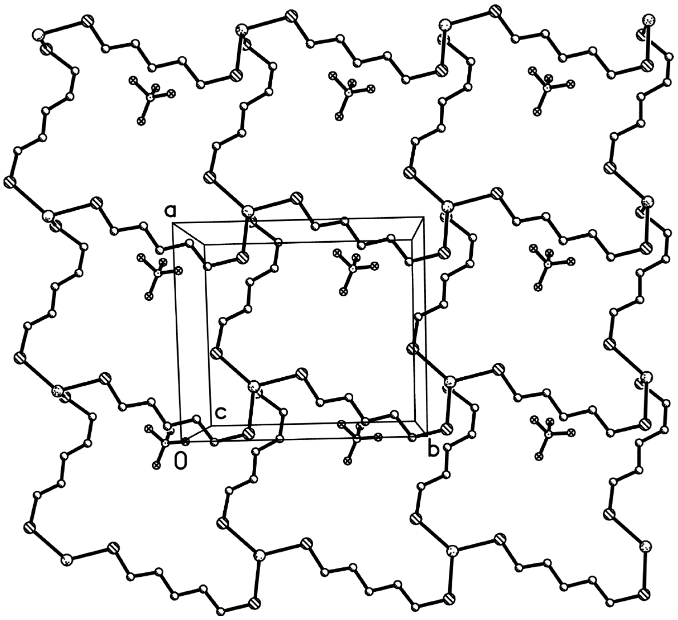


Figure 3
View of the two-dimensional rectanglar network of (I).

Experimental

1,5-Bis(phenylsulfanyl)pentane (*L*) was prepared according to the procedure reported by Shao *et al.* (1991). $AgBF_4$ (19 mg, 0.1 mmol) in acetone (5 ml) was added slowly to a solution of *L* (29 mg, 0.1 mmol) in chloroform (5 ml). The mixture was refluxed for 30 min and allowed to stand at room temperature. Colorless well shaped single crystals were obtained by slow evaporation of the solvent (yield 55%). IR (KBr pellet, cm^{-1}): 2929 (*s*), 2855 (*m*), 1584 (*s*), 1479 (*vs*), 1459 (*m*), 1438 (*s*), 1384 (*w*), 1301 (*m*), 1271 (*w*), 1232 (*m*), 1089 (*vs*), 1055 (*vs*), 738 (*vs*), 690 (*vs*), 616 (*w*), 534 (*m*), 522 (*m*), 482 (*m*), 473 (*m*). Analysis calculated for $C_{34}H_{40}AgBF_4S_4$: C 52.93, H 5.23%; found: C 52.84, H 5.11%.

Crystal data

$[Ag(C_{17}H_{20}S_2)_2]BF_4$
$M_r = 771.62$
Monoclinic, *Pn*
$a = 9.209$ (3) Å
$b = 10.182$ (3) Å
$c = 19.158$ (5) Å
$\beta = 103.507$ (5)°
$V = 1746.7$ (9) Å^3
$Z = 2$
$D_x = 1.467$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 981 reflections
$\theta = 3.1$–19.7°
$\mu = 0.86$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 diffractometer
ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 1997)
$T_{\min} = 0.782$, $T_{\max} = 0.847$
7056 measured reflections
5074 independent reflections
4519 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 25.0°$
$h = -10 \rightarrow 10$
$k = -8 \rightarrow 12$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.064$
$S = 1.07$
5074 reflections
425 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.43$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}
Absolute structure: Flack (1983); 1989 Friedel pairs
Flack parameter = 0.00 (2)

Table 1
Selected geometric parameters (Å, °).

Ag1—S1$^{\rm i}$	2.5884 (13)	Ag1—S2	2.6300 (13)
Ag1—S4	2.5985 (12)	Ag1—S3$^{\rm ii}$	2.6772 (12)
S1$^{\rm i}$—Ag1—S4	122.83 (4)	S1$^{\rm i}$—Ag1—S3$^{\rm ii}$	97.69 (4)
S1$^{\rm i}$—Ag1—S2	105.46 (3)	S4—Ag1—S3$^{\rm ii}$	99.69 (3)
S4—Ag1—S2	120.91 (4)	S2—Ag1—S3$^{\rm ii}$	105.81 (4)

Symmetry codes: (i) $x, y-1, z$; (ii) $1+x, y, z$.

Although most H atoms were visible in difference maps, all H atoms were placed in calculated positions (0.97 Å for methylene C—H and 0.93 Å for aromatic C—H) and included in the final refinement in the riding-model approximation, with displacement parameters $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$ (C).

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); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL*97.

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