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Poly[[bis[μ_2-1,3-bis(phenylsulfanyl)propane-$\kappa^2S:S'$]silver(I)] hexafluoridoantimonate diethyl ether hemisolvate]

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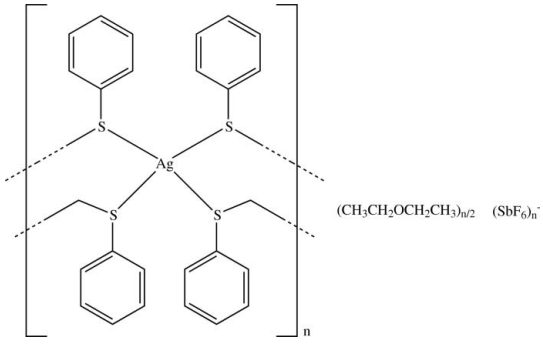
Key indicators: single-crystal X-ray study; T = 220 K; mean σ(C–C) = 0.008 Å; some non-H atoms missing; disorder in main residue; R factor = 0.044; wR factor = 0.114; data-to-parameter ratio = 18.9.

The title compound, $\{[Ag(C_{15}H_{16}S_2)_2]SbF_6\cdot 0.5C_4H_{10}O\}_n$, was obtained from the self-assembly of $AgSbF_6$ and 1,3-bis(phenylsulfanyl)propane. Each Ag^I ion is coordinated by four S atoms from different ligands, forming a distorted tethrahedral geometry. Each ligand links adjacent Ag^I ions, forming an extended two-dimensional grid-like framework. SbF_6^- ions, which are incorporated into the cavities of the network, complete and stabilize the structure. One of the phenyl rings is disordered over two sites, the ratio of occupancies being 0.508 (4):0.492 (4).

Related literature

For related literature, see: Awaleh *et al.* (2006*a*,*b*, 2007); Black *et al.* (1995); Blake *et al.* (1999); Bu *et al.* (2002); Carlucci *et al.* (2002); Hartley *et al.* (1979); Hou *et al.* (2005); Millward & Yaghi (2005); Noro *et al.* (2002); Sluis & Spek (1990); Spek (2003); Withersby *et al.* (1997, 1999); Wong-Foy, Matzger & Yaghi (2006).



Experimental

Crystal data

$[Ag(C_{15}H_{16}S_2)_2]SbF_6\cdot 0.5C_4H_{10}O$
M_r = 901.52
Monoclinic, $P2_1/c$
a = 13.5794 (2) Å
b = 13.0497 (2) Å
c = 20.5848 (3) Å
β = 97.791 (1)°
V = 3614.10 (9) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 12.87 mm^{-1}
T = 220 (2) K
0.27 × 0.14 × 0.11 mm

Data collection

Bruker SMART 2K diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.162, T_{max} = 0.239
43960 measured reflections
7095 independent reflections
5413 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 0.95
7095 reflections
375 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—S2	2.5293 (12)	Ag1—S4	2.5639 (12)
Ag1—S3	2.5621 (12)	Ag1—S1	2.6170 (12)
S2—Ag1—S3	118.58 (4)	S2—Ag1—S1	106.61 (4)
S2—Ag1—S4	114.28 (4)	S3—Ag1—S1	103.08 (4)
S3—Ag1—S4	109.98 (4)	S4—Ag1—S1	102.26 (4)

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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, 1997); software used to prepare material for publication: *UdMX* (Maris, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2544).

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supplementary materials

Acta Cryst. (2007). E**63**, m3013-m3014 [**doi:10.1107/S1600536807056371**]

Poly[[bis[μ_2-1,3-bis(phenylsulfanyl)propane-κ^2S:S']silver(I)] hexafluoridoantimonate diethyl ether hemisolvate\]

M. O. Awaleh, A. Badia and F. Brisse

Comment

The self-assembly of metal-organic coordination polymers has attracted a great attention because of their potential as functional materials (Millward & Yaghi, 2005; Wong-Foy *et al.*, 2006). When flexible ligands are involved in supramolecular architectures, the prediction of the topology of the coordination polymer is more difficult because there are several factors affecting the framework formation, such as the type of solvent, the counter-anion, and the metal-to-ligand ratio among others (Withersby *et al.*, 1999, 1997; Noro *et al.*, 2002; Black *et al.*, 1995; Blake *et al.*, 1999; Bu *et al.*, 2002; Carlucci *et al.*, 2002). Neverthless, in order to gain more information about those subtle factors, not yet well understood, we have studied the effect of one parameter at a time on the topology of the networks (Awaleh *et al.*, 2006*a*,b; 2007). In our continuous effort to study the structure of the metal-organic supramolecular architecture, we report herein a silver(I) coordination polymer forming a lamellar network by using a flexible dithioether, *viz*. 1,3-bis(phenylsulfanyl)propane ($L^{3\text{-Ph}}$), as building block, namely Poly[Silver(I)-di-μ-1,3-bis(phenylsulfanyl)propane]hexafluoroantimonate acetone solvate (I). In the title complex (I), each Ag^I center is linked in a tetrahedral manner to a sulfur atom of four different $L^{3\text{-Ph}}$ ligands (Fig. 1). The other sulfur atom of each ligand is bound to a neighbouring Ag^I ion thus forming a two-dimensional cationic coordination polymer where the repeat unit is a rectangular 24-membered macrometallocycle $Ag_4(L^{3\text{-Ph}})_4$ (Fig. 2). The phenyl groups of the $L^{3\text{-Ph}}$ ligands are located on the same side of the Ag_4 plane. The dihedral angle between the phenyl groups is 71.6(20°. The PF_6^- ions are incorporated in the cavities of the repeating unit to balance the charge of the cationic coordination polymer (Fig. 3). Neighbouring rectangular rings are fused in a parquet-like pattern to form an infinite lamellar (4,4) coordination network (Fig. 3).

Experimental

The ligand 1,3-bis(phenylsulfanyl)propane, $L^{3\text{-Ph}}$, was synthesized following a publish report (Hartley *et al.*, 1979). For the synthesis of the title compound (I), a solution of $AgSbF_6$ (164 mg, 0.48 mmol) in acetone (5 ml) was added a solution of $L^{3\text{-Ph}}$ (0.22 ml, 0.95 mmol) in diethyl ether (5 ml). The mixture was kept under reflux at 323 K for 2 h. The filtrate was recrystallized by diffusion of petroleum ether into the solution at room temperature. A few days later, single crystals suitable for X-ray analysis were deposited. Yield 74% based on $AgSbF_6$. Anal. Found: C, 42.46; H, 3.84. Calculated for $C_{32}H_{37}S_4O_{0.5}AgSbF_6$: C, 42.63; H, 4.14. ^{1}H NMR (DMSO-d_6, 400 MHz): d 1.84 (qt, 2H, –S-(CH_2)-(CH_2)-), 3.07 (t, 4H, –S-(CH_2)-), 7.28–7.59 (m, 10H, C_6H_5–). ^{19}F NMR (DMSO-d_6, 376.31 MHz): d −137.49 - −102.91 (m, F—Sb).

Refinement

All non-H atoms were refined by full-matrix least-squares with anisotropic displacement parameters. H atoms were generated geometrically (C—H distances of 0.93 A for aromatic H, 0.97 A for the other) and were included in the refinement in

the riding model approximation; their temperature factors were set to 1.2 times those of the equivalent isotropic temperature factors of the parent site. An electron density map showed two regions centered at (1/2, 0, 0) and (1/2, 1/2, 1/2), containing peaks due to severely disordered solvent. No consistent models for diethyl ether molecules, which was the only solvent present, could be assembled from these peaks. This part of the structure was modeled by using the SQUEEZE procedure of *PLATON* (Spek, 2003), which indicated the presence of two cavities of 205 Å^3, each occupied by 40 electrons, which is consistent with the presence of one $CH_3CH_2OCH_2CH_3$ molecule per cavity (half of diethyl ether molecule per asymmetric unit)·The contribution of the disordered solvent was calculated with BYPASS (van der Sluis & Spek, 1990) and a new data set without the solvent contribution was generated. The final model consisting of the ordered part only was refined. One phenyl group of one 1,3-bis(phenylsulfanul)propane ligand was found to be disordered·This group was split over two sites with occupancies of 58 and 42%.

Figures

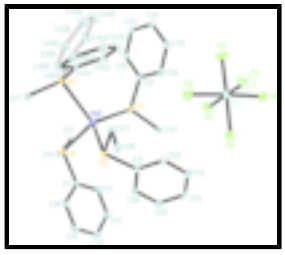

Fig. 1. The aysmmetric unit of the title compound. Ellipsoid are drawn at the 30% probability level. The disordered components are labeled with suffixes A and B.

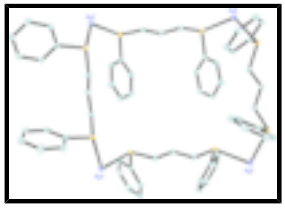

Fig. 2. View of the 24-membered $Ag_4(L^{3\text{-Ph}})_4$ macrometallocyclic repeat unit of the title compound.

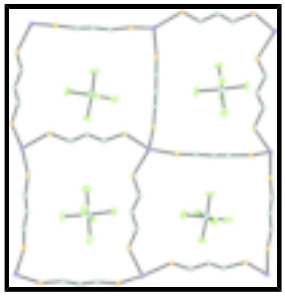

Fig. 3. View of the two-dimensional molecular-rectangle network of the title compound.

Poly[[bis[μ$_2$-1,3-bis(phenylsulfanyl)propane-κ^2*S*:*S*']silver(I)] hexafluoridoantimonate diethyl ether hemisolvate]

Crystal data

$[Ag(C_{15}H_{16}S_2)_2]SbF_6·0.5C_4H_{10}O$	F_{000} = 1712
M_r = 901.52	D_x = 1.657 Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation λ = 1.54178 Å
Hall symbol: -P 2ybc	Cell parameters from 7995 reflections
a = 13.5794 (2) Å	θ = 3.3–72.8º

b = 13.0497 (2) Å
c = 20.5848 (3) Å
β = 97.7910 (10)º
V = 3614.10 (9) Å^3
Z = 4

μ = 12.87 mm^{-1}
T = 220 (2) K
Block, colorless
0.27 × 0.14 × 0.11 mm

Data collection

Bruker SMART 2K diffractometer
Radiation source: X-ray Sealed Tube
Monochromator: graphite
Detector resolution: 5.5 pixels mm^{-1}
T = 220(2) K
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.162, T_{max} = 0.239
43960 measured reflections

7095 independent reflections
5413 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 72.9º
θ_{min} = 3.3º
h = −16→16
k = −13→15
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 0.95
7095 reflections
375 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}
Extinction correction: none

Special details

Experimental. X-ray crystallographic data for I were collected from a single-crystal sample, which was mounted on a loop fiber. Data were collected using a Bruker Platform diffractometer, equipped with a Bruker *SMART* 2 K Charged-Coupled Device (CCD) Area Detector using the program *SMART* and normal focus sealed tube source graphite monochromated Cu—Kα radiation. The crystal-to-detector distance was 4.908 cm, and the data collection was carried out in 512 *x* 512 pixel mode, utilizing 4 *x* 4 pixel binning. The initial unit-cell parameters were determined by a least-squares fit of the angular setting of strong reflections, collected by a 9.0 degree scan in 30 frames over four different parts of the reciprocal space (120 frames total). One complete sphere of data was collected, to better than 0.8Å resolution. Upon completion of the data collection, the first 101 frames were recollected in order to improve the decay correction analysis.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ag1	0.25367 (2)	0.61376 (3)	0.245888 (17)	0.02260 (10)	
Sb1	0.22596 (3)	0.08152 (3)	0.166843 (17)	0.03613 (11)	
S1	0.21540 (8)	0.77327 (9)	0.31534 (6)	0.0215 (2)	
S2	0.34586 (8)	0.48708 (9)	0.32496 (6)	0.0252 (3)	
S3	0.08207 (8)	0.56386 (9)	0.18682 (6)	0.0227 (2)	
S4	0.35897 (8)	0.69189 (9)	0.16407 (6)	0.0247 (3)	
F1	0.1398 (3)	0.1928 (3)	0.1844 (2)	0.0678 (12)	
F2	0.3345 (3)	0.1719 (4)	0.1855 (2)	0.0820 (15)	
F3	0.3054 (3)	−0.0257 (4)	0.1523 (2)	0.0916 (17)	
F4	0.1130 (3)	−0.0011 (3)	0.15182 (17)	0.0519 (9)	
F5	0.2087 (3)	0.1186 (4)	0.07860 (18)	0.0787 (15)	
F6	0.2400 (3)	0.0490 (3)	0.25589 (16)	0.0488 (9)	
C11	0.1783 (3)	0.7220 (4)	0.3894 (2)	0.0218 (10)	
C12	0.0832 (4)	0.6887 (4)	0.3940 (2)	0.0291 (11)	
H12	0.0343	0.6927	0.3578	0.035*	
C13	0.0607 (4)	0.6496 (4)	0.4522 (3)	0.0368 (13)	
H13	−0.0039	0.6285	0.4555	0.044*	
C14	0.1326 (5)	0.6415 (4)	0.5055 (3)	0.0444 (15)	
H14	0.1172	0.6140	0.5445	0.053*	
C15	0.2281 (5)	0.6742 (4)	0.5010 (3)	0.0394 (14)	
H15	0.2769	0.6687	0.5372	0.047*	
C16	0.2515 (4)	0.7153 (4)	0.4431 (3)	0.0330 (12)	
H16	0.3157	0.7382	0.4402	0.040*	
C17	0.1015 (4)	0.8260 (4)	0.2720 (2)	0.0251 (10)	
H17A	0.1135	0.8492	0.2290	0.030*	
H17B	0.0513	0.7726	0.2659	0.030*	
C18	0.0624 (3)	0.9153 (4)	0.3087 (2)	0.0231 (10)	
H18A	0.1110	0.9701	0.3135	0.028*	
H18B	0.0518	0.8931	0.3523	0.028*	
C21	0.2527 (3)	0.4021 (4)	0.3470 (2)	0.0244 (10)	
C22	0.2337 (4)	0.3056 (4)	0.3204 (3)	0.0284 (11)	
H22	0.2714	0.2799	0.2896	0.034*	
C23	0.1570 (4)	0.2476 (4)	0.3405 (3)	0.0317 (12)	
H23	0.1438	0.1824	0.3233	0.038*	
C24	0.1006 (4)	0.2860 (4)	0.3857 (3)	0.0339 (12)	
H24	0.0488	0.2472	0.3983	0.041*	
C25	0.1208 (4)	0.3818 (5)	0.4123 (3)	0.0394 (14)	
H25	0.0829	0.4073	0.4431	0.047*	

C26	0.1969 (4)	0.4401 (4)	0.3935 (3)	0.0318 (12)	
H26	0.2108	0.5044	0.4119	0.038*	
C27	0.4222 (4)	0.4080 (4)	0.2802 (3)	0.0278 (11)	
H27A	0.3797	0.3680	0.2480	0.033*	
H27B	0.4632	0.4517	0.2567	0.033*	
C28	0.4891 (4)	0.3357 (4)	0.3247 (2)	0.0270 (11)	
H28A	0.5309	0.3752	0.3575	0.032*	
H28B	0.4485	0.2901	0.3471	0.032*	
C31	0.1094 (3)	0.5131 (4)	0.1110 (2)	0.0211 (10)	
C32	0.1117 (4)	0.5836 (4)	0.0602 (2)	0.0277 (11)	
H32	0.0979	0.6523	0.0668	0.033*	
C33	0.1343 (4)	0.5510 (4)	0.0005 (3)	0.0329 (12)	
H33	0.1368	0.5982	−0.0331	0.040*	
C34	0.1534 (4)	0.4484 (4)	−0.0101 (3)	0.0377 (14)	
H34	0.1681	0.4267	−0.0507	0.045*	
C35	0.1503 (4)	0.3783 (4)	0.0401 (3)	0.0373 (13)	
H35	0.1629	0.3094	0.0330	0.045*	
C36	0.1286 (4)	0.4100 (4)	0.1007 (3)	0.0290 (11)	
H36	0.1268	0.3627	0.1344	0.035*	
C37	0.0354 (3)	0.4546 (4)	0.2285 (2)	0.0243 (10)	
H37A	0.0844	0.4001	0.2321	0.029*	
H37B	0.0251	0.4746	0.2724	0.029*	
C41A	0.4293 (6)	0.5788 (5)	0.1447 (4)	0.025 (2)	0.508 (4)
C42A	0.3748 (4)	0.4987 (6)	0.1131 (4)	0.0391 (19)	0.508 (4)
H42A	0.3068	0.5057	0.1007	0.047*	0.508 (4)
C43A	0.4222 (5)	0.4079 (5)	0.1002 (4)	0.052 (3)	0.508 (4)
H43A	0.3857	0.3543	0.0791	0.062*	0.508 (4)
C44A	0.5239 (5)	0.3973 (5)	0.1188 (4)	0.044 (2)	0.508 (4)
H44A	0.5556	0.3366	0.1102	0.053*	0.508 (4)
C45A	0.5784 (4)	0.4775 (7)	0.1504 (4)	0.035 (3)	0.508 (4)
H45A	0.6465	0.4704	0.1628	0.042*	0.508 (4)
C46A	0.5311 (6)	0.5682 (6)	0.1633 (4)	0.0285 (12)	0.508 (4)
H46A	0.5675	0.6218	0.1844	0.034*	0.508 (4)
C41B	0.4365 (7)	0.6062 (6)	0.1305 (4)	0.025 (2)	0.492 (4)
C42B	0.3977 (5)	0.5663 (6)	0.0698 (4)	0.0391 (19)	0.492 (4)
H42B	0.3347	0.5859	0.0502	0.047*	0.492 (4)
C43B	0.4529 (6)	0.4970 (7)	0.0383 (3)	0.052 (3)	0.492 (4)
H43B	0.4270	0.4703	−0.0023	0.062*	0.492 (4)
C44B	0.5470 (5)	0.4676 (6)	0.0676 (4)	0.044 (2)	0.492 (4)
H44B	0.5840	0.4213	0.0465	0.053*	0.492 (4)
C45B	0.5858 (5)	0.5075 (7)	0.1283 (4)	0.035 (3)	0.492 (4)
H45B	0.6487	0.4879	0.1479	0.042*	0.492 (4)
C46B	0.5305 (7)	0.5768 (7)	0.1598 (3)	0.0285 (12)	0.492 (4)
H46B	0.5565	0.6036	0.2004	0.034*	0.492 (4)
C47	0.4461 (3)	0.7731 (4)	0.2149 (2)	0.0264 (11)	
H47A	0.4094	0.8192	0.2398	0.032*	
H47B	0.4882	0.7307	0.2458	0.032*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.01757 (16)	0.02028 (19)	0.0306 (2)	−0.00137 (12)	0.00575 (13)	−0.00095 (13)
Sb1	0.0370 (2)	0.0407 (2)	0.0296 (2)	−0.00904 (16)	0.00059 (15)	0.00587 (15)
S1	0.0170 (5)	0.0194 (6)	0.0280 (6)	0.0012 (4)	0.0021 (4)	−0.0011 (4)
S2	0.0197 (6)	0.0202 (6)	0.0369 (7)	0.0017 (4)	0.0081 (5)	0.0011 (5)
S3	0.0186 (5)	0.0191 (6)	0.0307 (6)	−0.0026 (4)	0.0046 (5)	−0.0005 (4)
S4	0.0158 (5)	0.0276 (7)	0.0305 (6)	−0.0043 (4)	0.0028 (5)	0.0039 (5)
F1	0.079 (3)	0.044 (2)	0.072 (3)	0.024 (2)	−0.020 (2)	−0.0084 (19)
F2	0.069 (3)	0.106 (4)	0.067 (3)	−0.053 (3)	−0.006 (2)	0.015 (3)
F3	0.081 (3)	0.109 (4)	0.084 (3)	0.059 (3)	0.005 (3)	−0.019 (3)
F4	0.044 (2)	0.057 (2)	0.052 (2)	−0.0191 (18)	−0.0046 (17)	0.0042 (17)
F5	0.078 (3)	0.118 (4)	0.037 (2)	−0.032 (3)	−0.003 (2)	0.025 (2)
F6	0.056 (2)	0.050 (2)	0.038 (2)	−0.0002 (17)	−0.0038 (17)	0.0128 (15)
C11	0.024 (2)	0.018 (3)	0.023 (2)	0.0038 (18)	0.0019 (19)	−0.0032 (18)
C12	0.032 (3)	0.026 (3)	0.029 (3)	0.003 (2)	0.006 (2)	0.003 (2)
C13	0.039 (3)	0.038 (3)	0.037 (3)	0.007 (2)	0.017 (3)	0.003 (2)
C14	0.072 (5)	0.032 (3)	0.032 (3)	0.010 (3)	0.016 (3)	−0.001 (2)
C15	0.059 (4)	0.032 (3)	0.023 (3)	0.007 (3)	−0.009 (3)	−0.004 (2)
C16	0.039 (3)	0.024 (3)	0.033 (3)	0.001 (2)	−0.006 (2)	−0.004 (2)
C17	0.026 (3)	0.024 (3)	0.025 (3)	0.0081 (19)	0.003 (2)	−0.0015 (19)
C18	0.017 (2)	0.022 (3)	0.029 (3)	0.0027 (18)	0.0012 (19)	−0.0025 (19)
C21	0.021 (2)	0.021 (3)	0.031 (3)	0.0000 (18)	0.004 (2)	0.0051 (19)
C22	0.023 (2)	0.027 (3)	0.036 (3)	0.003 (2)	0.004 (2)	−0.001 (2)
C23	0.029 (3)	0.020 (3)	0.043 (3)	−0.004 (2)	−0.003 (2)	0.003 (2)
C24	0.031 (3)	0.025 (3)	0.046 (3)	−0.008 (2)	0.006 (2)	0.007 (2)
C25	0.042 (3)	0.044 (4)	0.036 (3)	−0.005 (3)	0.019 (3)	0.000 (3)
C26	0.039 (3)	0.020 (3)	0.039 (3)	−0.001 (2)	0.013 (2)	−0.001 (2)
C27	0.025 (3)	0.028 (3)	0.032 (3)	0.002 (2)	0.012 (2)	0.002 (2)
C28	0.021 (2)	0.028 (3)	0.032 (3)	0.0011 (19)	0.006 (2)	0.000 (2)
C31	0.014 (2)	0.020 (3)	0.028 (3)	−0.0007 (17)	0.0016 (18)	0.0035 (18)
C32	0.023 (2)	0.028 (3)	0.031 (3)	−0.0026 (19)	−0.001 (2)	0.008 (2)
C33	0.034 (3)	0.035 (3)	0.029 (3)	−0.012 (2)	0.000 (2)	0.009 (2)
C34	0.039 (3)	0.042 (4)	0.033 (3)	−0.019 (3)	0.009 (3)	−0.006 (2)
C35	0.045 (3)	0.025 (3)	0.042 (3)	0.002 (2)	0.009 (3)	−0.003 (2)
C36	0.031 (3)	0.020 (3)	0.037 (3)	0.0004 (19)	0.008 (2)	0.004 (2)
C37	0.022 (2)	0.028 (3)	0.022 (3)	−0.0086 (19)	0.0019 (19)	0.0016 (19)
C41A	0.018 (3)	0.031 (6)	0.027 (5)	−0.007 (3)	0.009 (3)	0.000 (4)
C42A	0.025 (4)	0.043 (5)	0.048 (5)	0.008 (3)	−0.003 (4)	−0.009 (3)
C43A	0.041 (5)	0.060 (7)	0.051 (6)	0.010 (4)	−0.010 (4)	−0.031 (4)
C44A	0.036 (5)	0.045 (6)	0.053 (6)	0.008 (4)	0.012 (4)	−0.012 (4)
C45A	0.023 (3)	0.050 (7)	0.033 (6)	−0.001 (4)	0.008 (4)	−0.005 (5)
C46A	0.022 (3)	0.030 (3)	0.032 (3)	−0.001 (2)	0.000 (2)	0.002 (2)
C41B	0.018 (3)	0.031 (6)	0.027 (5)	−0.007 (3)	0.009 (3)	0.000 (4)
C42B	0.025 (4)	0.043 (5)	0.048 (5)	0.008 (3)	−0.003 (4)	−0.009 (3)
C43B	0.041 (5)	0.060 (7)	0.051 (6)	0.010 (4)	−0.010 (4)	−0.031 (4)

C44B	0.036 (5)	0.045 (6)	0.053 (6)	0.008 (4)	0.012 (4)	−0.012 (4)
C45B	0.023 (3)	0.050 (7)	0.033 (6)	−0.001 (4)	0.008 (4)	−0.005 (5)
C46B	0.022 (3)	0.030 (3)	0.032 (3)	−0.001 (2)	0.000 (2)	0.002 (2)
C47	0.019 (2)	0.026 (3)	0.033 (3)	−0.0031 (19)	0.002 (2)	−0.004 (2)

Geometric parameters (Å, °)

Ag1—S2	2.5293 (12)	C26—H26	0.93
Ag1—S3	2.5621 (12)	C27—C28	1.526 (7)
Ag1—S4	2.5639 (12)	C27—H27a	0.97
Ag1—S1	2.6170 (12)	C27—H27b	0.97
Sb1—F3	1.816 (4)	C28—C47^{ii}	1.517 (6)
Sb1—F5	1.864 (4)	C28—H28a	0.97
Sb1—F6	1.866 (3)	C28—H28b	0.97
Sb1—F4	1.866 (3)	C31—C36	1.392 (7)
Sb1—F2	1.886 (4)	C31—C32	1.395 (6)
Sb1—F1	1.929 (4)	C32—C33	1.374 (7)
S1—C11	1.799 (5)	C32—H32	0.93
S1—C17	1.814 (5)	C33—C34	1.387 (8)
S2—C21	1.786 (5)	C33—H33	0.93
S2—C27	1.802 (5)	C34—C35	1.385 (8)
S3—C31	1.781 (5)	C34—H34	0.93
S3—C37	1.820 (5)	C35—C36	1.384 (7)
S4—C41b	1.741 (6)	C35—H35	0.93
S4—C47	1.811 (5)	C36—H36	0.93
S4—C41a	1.831 (6)	C37—C18^{iii}	1.530 (6)
C11—C12	1.378 (7)	C37—H37a	0.97
C11—C16	1.385 (7)	C37—H37b	0.97
C12—C13	1.374 (7)	C41a—C42a	1.39
C12—H12	0.93	C41a—C46a	1.39
C13—C14	1.371 (8)	C42a—C43a	1.39
C13—H13	0.93	C42a—H42a	0.93
C14—C15	1.379 (9)	C43a—C44a	1.39
C14—H14	0.93	C43a—H43a	0.93
C15—C16	1.384 (7)	C44a—C45a	1.39
C15—H15	0.93	C44a—H44a	0.93
C16—H16	0.93	C45a—C46a	1.39
C17—C18	1.523 (6)	C45a—H45a	0.93
C17—H17a	0.97	C46a—H46a	0.93
C17—H17b	0.97	C41b—C42b	1.39
C18—C37^{i}	1.530 (6)	C41b—C46b	1.39
C18—H18a	0.97	C42b—C43b	1.39
C18—H18b	0.97	C42b—H42b	0.93
C21—C22	1.384 (7)	C43b—C44b	1.39
C21—C26	1.390 (7)	C43b—H43b	0.93
C22—C23	1.396 (7)	C44b—C45b	1.39
C22—H22	0.93	C44b—H44b	0.93
C23—C24	1.377 (7)	C45b—C46b	1.39

C23—H23	0.93	C45b—H45b	0.93
C24—C25	1.378 (8)	C46b—H46b	0.93
C24—H24	0.93	C47—C28^{iv}	1.517 (6)
C25—C26	1.380 (7)	C47—H47a	0.97
C25—H25	0.93	C47—H47b	0.97
S2—Ag1—S3	118.58 (4)	C25—C26—H26	120.2
S2—Ag1—S4	114.28 (4)	C21—C26—H26	120.2
S3—Ag1—S4	109.98 (4)	C28—C27—S2	112.5 (4)
S2—Ag1—S1	106.61 (4)	C28—C27—H27A	109.1
S3—Ag1—S1	103.08 (4)	S2—C27—H27A	109.1
S4—Ag1—S1	102.26 (4)	C28—C27—H27B	109.1
F3—SB1—F5	92.2 (2)	S2—C27—H27B	109.1
F3—SB1—F6	90.18 (19)	H27A—C27—H27B	107.8
F5—SB1—F6	177.6 (2)	C47^{ii}—C28—C27	110.6 (4)
F3—SB1—F4	91.2 (2)	C47^{ii}—C28—H28A	109.5
F5—SB1—F4	89.82 (17)	C27—C28—H28A	109.5
F6—SB1—F4	90.21 (15)	C47^{ii}—C28—H28B	109.5
F3—SB1—F2	92.9 (2)	C27—C28—H28B	109.5
F5—SB1—F2	91.56 (18)	H28A—C28—H28B	108.1
F6—SB1—F2	88.24 (17)	C36—C31—C32	120.0 (5)
F4—SB1—F2	175.6 (2)	C36—C31—S3	123.9 (4)
F3—SB1—F1	178.1 (2)	C32—C31—S3	116.1 (4)
F5—SB1—F1	89.3 (2)	C33—C32—C31	119.8 (5)
F6—SB1—F1	88.32 (16)	C33—C32—H32	120.1
F4—SB1—F1	87.73 (18)	C31—C32—H32	120.1
F2—SB1—F1	88.2 (2)	C32—C33—C34	120.6 (5)
C11—S1—C17	103.9 (2)	C32—C33—H33	119.7
C11—S1—AG1	105.44 (15)	C34—C33—H33	119.7
C17—S1—AG1	104.63 (16)	C35—C34—C33	119.7 (5)
C21—S2—C27	104.6 (2)	C35—C34—H34	120.2
C21—S2—AG1	105.26 (16)	C33—C34—H34	120.2
C27—S2—AG1	108.28 (17)	C34—C35—C36	120.5 (5)
C31—S3—C37	104.4 (2)	C34—C35—H35	119.7
C31—S3—AG1	103.08 (15)	C36—C35—H35	119.7
C37—S3—AG1	109.11 (16)	C35—C36—C31	119.5 (5)
C41B—S4—C47	102.9 (3)	C35—C36—H36	120.3
C47—S4—C41A	106.2 (3)	C31—C36—H36	120.3
C41B—S4—AG1	115.2 (3)	C18^{iii}—C37—S3	111.2 (3)
C47—S4—AG1	103.42 (16)	C18^{iii}—C37—H37A	109.4
C41A—S4—AG1	100.2 (3)	S3—C37—H37A	109.4
C12—C11—C16	120.3 (5)	C18^{iii}—C37—H37B	109.4
C12—C11—S1	123.2 (4)	S3—C37—H37B	109.4
C16—C11—S1	116.5 (4)	H37A—C37—H37B	108
C13—C12—C11	119.9 (5)	C42A—C41A—C46A	120
C13—C12—H12	120.1	C42A—C41A—S4	116.6 (5)
C11—C12—H12	120.1	C46A—C41A—S4	123.3 (5)
C14—C13—C12	120.5 (6)	C41A—C42A—C43A	120

C14—C13—H13	119.8	C41A—C42A—H42A	120
C12—C13—H13	119.8	C43A—C42A—H42A	120
C13—C14—C15	119.8 (6)	C42A—C43A—C44A	120
C13—C14—H14	120.1	C42A—C43A—H43A	120
C15—C14—H14	120.1	C44A—C43A—H43A	120
C14—C15—C16	120.3 (5)	C45A—C44A—C43A	120
C14—C15—H15	119.8	C45A—C44A—H44A	120
C16—C15—H15	119.8	C43A—C44A—H44A	120
C15—C16—C11	119.2 (5)	C46A—C45A—C44A	120
C15—C16—H16	120.4	C46A—C45A—H45A	120
C11—C16—H16	120.4	C44A—C45A—H45A	120
C18—C17—S1	112.2 (3)	C45A—C46A—C41A	120
C18—C17—H17A	109.2	C45A—C46A—H46A	120
S1—C17—H17A	109.2	C41A—C46A—H46A	120
C18—C17—H17B	109.2	C42B—C41B—C46B	120
S1—C17—H17B	109.2	C42B—C41B—S4	114.9 (5)
H17A—C17—H17B	107.9	C46B—C41B—S4	125.1 (5)
C17—C18—C37^{i}	110.2 (4)	C43B—C42B—C41B	120
C17—C18—H18A	109.6	C43B—C42B—H42B	120
C37^{i}—C18—H18A	109.6	C41B—C42B—H42B	120
C17—C18—H18B	109.6	C42B—C43B—C44B	120
C37^{i}—C18—H18B	109.6	C42B—C43B—H43B	120
H18A—C18—H18B	108.1	C44B—C43B—H43B	120
C22—C21—C26	120.5 (5)	C43B—C44B—C45B	120
C22—C21—S2	124.4 (4)	C43B—C44B—H44B	120
C26—C21—S2	115.1 (4)	C45B—C44B—H44B	120
C21—C22—C23	118.9 (5)	C46B—C45B—C44B	120
C21—C22—H22	120.6	C46B—C45B—H45B	120
C23—C22—H22	120.6	C44B—C45B—H45B	120
C24—C23—C22	120.6 (5)	C45B—C46B—C41B	120
C24—C23—H23	119.7	C45B—C46B—H46B	120
C22—C23—H23	119.7	C41B—C46B—H46B	120
C25—C24—C23	120.0 (5)	C28^{iv}—C47—S4	112.7 (3)
C25—C24—H24	120	C28^{iv}—C47—H47A	109
C23—C24—H24	120	S4—C47—H47A	109
C24—C25—C26	120.4 (5)	C28^{iv}—C47—H47B	109
C24—C25—H25	119.8	S4—C47—H47B	109
C26—C25—H25	119.8	H47A—C47—H47B	107.8
C25—C26—C21	119.7 (5)		
S2—AG1—S1—C11	−41.29 (16)	C24—C25—C26—C21	0.7 (9)
S3—AG1—S1—C11	84.28 (16)	C22—C21—C26—C25	−1.3 (8)
S4—AG1—S1—C11	−161.55 (16)	S2—C21—C26—C25	177.8 (4)
S2—AG1—S1—C17	−150.52 (17)	C21—S2—C27—C28	−73.9 (4)
S3—AG1—S1—C17	−24.95 (18)	AG1—S2—C27—C28	174.3 (3)
S4—AG1—S1—C17	89.22 (17)	S2—C27—C28—C47^{ii}	−178.4 (3)
S3—AG1—S2—C21	−20.62 (18)	C37—S3—C31—C36	−22.9 (5)
S4—AG1—S2—C21	−152.88 (17)	AG1—S3—C31—C36	91.1 (4)

S1—AG1—S2—C21	94.94 (18)	C37—S3—C31—C32	157.5 (4)
S3—AG1—S2—C27	90.76 (18)	AG1—S3—C31—C32	−88.5 (4)
S4—AG1—S2—C27	−41.50 (19)	C36—C31—C32—C33	−1.0 (7)
S1—AG1—S2—C27	−153.68 (18)	S3—C31—C32—C33	178.6 (4)
S2—AG1—S3—C31	−94.61 (16)	C31—C32—C33—C34	1.0 (8)
S4—AG1—S3—C31	39.51 (16)	C32—C33—C34—C35	−0.5 (8)
S1—AG1—S3—C31	147.95 (16)	C33—C34—C35—C36	−0.2 (9)
S2—AG1—S3—C37	15.91 (18)	C34—C35—C36—C31	0.2 (8)
S4—AG1—S3—C37	150.04 (18)	C32—C31—C36—C35	0.4 (7)
S1—AG1—S3—C37	−101.52 (18)	S3—C31—C36—C35	−179.2 (4)
S2—AG1—S4—C41B	42.0 (3)	C31—S3—C37—C18^{iii}	−64.9 (4)
S3—AG1—S4—C41B	−94.2 (3)	AG1—S3—C37—C18^{iii}	−174.5 (3)
S1—AG1—S4—C41B	156.8 (3)	C41B—S4—C41A—C42A	−109 (2)
S2—AG1—S4—C47	−69.39 (17)	C47—S4—C41A—C42A	171.7 (4)
S3—AG1—S4—C47	154.36 (17)	AG1—S4—C41A—C42A	64.4 (4)
S1—AG1—S4—C47	45.38 (17)	C41B—S4—C41A—C46A	75 (2)
S2—AG1—S4—C41A	40.1 (3)	C47—S4—C41A—C46A	−4.4 (5)
S3—AG1—S4—C41A	−96.2 (3)	AG1—S4—C41A—C46A	−111.7 (4)
S1—AG1—S4—C41A	154.9 (3)	C46A—C41A—C42A—C43A	0
C17—S1—C11—C12	27.0 (5)	S4—C41A—C42A—C43A	−176.3 (6)
AG1—S1—C11—C12	−82.7 (4)	C41A—C42A—C43A—C44A	0
C17—S1—C11—C16	−154.1 (4)	C42A—C43A—C44A—C45A	0
AG1—S1—C11—C16	96.2 (4)	C43A—C44A—C45A—C46A	0
C16—C11—C12—C13	0.6 (8)	C44A—C45A—C46A—C41A	0
S1—C11—C12—C13	179.5 (4)	C42A—C41A—C46A—C45A	0
C11—C12—C13—C14	−1.3 (8)	S4—C41A—C46A—C45A	176.0 (6)
C12—C13—C14—C15	1.0 (9)	C47—S4—C41B—C42B	−152.3 (4)
C13—C14—C15—C16	0.0 (9)	C41A—S4—C41B—C42B	103 (2)
C14—C15—C16—C11	−0.8 (8)	AG1—S4—C41B—C42B	95.9 (5)
C12—C11—C16—C15	0.4 (7)	C47—S4—C41B—C46B	27.7 (6)
S1—C11—C16—C15	−178.5 (4)	C41A—S4—C41B—C46B	−77 (2)
C11—S1—C17—C18	64.8 (4)	AG1—S4—C41B—C46B	−84.0 (5)
AG1—S1—C17—C18	175.1 (3)	C46B—C41B—C42B—C43B	0
S1—C17—C18—C37^{i}	−178.1 (3)	S4—C41B—C42B—C43B	−179.9 (6)
C27—S2—C21—C22	−13.7 (5)	C41B—C42B—C43B—C44B	0
AG1—S2—C21—C22	100.3 (4)	C42B—C43B—C44B—C45B	0
C27—S2—C21—C26	167.2 (4)	C43B—C44B—C45B—C46B	0
AG1—S2—C21—C26	−78.8 (4)	C44B—C45B—C46B—C41B	0
C26—C21—C22—C23	0.7 (7)	C42B—C41B—C46B—C45B	0
S2—C21—C22—C23	−178.4 (4)	S4—C41B—C46B—C45B	179.9 (7)
C21—C22—C23—C24	0.5 (8)	C41B—S4—C47—C28^{iv}	65.1 (5)
C22—C23—C24—C25	−1.1 (8)	C41A—S4—C47—C28^{iv}	80.4 (5)
C23—C24—C25—C26	0.5 (9)	AG1—S4—C47—C28^{iv}	−174.7 (3)

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) −*x*, *y*−1/2, −*z*+1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

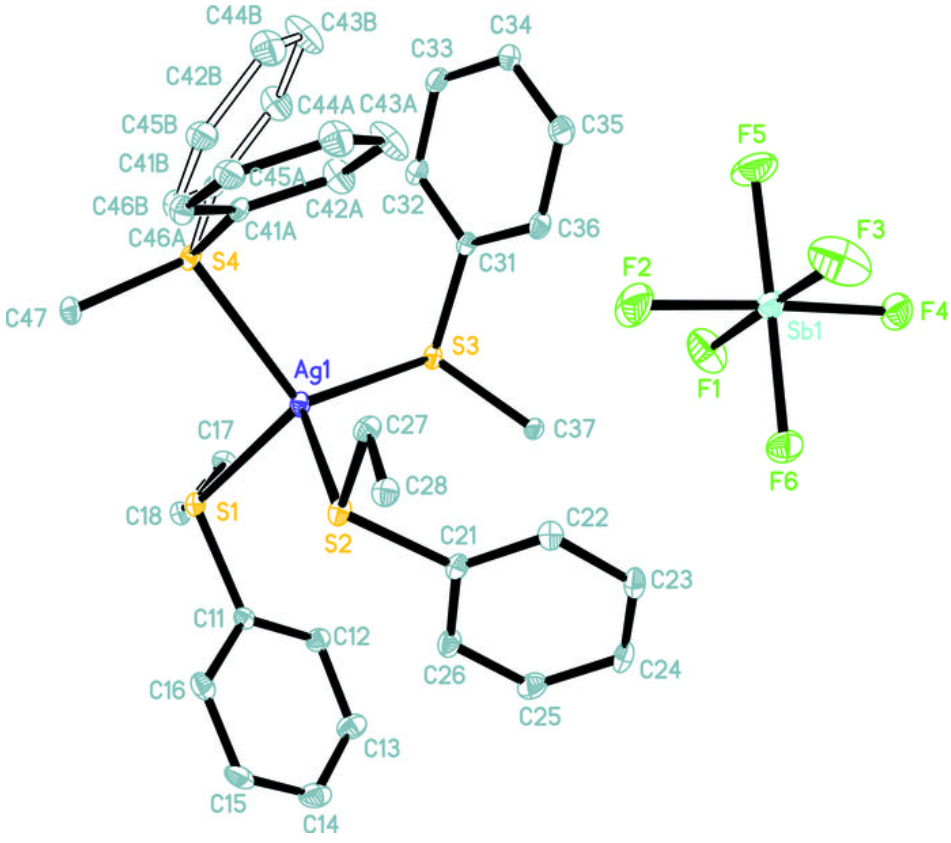
C44B
C43B
C34
C33
C42B
C44A
C43A
C35
C45B
F5
C41B
C45A
C32
F3
C46B
C42A
C36
C46A
C41A
C31
F2
S4
F4
C47
S3
Sb1
Ag1
F1
C17
C27
C37
F6
C28
C18
S1
S2
C22
C21
C23
C11
C12
C26
C24
C16
C25
C13
C15
C14

Fig. 2

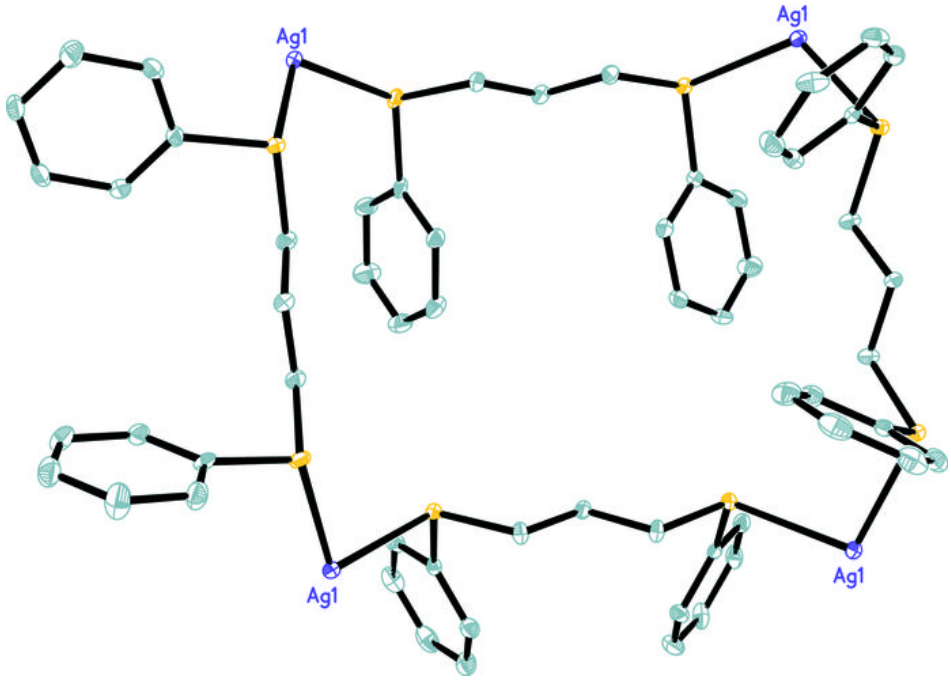

Fig. 3