Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[bis[μ-1,4-bis(2-pyrimidinylthio)butane-κ^2N:N']disilver(I) diperchlorate chloroform sesquisolvate]

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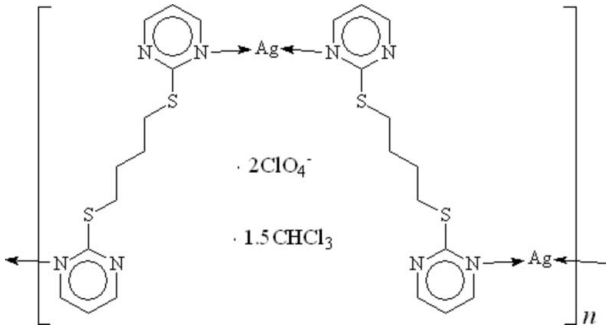
Received 11 August 2007; accepted 6 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; disorder in solvent or counterion; R factor = 0.053; wR factor = 0.167; data-to-parameter ratio = 13.5.

The crystal structure of the title complex, $\{[Ag_2(C_{12}H_{14}N_4S_2)_2](ClO_4)_2\cdot 1.5CHCl_3\}_n$, consists of $[Ag_2(C_{12}H_{14}N_4S_2)_2]_n^{2n+}$ one-dimensional chain cations, ClO_4^- anions and solvent chloroform molecules. There are two crystallographically independent Ag^I centers. The ligand coordinates to the Ag^I centers in an N,N'-bidentate bridging mode in an *anti* conformation, resulting in infinite corrugated chains. The one-dimensional chains are linked to form a two-dimensional framework by weak Ag···S interactions [3.052 (4) and 3.348 (5) Å]. One of the perchlorate ions and all of the solvent chloroform molecules are disordered.

Related literature

For related literature, see: Bu *et al.* (2003); Li *et al.* (2005); Xie *et al.* (2004, 2005); Zheng *et al.* (2003, 2005).



Experimental

Crystal data

$[Ag_2(C_{12}H_{14}N_4S_2)_2](ClO_4)_2\cdot 1.5CHCl_3$
M_r = 2300.95
Triclinic, $P\overline{1}$
a = 11.197 (4) Å
b = 12.394 (4) Å
c = 16.897 (6) Å
α = 73.715 (5)°
β = 73.060 (6)°
γ = 86.618 (6)°
V = 2152.5 (13) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 293 (2) K
0.28 × 0.26 × 0.22 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.834, T_{max} = 1.000
(expected range = 0.592–0.710)
12535 measured reflections
8803 independent reflections
4653 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.167
S = 1.02
8803 reflections
652 parameters
494 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.188 (4)	Ag2—N7	2.171 (5)
Ag1—N5	2.201 (5)	Ag2—N3^{i}	2.177 (5)
N1—Ag1—N5	161.96 (18)	N7—Ag2—N3^{i}	168.73 (19)

Symmetry code: (i) $x, y, z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART* (Bruker, 1998); data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors gratefully acknowledge financial support from the Department of Chemistry, Tianjin University, People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2189).

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  doi:10.1107/S1600536807043802

supplementary materials

Acta Cryst. (2007). E**63**, m2528 [**doi:10.1107/S1600536807043802**]

catena-Poly[bis[μ-1,4-bis(2-pyrimidinylthio)butane-κ^2N:N']disilver(I) diperchlorate chloroform sesquisolvate]

S.-L. Wang and Y. Zheng

Comment

Some Ag^I complexes of flexible bis(arylthio)alkyl ligands (aryl = phenyl, benzyl, pyridyl, pyrimidinyl, 4-methyl-2-pyrimidinyl or 5-methyl-1,3,4-thiadiazolyl) have been reported by us and others [Bu *et al.*, 2003; Li *et al.*, 2005; Xie *et al.*, 2004, 2005; Zheng *et al.*, 2003, 2005], which show different structure features. Herein, we report a 1,4-bis(2-pyrimidinylthio)butane(*L*)—Ag^I complex, $\{[Ag_2(C_{12}H_{14}N_4S_2)_2]\cdot 2ClO_4\cdot 1.5CHCl_3\}_n$ (I). The crystal structure of the title complex (I) consists of $[AgL]_n$ one-dimensional chain cations, ClO_4^- anions (as shown in Fig. 1) and solvent chloroform molecules. In the cationic chain, there are two crystallographic independent Ag^I centers (Ag1 and Ag2), both of which adopt near linear coordination geometry coordinated by two pyrimidine N atoms from two crystallographic independent *L* ligands. Selected bond distances and angles are listed in Table 1. The ligand coordinates to the Ag^I centers in a N,*N*'-bidentate bridging mode with two N donors in an anti-conformation, resulting in an infinite corrugated chain with the intra-molecular Ag—Ag separations of 13.089 (5) and 13.228 (5) Å. It is interesting that by the Ag—S weak coordinations (Ag1—S1B = 3.052 (4) and Ag2—S4C = 3.348 (5) Å) such one-dimensional chains are linked to form a two-dimensional supramolecular framework as shown in Fig. 2.

Experimental

The ligand 1,4-bis(2-pyrimidinylthio)butane (*L*) was synthesized by simulating a reported procedures [Bu *et al.*, 2003]. The solution of $AgClO_4\cdot H_2O$ (23 mg, 0.1 mmol) in MeOH was carefully layered on top of a solution of *L* (28 mg, 0.1 mmol) in toluene in a test-tube. After ten days at room temperature, colorless block single crystals appeared at the boundary between two solvents with a yield of 40%.

Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93, 0.97 and 0.98 Å and U_{iso}(H) = 1.2 U_{eq}(C). One of perchlorate ions and all of solvent chloroform molecuels are disordered. For the disordered perchlorate ion, each one O atom was refined in two positions with a near 1:1 occupation factors ratio. The Cl—O lengths were restrained to 1.44 (1) Å. Additionally, the displacement parameters were restrained to be nearly isotropic. For chloroform molecuels, C and Cl atoms were refined in three positions with a 1:1:1 occupation factors ratio for one, and in two positions with a 3:1 ratio for half one. All of Cl—O lengths were restrained to 1.72 (1) Å and Cl—O distances to 2.81 (1) Å

Figures

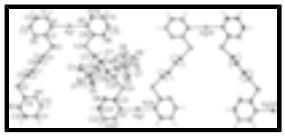

Fig. 1. Displacement ellipsoid plot (30% probability) of a fragment of the one-dimensional structure of (I) with disordered solvent chloroform molecules omitted for clarity. [symmetry codes: (A) *x*, *y*, 1 + *z*]

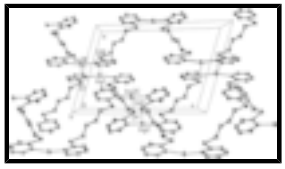

Fig. 2. Two-dimensional supramolecular layer of (I) showing Ag—S weak coordinaolyPtion. [symmetry codes: (B) 1 − *x*, −*y*, −*z*; (C) −*x*, 1 − *y*, 1 − *z*]

catena-Poly[bis[μ-1,4-bis(2-pyrimidinylthio)butane-κ2 N:*N*']disilver(I) diperchlorate chloroform sesquisolvate]

Crystal data

$[Ag_2(C_{12}H_{14}N_4S_2)_2](ClO_4)_2·1.5CHCl_3$	$Z = 1$
$M_r = 2300.95$	$F_{000} = 1142$
Triclinic, $P\overline{1}$	$D_x = 1.775$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.197$ (4) Å	Cell parameters from 883 reflections
$b = 12.394$ (4) Å	$\theta = 3.3$–$25.5°$
$c = 16.897$ (6) Å	$\mu = 1.56$ mm^{-1}
$\alpha = 73.715$ (5)°	$T = 293$ (2) K
$\beta = 73.060$ (6)°	Block, colorless
$\gamma = 86.618$ (6)°	0.28 × 0.26 × 0.22 mm
$V = 2152.5$ (13) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	8803 independent reflections
Radiation source: fine-focus sealed tube	4653 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 293(2)$ K	$\theta_{max} = 26.5°$
φ and ω scan	$\theta_{min} = 1.3°$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -14 \rightarrow 7$
$T_{min} = 0.834$, $T_{max} = 1.000$	$k = -15 \rightarrow 14$
12535 measured reflections	$l = -20 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained

$wR(F^2) = 0.167$	$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2 + 1.7172P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
8803 reflections	$\Delta\rho_{max} = 0.74$ e Å^{-3}
652 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
494 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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	0.42920 (6)	−0.16870 (5)	0.08567 (3)	0.0729 (2)	
Ag2	−0.16104 (6)	0.47906 (5)	0.57281 (3)	0.0785 (2)	
S1	0.33368 (16)	0.03171 (13)	−0.04970 (10)	0.0557 (4)	
S2	−0.06388 (16)	0.26616 (15)	−0.29450 (11)	0.0639 (5)	
S3	0.30282 (17)	0.00309 (15)	0.19341 (11)	0.0657 (5)	
S4	−0.03039 (19)	0.30037 (18)	0.47281 (13)	0.0812 (6)	
N1	0.4087 (4)	−0.1739 (4)	−0.0381 (3)	0.0470 (11)	
N2	0.3745 (5)	−0.0766 (5)	−0.1712 (3)	0.0623 (14)	
N3	−0.1815 (5)	0.4539 (4)	−0.2911 (3)	0.0578 (13)	
N4	−0.1477 (5)	0.3492 (5)	−0.1600 (3)	0.0661 (15)	
N5	0.3957 (4)	−0.1960 (4)	0.2249 (3)	0.0506 (12)	
N6	0.3364 (5)	−0.1174 (5)	0.3424 (3)	0.0678 (15)	
N7	−0.1665 (5)	0.4764 (4)	0.4460 (3)	0.0569 (13)	
N8	−0.1288 (6)	0.3764 (6)	0.3418 (4)	0.092 (2)	
C1	0.4380 (6)	−0.2656 (5)	−0.0663 (4)	0.0578 (16)	
H1	0.4620	−0.3295	−0.0306	0.069*	
C2	0.4338 (7)	−0.2683 (6)	−0.1456 (4)	0.0695 (19)	
H2	0.4505	−0.3332	−0.1640	0.083*	
C3	0.4035 (7)	−0.1699 (6)	−0.1966 (4)	0.071 (2)	
H3	0.4033	−0.1680	−0.2520	0.085*	
C4	0.3755 (5)	−0.0837 (5)	−0.0925 (4)	0.0468 (14)	
C5	0.2764 (6)	0.1281 (5)	−0.1320 (4)	0.0593 (17)	
H5A	0.2736	0.2025	−0.1234	0.071*	
H5B	0.3355	0.1318	−0.1876	0.071*	

C6	0.1485 (6)	0.0977 (5)	−0.1340 (4)	0.0560 (16)	
H6A	0.0898	0.0860	−0.0771	0.067*	
H6B	0.1524	0.0285	−0.1506	0.067*	
C7	0.1041 (6)	0.1919 (5)	−0.1980 (4)	0.0579 (16)	
H7A	0.0925	0.2588	−0.1778	0.069*	
H7B	0.1681	0.2093	−0.2530	0.069*	
C8	−0.0167 (6)	0.1621 (5)	−0.2106 (4)	0.0626 (17)	
H8A	−0.0824	0.1525	−0.1568	0.075*	
H8B	−0.0076	0.0907	−0.2245	0.075*	
C9	−0.1360 (6)	0.3644 (5)	−0.2418 (4)	0.0516 (15)	
C10	−0.2405 (7)	0.5294 (6)	−0.2526 (5)	0.076 (2)	
H10	−0.2724	0.5917	−0.2849	0.091*	
C11	−0.2563 (8)	0.5199 (6)	−0.1689 (5)	0.084 (2)	
H11	−0.2990	0.5733	−0.1428	0.101*	
C12	−0.2065 (7)	0.4279 (7)	−0.1241 (5)	0.081 (2)	
H12	−0.2140	0.4200	−0.0665	0.097*	
C13	0.4284 (6)	−0.2900 (6)	0.2747 (4)	0.0578 (16)	
H13	0.4594	−0.3490	0.2512	0.069*	
C14	0.4171 (6)	−0.3015 (6)	0.3597 (4)	0.0686 (19)	
H14	0.4403	−0.3667	0.3945	0.082*	
C15	0.3699 (7)	−0.2118 (7)	0.3907 (5)	0.080 (2)	
H15	0.3610	−0.2174	0.4482	0.096*	
C16	0.3492 (5)	−0.1141 (5)	0.2626 (4)	0.0523 (15)	
C17	0.2660 (6)	0.1047 (6)	0.2555 (5)	0.0723 (19)	
H17A	0.3298	0.1024	0.2843	0.087*	
H17B	0.2697	0.1792	0.2161	0.087*	
C18	0.1413 (6)	0.0876 (6)	0.3214 (5)	0.073 (2)	
H18A	0.1416	0.0210	0.3682	0.087*	
H18B	0.0773	0.0773	0.2959	0.087*	
C19	0.1135 (7)	0.1928 (7)	0.3564 (5)	0.079 (2)	
H19A	0.1816	0.2050	0.3779	0.095*	
H19B	0.1109	0.2581	0.3091	0.095*	
C20	−0.0037 (8)	0.1840 (7)	0.4250 (6)	0.094 (3)	
H20A	−0.0043	0.1149	0.4698	0.113*	
H20B	−0.0723	0.1788	0.4019	0.113*	
C21	−0.1173 (6)	0.3937 (6)	0.4123 (4)	0.0617 (17)	
C22	−0.2316 (7)	0.5505 (6)	0.4029 (4)	0.0705 (19)	
H22	−0.2652	0.6111	0.4236	0.085*	
C23	−0.2506 (7)	0.5406 (7)	0.3290 (5)	0.080 (2)	
H23	−0.2977	0.5920	0.2998	0.096*	
C24	−0.1982 (8)	0.4534 (8)	0.3005 (5)	0.095 (3)	
H24	−0.2097	0.4450	0.2502	0.114*	
Cl1	0.6523 (2)	0.60581 (16)	0.06711 (13)	0.0779 (5)	
O1	0.6813 (9)	0.7093 (7)	0.0011 (6)	0.177 (4)	
O2	0.7267 (9)	0.5929 (7)	0.1195 (6)	0.184 (4)	
O3	0.6527 (11)	0.5225 (6)	0.0323 (6)	0.200 (5)	
O4	0.5317 (8)	0.6208 (9)	0.1100 (5)	0.192 (4)	
Cl2	0.4539 (2)	0.34556 (17)	0.39794 (12)	0.0774 (5)	
O5	0.3219 (6)	0.3444 (10)	0.4326 (7)	0.094 (4)	0.667 (14)

O6	0.4963 (10)	0.4271 (9)	0.3167 (5)	0.112 (5)	0.667 (14)
O7	0.5051 (12)	0.3800 (14)	0.4553 (6)	0.167 (7)	0.667 (14)
O8	0.4962 (14)	0.2406 (7)	0.3917 (10)	0.215 (9)	0.667 (14)
O5'	0.3346 (15)	0.292 (2)	0.4241 (19)	0.214 (19)	0.333 (14)
O6'	0.438 (2)	0.4639 (9)	0.3833 (18)	0.152 (10)	0.333 (14)
O7'	0.525 (2)	0.325 (3)	0.3191 (11)	0.237 (16)	0.333 (14)
O8'	0.518 (2)	0.3029 (17)	0.4592 (13)	0.134 (10)	0.333 (14)
C25	0.2886 (11)	0.0715 (10)	0.5631 (9)	0.055 (5)	0.422 (11)
H25	0.3190	0.1255	0.5063	0.066*	0.422 (11)
Cl3	0.1298 (9)	0.0784 (11)	0.6004 (10)	0.153 (5)	0.422 (11)
Cl4	0.3558 (12)	0.1004 (13)	0.6321 (10)	0.169 (5)	0.422 (11)
Cl5	0.3221 (11)	−0.0635 (12)	0.5547 (14)	0.240 (8)	0.422 (11)
C25'	0.2522 (15)	0.0247 (15)	0.5881 (9)	0.109 (11)	0.328 (11)
H25'	0.2008	−0.0428	0.6227	0.131*	0.328 (11)
Cl3'	0.1541 (12)	0.1336 (15)	0.5820 (9)	0.128 (6)	0.328 (11)
Cl4'	0.3563 (16)	0.0365 (14)	0.6398 (10)	0.146 (5)	0.328 (11)
Cl5'	0.3181 (10)	0.0060 (9)	0.4887 (6)	0.116 (4)	0.328 (11)
C26	0.0137 (18)	0.7237 (10)	0.9183 (10)	0.069 (7)	0.283 (5)
H26	−0.0765	0.7169	0.9461	0.083*	0.283 (5)
Cl6	0.0834 (17)	0.7822 (11)	0.9757 (8)	0.075 (4)	0.283 (5)
Cl7	0.0710 (13)	0.5926 (8)	0.9178 (7)	0.130 (4)	0.283 (5)
Cl8	0.041 (2)	0.8061 (12)	0.8154 (9)	0.166 (8)	0.283 (5)
C26'	−0.0228 (17)	0.7372 (12)	0.9237 (9)	0.072 (7)	0.317 (5)
H26'	−0.0895	0.6816	0.9594	0.086*	0.317 (5)
Cl6'	0.081 (2)	0.7375 (16)	0.9808 (12)	0.120 (6)	0.317 (5)
Cl7'	0.0455 (14)	0.7020 (13)	0.8312 (7)	0.175 (6)	0.317 (5)
Cl8'	−0.0879 (7)	0.8663 (5)	0.9019 (4)	0.096 (3)	0.317 (5)
Cl6"	−0.019 (3)	0.616 (2)	0.897 (2)	0.191 (12)	0.15
Cl7"	0.108 (2)	0.818 (3)	0.7986 (16)	0.123 (9)	0.15
Cl8"	0.028 (2)	0.770 (3)	0.9793 (17)	0.103 (9)	0.15
C26"	0.084 (2)	0.715 (2)	0.8939 (15)	0.106 (12)	0.15
H26"	0.1639	0.6790	0.8968	0.128*	0.15

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.1018 (5)	0.0786 (4)	0.0495 (3)	0.0385 (3)	−0.0379 (3)	−0.0256 (3)
Ag2	0.0922 (4)	0.0976 (5)	0.0553 (3)	0.0323 (3)	−0.0377 (3)	−0.0253 (3)
S1	0.0675 (11)	0.0551 (9)	0.0569 (9)	0.0170 (8)	−0.0354 (8)	−0.0198 (8)
S2	0.0710 (11)	0.0731 (11)	0.0608 (10)	0.0258 (9)	−0.0383 (9)	−0.0239 (9)
S3	0.0695 (11)	0.0720 (11)	0.0593 (10)	0.0208 (9)	−0.0230 (8)	−0.0230 (9)
S4	0.0862 (14)	0.0928 (14)	0.0760 (13)	0.0394 (11)	−0.0336 (10)	−0.0379 (11)
N1	0.059 (3)	0.043 (3)	0.045 (3)	0.009 (2)	−0.023 (2)	−0.013 (2)
N2	0.075 (4)	0.075 (4)	0.049 (3)	0.023 (3)	−0.033 (3)	−0.024 (3)
N3	0.075 (4)	0.053 (3)	0.057 (3)	0.013 (3)	−0.036 (3)	−0.016 (3)
N4	0.079 (4)	0.073 (4)	0.049 (3)	0.021 (3)	−0.029 (3)	−0.014 (3)
N5	0.047 (3)	0.062 (3)	0.045 (3)	0.009 (2)	−0.018 (2)	−0.015 (2)
N6	0.076 (4)	0.086 (4)	0.051 (3)	0.015 (3)	−0.030 (3)	−0.024 (3)

N7	0.058 (3)	0.063 (3)	0.050 (3)	0.012 (3)	−0.019 (2)	−0.016 (3)
N8	0.096 (5)	0.124 (6)	0.087 (5)	0.037 (4)	−0.048 (4)	−0.062 (4)
C1	0.070 (4)	0.056 (4)	0.054 (4)	0.014 (3)	−0.026 (3)	−0.018 (3)
C2	0.075 (5)	0.073 (5)	0.073 (5)	0.019 (4)	−0.026 (4)	−0.040 (4)
C3	0.084 (5)	0.087 (5)	0.053 (4)	0.021 (4)	−0.029 (4)	−0.031 (4)
C4	0.047 (3)	0.051 (3)	0.047 (3)	0.008 (3)	−0.021 (3)	−0.014 (3)
C5	0.069 (4)	0.048 (4)	0.068 (4)	0.010 (3)	−0.038 (3)	−0.009 (3)
C6	0.058 (4)	0.051 (4)	0.064 (4)	0.008 (3)	−0.031 (3)	−0.011 (3)
C7	0.062 (4)	0.051 (4)	0.067 (4)	0.013 (3)	−0.033 (3)	−0.014 (3)
C8	0.067 (4)	0.058 (4)	0.072 (4)	0.016 (3)	−0.038 (4)	−0.016 (3)
C9	0.051 (4)	0.053 (4)	0.053 (4)	0.003 (3)	−0.026 (3)	−0.008 (3)
C10	0.101 (6)	0.065 (5)	0.079 (5)	0.017 (4)	−0.055 (5)	−0.021 (4)
C11	0.117 (7)	0.078 (5)	0.080 (5)	0.039 (5)	−0.052 (5)	−0.039 (4)
C12	0.100 (6)	0.093 (6)	0.054 (4)	0.020 (5)	−0.033 (4)	−0.019 (4)
C13	0.053 (4)	0.064 (4)	0.054 (4)	0.004 (3)	−0.015 (3)	−0.015 (3)
C14	0.072 (5)	0.078 (5)	0.055 (4)	0.012 (4)	−0.027 (3)	−0.010 (4)
C15	0.088 (6)	0.110 (7)	0.049 (4)	0.011 (5)	−0.024 (4)	−0.029 (4)
C16	0.045 (4)	0.064 (4)	0.051 (4)	0.005 (3)	−0.015 (3)	−0.019 (3)
C17	0.063 (5)	0.077 (5)	0.081 (5)	0.011 (4)	−0.017 (4)	−0.033 (4)
C18	0.063 (5)	0.080 (5)	0.078 (5)	0.010 (4)	−0.016 (4)	−0.032 (4)
C19	0.074 (5)	0.095 (6)	0.070 (5)	0.008 (4)	−0.018 (4)	−0.027 (4)
C20	0.085 (6)	0.082 (6)	0.106 (7)	0.014 (5)	−0.006 (5)	−0.035 (5)
C21	0.049 (4)	0.083 (5)	0.056 (4)	0.010 (3)	−0.014 (3)	−0.028 (4)
C22	0.082 (5)	0.070 (5)	0.064 (4)	0.018 (4)	−0.033 (4)	−0.018 (4)
C23	0.087 (6)	0.087 (6)	0.070 (5)	0.007 (5)	−0.039 (4)	−0.011 (4)
C24	0.104 (7)	0.131 (8)	0.078 (6)	0.027 (6)	−0.052 (5)	−0.049 (5)
Cl1	0.1006 (15)	0.0713 (12)	0.0836 (13)	0.0258 (11)	−0.0431 (12)	−0.0431 (11)
O1	0.219 (9)	0.123 (6)	0.202 (9)	−0.044 (6)	−0.141 (8)	0.031 (6)
O2	0.260 (11)	0.137 (6)	0.210 (9)	0.036 (7)	−0.186 (9)	−0.015 (6)
O3	0.373 (14)	0.105 (5)	0.167 (8)	0.045 (7)	−0.098 (9)	−0.097 (6)
O4	0.171 (8)	0.297 (12)	0.091 (5)	0.111 (8)	−0.031 (5)	−0.054 (6)
Cl2	0.0968 (15)	0.0741 (13)	0.0672 (12)	0.0153 (11)	−0.0386 (11)	−0.0156 (10)
O5	0.081 (7)	0.116 (10)	0.085 (7)	0.032 (6)	−0.017 (5)	−0.039 (6)
O6	0.143 (9)	0.102 (8)	0.080 (7)	−0.014 (7)	−0.054 (6)	0.020 (6)
O7	0.153 (11)	0.258 (19)	0.084 (8)	−0.054 (12)	−0.074 (7)	0.013 (10)
O8	0.286 (18)	0.105 (9)	0.156 (14)	0.063 (10)	0.059 (12)	−0.023 (9)
O5'	0.25 (3)	0.12 (2)	0.30 (4)	−0.08 (2)	−0.22 (3)	0.07 (2)
O6'	0.21 (2)	0.091 (15)	0.18 (2)	0.056 (15)	−0.074 (19)	−0.058 (15)
O7'	0.38 (4)	0.27 (4)	0.10 (2)	0.13 (3)	−0.10 (2)	−0.12 (2)
O8'	0.19 (2)	0.098 (16)	0.146 (19)	0.057 (16)	−0.128 (17)	−0.007 (14)
C25	0.082 (12)	0.038 (9)	0.059 (10)	0.013 (8)	−0.042 (9)	−0.017 (7)
Cl3	0.121 (8)	0.157 (10)	0.181 (12)	−0.005 (6)	−0.026 (6)	−0.066 (8)
Cl4	0.147 (8)	0.201 (14)	0.189 (11)	0.049 (9)	−0.061 (7)	−0.097 (10)
Cl5	0.188 (10)	0.206 (13)	0.36 (2)	0.014 (9)	−0.034 (12)	−0.183 (15)
C25'	0.090 (18)	0.13 (2)	0.092 (18)	0.015 (17)	−0.013 (15)	−0.022 (17)
Cl3'	0.086 (7)	0.208 (15)	0.093 (7)	0.054 (8)	−0.030 (5)	−0.053 (9)
Cl4'	0.176 (11)	0.161 (13)	0.137 (8)	0.050 (10)	−0.102 (8)	−0.047 (9)
Cl5'	0.129 (7)	0.106 (7)	0.130 (8)	0.033 (5)	−0.045 (6)	−0.057 (6)
C26	0.042 (15)	0.093 (15)	0.091 (15)	0.031 (12)	−0.028 (11)	−0.049 (13)

Cl6	0.072 (8)	0.092 (8)	0.070 (5)	0.006 (7)	−0.035 (6)	−0.022 (5)
Cl7	0.160 (10)	0.104 (7)	0.139 (9)	0.040 (7)	−0.043 (8)	−0.060 (6)
Cl8	0.26 (2)	0.143 (12)	0.129 (11)	−0.003 (13)	−0.142 (14)	−0.001 (9)
C26'	0.048 (13)	0.101 (14)	0.083 (13)	0.050 (11)	−0.034 (10)	−0.045 (12)
Cl6'	0.144 (11)	0.127 (12)	0.132 (9)	0.073 (9)	−0.099 (9)	−0.055 (8)
Cl7'	0.245 (14)	0.205 (13)	0.111 (8)	0.104 (12)	−0.071 (8)	−0.100 (9)
Cl8'	0.114 (6)	0.089 (5)	0.085 (5)	0.028 (4)	−0.045 (4)	−0.013 (4)
Cl6"	0.17 (2)	0.22 (2)	0.18 (2)	−0.085 (19)	0.005 (19)	−0.08 (2)
Cl7"	0.117 (16)	0.16 (2)	0.106 (14)	−0.044 (14)	−0.066 (12)	−0.018 (13)
Cl8"	0.079 (15)	0.137 (19)	0.131 (16)	0.023 (13)	−0.047 (13)	−0.081 (15)
C26"	0.12 (2)	0.108 (19)	0.105 (19)	0.007 (19)	−0.038 (18)	−0.046 (18)

Geometric parameters (Å, °)

Ag1—N1	2.188 (4)	C14—C15	1.373 (10)
Ag1—N5	2.201 (5)	C14—H14	0.9300
Ag2—N7	2.171 (5)	C15—H15	0.9300
Ag2—N3^{i}	2.177 (5)	C17—C18	1.493 (9)
S1—C4	1.758 (6)	C17—H17A	0.9700
S1—C5	1.808 (6)	C17—H17B	0.9700
S2—C9	1.732 (6)	C18—C19	1.556 (10)
S2—C8	1.812 (6)	C18—H18A	0.9700
S3—C16	1.749 (6)	C18—H18B	0.9700
S3—C17	1.812 (7)	C19—C20	1.462 (10)
S4—C21	1.764 (7)	C19—H19A	0.9700
S4—C20	1.812 (8)	C19—H19B	0.9700
N1—C1	1.339 (7)	C20—H20A	0.9700
N1—C4	1.344 (7)	C20—H20B	0.9700
N2—C4	1.312 (7)	C22—C23	1.364 (9)
N2—C3	1.335 (8)	C22—H22	0.9300
N3—C10	1.324 (9)	C23—C24	1.341 (11)
N3—C9	1.359 (7)	C23—H23	0.9300
N3—Ag2^{ii}	2.177 (5)	C24—H24	0.9300
N4—C9	1.310 (7)	Cl1—O3	1.323 (6)
N4—C12	1.333 (9)	Cl1—O2	1.356 (7)
N5—C13	1.333 (7)	Cl1—O4	1.363 (8)
N5—C16	1.347 (7)	Cl1—O1	1.424 (7)
N6—C16	1.303 (7)	Cl2—O8	1.380 (7)
N6—C15	1.330 (9)	Cl2—O8'	1.398 (9)
N7—C21	1.324 (8)	Cl2—O5'	1.419 (10)
N7—C22	1.327 (8)	Cl2—O5	1.422 (7)
N8—C21	1.312 (8)	Cl2—O7'	1.424 (9)
N8—C24	1.361 (10)	Cl2—O6	1.425 (6)
C1—C2	1.366 (8)	Cl2—O7	1.427 (8)
C1—H1	0.9300	Cl2—O6'	1.427 (9)
C2—C3	1.370 (9)	C25—Cl4	1.684 (9)
C2—H2	0.9300	C25—Cl3	1.710 (9)
C3—H3	0.9300	C25—Cl5	1.728 (9)
C5—C6	1.515 (8)	C25—H25	0.9800

C5—H5A	0.9700	C25'—Cl4'	1.682 (10)
C5—H5B	0.9700	C25'—Cl3'	1.688 (10)
C6—C7	1.522 (8)	C25'—Cl5'	1.701 (10)
C6—H6A	0.9700	C25'—H25'	0.9800
C6—H6B	0.9700	C26—Cl8	1.701 (10)
C7—C8	1.511 (8)	C26—Cl7	1.713 (10)
C7—H7A	0.9700	C26—Cl6	1.724 (10)
C7—H7B	0.9700	C26—H26	0.9800
C8—H8A	0.9700	C26'—Cl7'	1.692 (10)
C8—H8B	0.9700	C26'—Cl8'	1.708 (10)
C10—C11	1.345 (9)	C26'—Cl6'	1.717 (10)
C10—H10	0.9300	C26'—H26'	0.9800
C11—C12	1.368 (9)	Cl6"—C26"	1.709 (10)
C11—H11	0.9300	Cl7"—C26"	1.714 (10)
C12—H12	0.9300	Cl8"—C26"	1.713 (10)
C13—C14	1.372 (8)	C26"—H26"	0.9800
C13—H13	0.9300		
N1—Ag1—N5	161.96 (18)	C17—C18—H18B	110.0
N7—Ag2—N3^{i}	168.73 (19)	C19—C18—H18B	110.0
C4—S1—C5	101.9 (3)	H18A—C18—H18B	108.3
C9—S2—C8	102.3 (3)	C20—C19—C18	114.0 (7)
C16—S3—C17	103.4 (3)	C20—C19—H19A	108.7
C21—S4—C20	103.4 (4)	C18—C19—H19A	108.7
C1—N1—C4	116.4 (5)	C20—C19—H19B	108.7
C1—N1—Ag1	121.1 (4)	C18—C19—H19B	108.7
C4—N1—Ag1	122.3 (4)	H19A—C19—H19B	107.6
C4—N2—C3	115.9 (5)	C19—C20—S4	114.4 (6)
C10—N3—C9	116.8 (5)	C19—C20—H20A	108.7
C10—N3—Ag2^{ii}	119.4 (4)	S4—C20—H20A	108.7
C9—N3—Ag2^{ii}	123.8 (4)	C19—C20—H20B	108.7
C9—N4—C12	117.2 (6)	S4—C20—H20B	108.7
C13—N5—C16	116.8 (5)	H20A—C20—H20B	107.6
C13—N5—Ag1	122.2 (4)	N8—C21—N7	126.5 (6)
C16—N5—Ag1	120.9 (4)	N8—C21—S4	119.8 (5)
C16—N6—C15	116.2 (6)	N7—C21—S4	113.7 (5)
C21—N7—C22	116.7 (6)	N7—C22—C23	122.0 (7)
C21—N7—Ag2	121.6 (4)	N7—C22—H22	119.0
C22—N7—Ag2	121.3 (4)	C23—C22—H22	119.0
C21—N8—C24	114.8 (7)	C24—C23—C22	116.9 (7)
N1—C1—C2	122.2 (6)	C24—C23—H23	121.5
N1—C1—H1	118.9	C22—C23—H23	121.5
C2—C1—H1	118.9	C23—C24—N8	123.1 (7)
C1—C2—C3	116.0 (6)	C23—C24—H24	118.5
C1—C2—H2	122.0	N8—C24—H24	118.5
C3—C2—H2	122.0	O3—Cl1—O2	115.5 (6)
N2—C3—C2	123.6 (6)	O3—Cl1—O4	107.7 (7)
N2—C3—H3	118.2	O2—Cl1—O4	110.6 (6)
C2—C3—H3	118.2	O3—Cl1—O1	109.6 (6)

N2—C4—N1	125.8 (5)	O2—Cl1—O1	110.6 (5)
N2—C4—S1	120.5 (4)	O4—Cl1—O1	101.8 (6)
N1—C4—S1	113.7 (4)	O8—Cl2—O8'	71.6 (10)
C6—C5—S1	114.9 (4)	O8—Cl2—O5'	83.4 (14)
C6—C5—H5A	108.5	O8'—Cl2—O5'	111.0 (9)
S1—C5—H5A	108.5	O8—Cl2—O5	111.4 (7)
C6—C5—H5B	108.5	O8'—Cl2—O5	114.4 (13)
S1—C5—H5B	108.5	O5'—Cl2—O5	28.4 (13)
H5A—C5—H5B	107.5	O8—Cl2—O7'	56.9 (12)
C5—C6—C7	109.8 (5)	O8'—Cl2—O7'	108.1 (9)
C5—C6—H6A	109.7	O5'—Cl2—O7'	109.1 (10)
C7—C6—H6A	109.7	O5—Cl2—O7'	128.6 (14)
C5—C6—H6B	109.7	O8—Cl2—O6	110.4 (6)
C7—C6—H6B	109.7	O8'—Cl2—O6	128.3 (11)
H6A—C6—H6B	108.2	O5'—Cl2—O6	120.7 (11)
C8—C7—C6	112.7 (5)	O5—Cl2—O6	112.2 (6)
C8—C7—H7A	109.0	O7'—Cl2—O6	53.5 (11)
C6—C7—H7A	109.0	O8—Cl2—O7	109.8 (7)
C8—C7—H7B	109.0	O8'—Cl2—O7	39.1 (8)
C6—C7—H7B	109.0	O5'—Cl2—O7	123.1 (15)
H7A—C7—H7B	107.8	O5—Cl2—O7	106.6 (6)
C7—C8—S2	113.9 (5)	O7'—Cl2—O7	124.7 (14)
C7—C8—H8A	108.8	O6—Cl2—O7	106.2 (6)
S2—C8—H8A	108.8	O8—Cl2—O6'	164.1 (12)
C7—C8—H8B	108.8	O8'—Cl2—O6'	111.6 (9)
S2—C8—H8B	108.8	O5'—Cl2—O6'	108.7 (9)
H8A—C8—H8B	107.7	O5—Cl2—O6'	81.9 (11)
N4—C9—N3	124.0 (6)	O7'—Cl2—O6'	108.3 (10)
N4—C9—S2	121.1 (5)	O6—Cl2—O6'	54.8 (10)
N3—C9—S2	114.8 (4)	O7—Cl2—O6'	72.7 (9)
N3—C10—C11	122.8 (6)	Cl4—C25—Cl3	109.9 (7)
N3—C10—H10	118.6	Cl4—C25—Cl5	110.4 (7)
C11—C10—H10	118.6	Cl3—C25—Cl5	107.3 (7)
C10—C11—C12	116.8 (7)	Cl4—C25—H25	109.7
C10—C11—H11	121.6	Cl3—C25—H25	109.7
C12—C11—H11	121.6	Cl5—C25—H25	109.7
N4—C12—C11	122.4 (7)	Cl4'—C25'—Cl3'	112.3 (8)
N4—C12—H12	118.8	Cl4'—C25'—Cl5'	113.8 (9)
C11—C12—H12	118.8	Cl3'—C25'—Cl5'	110.2 (8)
N5—C13—C14	121.3 (6)	Cl4'—C25'—H25'	106.7
N5—C13—H13	119.3	Cl3'—C25'—H25'	106.7
C14—C13—H13	119.3	Cl5'—C25'—H25'	106.7
C13—C14—C15	116.7 (6)	Cl8—C26—Cl7	109.6 (8)
C13—C14—H14	121.7	Cl8—C26—Cl6	110.6 (8)
C15—C14—H14	121.7	Cl7—C26—Cl6	109.8 (8)
N6—C15—C14	123.1 (6)	Cl8—C26—H26	108.9
N6—C15—H15	118.5	Cl7—C26—H26	108.9
C14—C15—H15	118.5	Cl6—C26—H26	108.9
N6—C16—N5	126.0 (6)	Cl7'—C26'—Cl8'	110.1 (8)

N6—C16—S3	120.8 (5)	Cl7'—C26'—Cl6'	111.8 (8)
N5—C16—S3	113.3 (4)	Cl8'—C26'—Cl6'	109.7 (8)
C18—C17—S3	115.2 (5)	Cl7'—C26'—H26'	108.4
C18—C17—H17A	108.5	Cl8'—C26'—H26'	108.4
S3—C17—H17A	108.5	Cl6'—C26'—H26'	108.4
C18—C17—H17B	108.5	Cl6"—C26"—Cl8"	110.6 (9)
S3—C17—H17B	108.5	Cl6"—C26"—Cl7"	108.9 (9)
H17A—C17—H17B	107.5	Cl8"—C26"—Cl7"	110.6 (9)
C17—C18—C19	108.7 (6)	Cl6"—C26"—H26"	108.9
C17—C18—H18A	110.0	Cl8"—C26"—H26"	108.9
C19—C18—H18A	110.0	Cl7"—C26"—H26"	108.9
N5—Ag1—N1—C1	−76.7 (8)	N3—C10—C11—C12	0.8 (12)
N5—Ag1—N1—C4	108.5 (6)	C9—N4—C12—C11	1.8 (11)
N1—Ag1—N5—C13	81.4 (7)	C10—C11—C12—N4	−1.7 (13)
N1—Ag1—N5—C16	−103.6 (7)	C16—N5—C13—C14	−1.2 (9)
$N3^{i}$—Ag2—N7—C21	−69.4 (12)	Ag1—N5—C13—C14	174.0 (5)
$N3^{i}$—Ag2—N7—C22	102.8 (11)	N5—C13—C14—C15	0.5 (10)
C4—N1—C1—C2	−0.5 (9)	C16—N6—C15—C14	0.8 (11)
Ag1—N1—C1—C2	−175.6 (5)	C13—C14—C15—N6	−0.3 (11)
N1—C1—C2—C3	3.0 (10)	C15—N6—C16—N5	−1.7 (10)
C4—N2—C3—C2	−0.3 (10)	C15—N6—C16—S3	177.5 (5)
C1—C2—C3—N2	−2.6 (11)	C13—N5—C16—N6	1.9 (9)
C3—N2—C4—N1	3.3 (9)	Ag1—N5—C16—N6	−173.4 (5)
C3—N2—C4—S1	−177.8 (5)	C13—N5—C16—S3	−177.3 (4)
C1—N1—C4—N2	−2.9 (9)	Ag1—N5—C16—S3	7.4 (6)
Ag1—N1—C4—N2	172.1 (5)	C17—S3—C16—N6	8.4 (6)
C1—N1—C4—S1	178.1 (4)	C17—S3—C16—N5	−172.4 (4)
Ag1—N1—C4—S1	−6.8 (6)	C16—S3—C17—C18	−79.3 (6)
C5—S1—C4—N2	8.1 (6)	S3—C17—C18—C19	−169.3 (5)
C5—S1—C4—N1	−172.9 (4)	C17—C18—C19—C20	−177.0 (7)
C4—S1—C5—C6	74.8 (5)	C18—C19—C20—S4	174.7 (6)
S1—C5—C6—C7	173.0 (5)	C21—S4—C20—C19	92.6 (7)
C5—C6—C7—C8	173.7 (5)	C24—N8—C21—N7	0.5 (12)
C6—C7—C8—S2	−173.9 (5)	C24—N8—C21—S4	179.8 (6)
C9—S2—C8—C7	−82.1 (5)	C22—N7—C21—N8	−1.7 (11)
C12—N4—C9—N3	−1.1 (10)	Ag2—N7—C21—N8	170.9 (6)
C12—N4—C9—S2	−178.8 (5)	C22—N7—C21—S4	179.1 (5)
C10—N3—C9—N4	0.3 (9)	Ag2—N7—C21—S4	−8.4 (7)
$Ag2^{ii}$—N3—C9—N4	179.8 (5)	C20—S4—C21—N8	−10.7 (7)
C10—N3—C9—S2	178.1 (5)	C20—S4—C21—N7	168.6 (5)
$Ag2^{ii}$—N3—C9—S2	−2.4 (7)	C21—N7—C22—C23	2.0 (11)
C8—S2—C9—N4	−2.0 (6)	Ag2—N7—C22—C23	−170.5 (6)
C8—S2—C9—N3	−180.0 (5)	N7—C22—C23—C24	−1.3 (12)
C9—N3—C10—C11	−0.2 (11)	C22—C23—C24—N8	0.1 (14)
$Ag2^{ii}$—N3—C10—C11	−179.7 (6)	C21—N8—C24—C23	0.3 (13)

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

Fig. 1

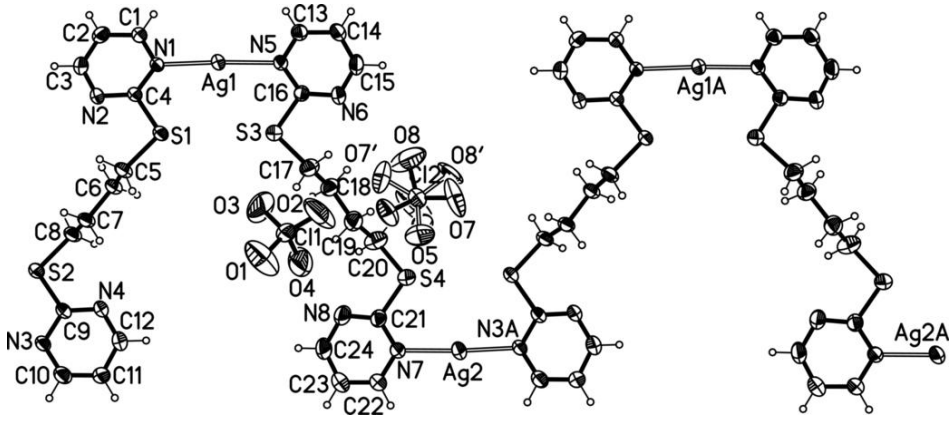
C1
C2
N1
C3
C4
N2
S1
C5
C6
C7
C8
S2
N4
C9
C12
N3
C10
C11
Ag1
C13
C14
N5
C15
C16
N6
S3
C17
C18
O7′
O8
O8′
Cl2
O3
O2
Cl1
O1
O4
C19
C20
O5
O7
S4
N8
C21
C24
C23
C22
N7
Ag2
N3A
Ag1A
Ag2A

Fig. 2