

catena-Poly[[silver(I)- μ -1,4-di-4-pyridyl-2,3-diazabuta-1,3-diene] methane-sulfonate]

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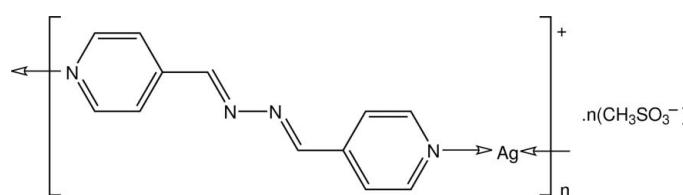
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Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å;
 R factor = 0.054; wR factor = 0.132; data-to-parameter ratio = 15.5.

The asymmetric unit in the polymeric title compound, $\{[\text{Ag}(\text{C}_{12}\text{H}_{10}\text{N}_4)]\text{CH}_3\text{SO}_3\}_n$, comprises two Ag atoms, a 4-pyridinealdazine molecule in a general position, two 4-pyridinealdazine molecules each disposed about a centre of inversion, and two methanesulfonate anions. The Ag atoms are in linear geometries within N_2 donor sets. The topology of the polymer is linear and the strands are connected into double chains via weak argentophilic $\text{Ag}\cdots\text{Ag}$ [3.2088 (10) Å] interactions that stack along the b axis interspersed by the methanesulfonate anions. These layers are consolidated in the crystal structure primarily via weak $\text{Ag}\cdots\text{O}$ contacts ($\text{Ag}\cdots\text{O} > 2.69$ Å).

Related literature

For related polymeric silver salts containing the 4-pyridine-aldazine ligand, see: Shi *et al.* (2002); Patra & Goldberg (2003); Kennedy *et al.* (2005). For related literature, see: Broker & Tiekink (2007a,b).



Experimental

Crystal data

$[\text{Ag}(\text{C}_{12}\text{H}_{10}\text{N}_4)]\text{CH}_3\text{O}_3\text{S}$
 $M_r = 413.22$

Monoclinic, $C2/c$
 $a = 25.083$ (9) Å

$b = 12.284$ (4) Å
 $c = 21.009$ (7) Å
 $\beta = 113.790$ (7)°
 $V = 5923$ (3) Å³
 $Z = 16$

Mo $K\alpha$ radiation
 $\mu = 1.52$ mm⁻¹
 $T = 153$ (2) K
 $0.30 \times 0.08 \times 0.07$ mm

Data collection

Rigaku AFC12κ/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.645$, $T_{\max} = 1.000$
(expected range = 0.580–0.899)

37758 measured reflections
6151 independent reflections
5879 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.132$
 $S = 1.16$
6151 reflections

397 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 1.98$ e Å⁻³
 $\Delta\rho_{\min} = -1.28$ e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.179 (4)	Ag2—N7	2.158 (4)
Ag1—N5	2.177 (4)	Ag1—Ag2 ⁱ	3.2088 (10)
Ag2—N4	2.165 (4)		
N1—Ag1—N5	169.88 (15)	N4—Ag2—N7	169.32 (15)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2517).

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Acta Cryst. (2007). E63, m2436 [doi:10.1107/S1600536807041645]

[*catena-Poly[[silver(I)-μ-1,4-di-4-pyridyl-2,3-diazabuta-1,3-diene] methanesulfonate*]]

G. A. Broker and E. R. T. Tiekink

Comment

The polymeric title compound, $[\text{Ag}(\text{C}_{12}\text{H}_{10}\text{N}_4)]_n \cdot n(\text{CH}_3\text{SO}_3)$ or $[\text{Ag}(4-\text{PA})]_n \cdot n(\text{CH}_3\text{SO}_3)$, (I), was investigated as a part of an on-going study of the structural chemistry of Ag salts of isomeric n-pyridinealdazine molecules, $n = 2, 3$ and 4 (Broker & Tiekink, 2007a,b). The asymmetric unit of (I) comprises two Ag atoms, a 4-pyridinealdazine (4-PA) molecule in a general position, two 4-PA molecules each disposed about a centre of inversion, and two methanesulfonate anions (Fig. 1). All the 4-PA ligands are bidentate bridging, resulting in polymeric chains and linear N_2 geometries for each Ag atom (Table 1). A small twist in the $\text{N}-\text{C}-\text{C}-\text{N}$ portions of the bridging ligand occupying the general position [$\text{C}_6-\text{N}_2-\text{N}_3-\text{C}_7 = 163.0(4)^\circ$] dictates that the chain is not strictly flat. The linear chains are connected into supramolecular double chains *via* weak $\text{Ag}_1 \cdots \text{Ag}_2$ agentophilic interactions [$\text{Ag} \cdots \text{Ag} = 3.2088(10) \text{\AA}$]. The double chains stack along the b axis being interspersed by anions to form a layer structure (Fig. 2). Connections between layers are afforded by $\text{Ag} \cdots \text{O}$ interactions with the most significant being $\text{Ag}_1 \cdots \text{O}_1$, O_4^i and O_5^i of $2.694(4)$, $2.797(4)$, and $2.770(4) \text{\AA}$, respectively ($i: 1-x, -y, 1-z$), and $\text{Ag}_2 \cdots \text{O}_4$, O_1^{ii} and O_3^{ii} of $2.743(4)$, $2.811(4)$ and $2.993(4) \text{\AA}$, respectively ($ii: 1-x, -y, 1-z$). A view of the unit-cell contents highlighting the stacking of layers is shown in Fig. 3.

Similar $[\text{Ag}(4-\text{PA})]_n$ polymeric chains as seen for (I) are found in the following salts: perchlorate, tetrafluoroborate (as acetonitrile solvates, Kennedy *et al.*, 2005), hexafluoroantimonate (as the acetonitrile water solvate, Kennedy *et al.*, 2005), and nitrate, for which two polymorphs have been reported (Shi *et al.*, 2002; Patra & Goldberg, 2003 & Kennedy *et al.*, 2005). In all but the nitrate polymorphs, the chains are essentially flat. In none of the above compounds are $\text{Ag} \cdots \text{Ag}$ interactions found.

Experimental

$\text{Ag}(\text{CH}_3\text{SO}_3)$ (Aldrich, 0.05 g, 0.25 mmol) was dissolved in CH_3CN (20 ml) and layered on top of a CH_2Cl_2 solution (20 ml) containing 0.05 g (0.25 mmol) of 4-pyridinealdazine (Aldrich). After three days, yellow prisms of (I) were observed at the interface between the two layers; m. pt. 522 – 524 K.

Refinement

All the H atoms were included in the riding-model approximation, with $\text{C}-\text{H} = 0.95\text{--}0.98 \text{\AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}$ (methyl C). The maximum and minimum difference peaks are located 1.14 and 0.84\AA , respectively, from Ag_1 .

Figures

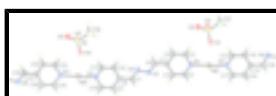


Fig. 1. The asymmetric unit of (I) showing atom-labelling scheme and displacement ellipsoids at the 70% probability level (arbitrary spheres for the H atoms).

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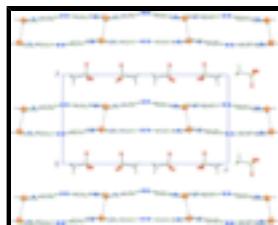


Fig. 2. View of the layers in (I) down the *c* axis highlighting the Ag···Ag interactions leading to supramolecular double chains. Colour code: orange (silver), yellow (sulfur), red (oxygen), blue (nitrogen), grey (carbon) and green (hydrogen).

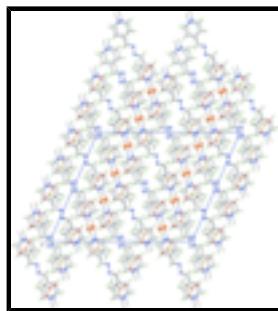


Fig. 3. View of the unit-cell contents in (I) down the *b* axis. Colour code as for Fig. 2.

catena-Poly[[silver(I)- μ -1,4-di-4-pyridyl-2,3-diazabuta-1,3-diene] methanesulfonate]

Crystal data

[Ag(C ₁₂ H ₁₀ N ₄)]CH ₃ O ₃ S	$F_{000} = 3296$
$M_r = 413.22$	$D_x = 1.853 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
Hall symbol: -C 2yc	$\lambda = 0.71070 \text{ \AA}$
$a = 25.083 (9) \text{ \AA}$	Cell parameters from 10582 reflections
$b = 12.284 (4) \text{ \AA}$	$\theta = 1.9\text{--}25.0^\circ$
$c = 21.009 (7) \text{ \AA}$	$\mu = 1.52 \text{ mm}^{-1}$
$\beta = 113.790 (7)^\circ$	$T = 153 (2) \text{ K}$
$V = 5923 (3) \text{ \AA}^3$	Prism, yellow
$Z = 16$	$0.30 \times 0.08 \times 0.07 \text{ mm}$

Data collection

Rigaku AFC12K/SATURN724 diffractometer	6151 independent reflections
Radiation source: fine-focus sealed tube	5879 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.048$
$T = 153(2) \text{ K}$	$\theta_{\text{max}} = 26.5^\circ$
ω scans	$\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -29 \rightarrow 31$
$T_{\text{min}} = 0.645$, $T_{\text{max}} = 1.000$	$k = -15 \rightarrow 15$
37758 measured reflections	$l = -26 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.132$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 41.7048P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.16$	$(\Delta/\sigma)_{\max} = 0.002$
6151 reflections	$\Delta\rho_{\max} = 1.98 \text{ e \AA}^{-3}$
397 parameters	$\Delta\rho_{\min} = -1.28 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.264234 (14)	0.11412 (3)	0.115089 (16)	0.02522 (12)
Ag2	0.761261 (15)	0.13780 (3)	0.867951 (17)	0.02714 (12)
S1	0.14174 (4)	-0.00296 (9)	0.18189 (5)	0.0232 (2)
S2	0.63856 (4)	0.00487 (9)	0.93140 (5)	0.0227 (2)
O1	0.17575 (14)	0.0433 (3)	0.14587 (17)	0.0349 (8)
O2	0.15577 (14)	0.0447 (3)	0.24999 (17)	0.0355 (8)
O3	0.14380 (15)	-0.1215 (3)	0.1835 (2)	0.0354 (8)
O4	0.66998 (14)	0.0630 (3)	0.89604 (16)	0.0297 (7)
O5	0.64598 (14)	-0.1133 (3)	0.92975 (17)	0.0282 (7)
O6	0.65091 (14)	0.0461 (3)	1.00060 (16)	0.0331 (8)
N1	0.32271 (16)	0.1270 (3)	0.2246 (2)	0.0233 (8)
N2	0.49505 (16)	0.1637 (3)	0.45649 (18)	0.0272 (8)
N3	0.52542 (16)	0.1634 (4)	0.52935 (19)	0.0273 (8)
N4	0.70009 (16)	0.1535 (3)	0.76056 (19)	0.0225 (8)
N5	0.19914 (16)	0.1277 (3)	0.00882 (19)	0.0233 (8)
N6	0.01700 (17)	0.1235 (3)	-0.21380 (19)	0.0281 (9)
N7	0.81773 (16)	0.1530 (3)	0.97678 (19)	0.0225 (8)
N8	0.98552 (16)	0.1972 (3)	1.21342 (18)	0.0269 (8)

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C1	0.38045 (19)	0.1436 (4)	0.2423 (2)	0.0235 (9)
H1	0.3938	0.1523	0.2062	0.028*
C2	0.42060 (19)	0.1483 (4)	0.3104 (2)	0.0243 (9)
H2	0.4606	0.1615	0.3208	0.029*
C3	0.40169 (19)	0.1335 (4)	0.3639 (2)	0.0229 (9)
C4	0.34180 (19)	0.1144 (4)	0.3451 (2)	0.0235 (9)
H4	0.3274	0.1026	0.3800	0.028*
C5	0.30417 (19)	0.1131 (4)	0.2757 (2)	0.0224 (9)
H5	0.2638	0.1018	0.2637	0.027*
C6	0.4412 (2)	0.1367 (4)	0.4377 (2)	0.0249 (9)
H6	0.4269	0.1187	0.4720	0.030*
C7	0.58074 (19)	0.1619 (4)	0.5471 (2)	0.0232 (9)
H7	0.5959	0.1612	0.5124	0.028*
C8	0.62066 (18)	0.1611 (4)	0.6211 (2)	0.0224 (9)
C9	0.68083 (19)	0.1661 (4)	0.6398 (2)	0.0250 (9)
H9	0.6955	0.1719	0.6048	0.030*
C10	0.71890 (19)	0.1625 (4)	0.7088 (2)	0.0252 (9)
H10	0.7596	0.1664	0.7204	0.030*
C11	0.64189 (19)	0.1490 (4)	0.7429 (2)	0.0244 (9)
H11	0.6283	0.1422	0.7789	0.029*
C12	0.60160 (19)	0.1539 (4)	0.6752 (2)	0.0240 (9)
H12	0.5611	0.1525	0.6651	0.029*
C13	0.1417 (2)	0.1261 (4)	-0.0053 (2)	0.0247 (9)
H13	0.1302	0.1240	0.0327	0.030*
C14	0.0987 (2)	0.1274 (4)	-0.0716 (2)	0.0248 (9)
H14	0.0588	0.1280	-0.0790	0.030*
C15	0.11503 (19)	0.1277 (4)	-0.1282 (2)	0.0224 (9)
C16	0.1747 (2)	0.1291 (4)	-0.1137 (2)	0.0252 (9)
H16	0.1873	0.1296	-0.1507	0.030*
C17	0.2149 (2)	0.1297 (4)	-0.0456 (2)	0.0249 (9)
H17	0.2551	0.1316	-0.0365	0.030*
C18	0.0717 (2)	0.1261 (4)	-0.2006 (2)	0.0245 (9)
H18	0.0842	0.1271	-0.2377	0.029*
C19	0.87543 (19)	0.1692 (4)	0.9965 (2)	0.0255 (9)
H19	0.8900	0.1758	0.9614	0.031*
C20	0.91447 (19)	0.1767 (4)	1.0653 (2)	0.0252 (9)
H20	0.9547	0.1892	1.0768	0.030*
C21	0.89386 (19)	0.1656 (4)	1.1176 (2)	0.0226 (9)
C22	0.83412 (19)	0.1478 (4)	1.0970 (2)	0.0235 (9)
H22	0.8186	0.1389	1.1311	0.028*
C23	0.7977 (2)	0.1432 (4)	1.0272 (2)	0.0245 (9)
H23	0.7572	0.1326	1.0142	0.029*
C24	0.93200 (19)	0.1704 (4)	1.1924 (2)	0.0245 (9)
H24	0.9164	0.1531	1.2255	0.029*
C25	0.06786 (19)	0.0330 (4)	0.1304 (3)	0.0315 (10)
H25A	0.0561	0.0026	0.0836	0.047*
H25B	0.0642	0.1125	0.1275	0.047*
H25C	0.0427	0.0038	0.1519	0.047*
C26	0.56288 (19)	0.0300 (4)	0.8806 (2)	0.0279 (10)

H26A	0.5524	0.0033	0.8331	0.042*
H26B	0.5553	0.1084	0.8794	0.042*
H26C	0.5395	-0.0080	0.9014	0.042*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.01883 (19)	0.0370 (2)	0.01557 (19)	0.00061 (13)	0.00254 (14)	-0.00006 (13)
Ag2	0.02145 (19)	0.0376 (2)	0.01613 (19)	-0.00067 (13)	0.00110 (14)	-0.00008 (13)
S1	0.0180 (5)	0.0310 (6)	0.0190 (5)	0.0005 (4)	0.0058 (4)	0.0016 (4)
S2	0.0180 (5)	0.0311 (6)	0.0183 (5)	0.0000 (4)	0.0065 (4)	-0.0001 (4)
O1	0.0228 (16)	0.057 (2)	0.0242 (17)	-0.0014 (15)	0.0087 (14)	0.0060 (15)
O2	0.0267 (17)	0.055 (2)	0.0223 (17)	0.0054 (16)	0.0080 (14)	-0.0057 (15)
O3	0.0268 (18)	0.0336 (19)	0.041 (2)	0.0013 (14)	0.0085 (16)	0.0017 (15)
O4	0.0237 (16)	0.042 (2)	0.0261 (16)	-0.0039 (14)	0.0127 (13)	0.0020 (14)
O5	0.0231 (17)	0.0316 (18)	0.0289 (18)	0.0043 (13)	0.0095 (14)	0.0021 (13)
O6	0.0284 (17)	0.049 (2)	0.0205 (16)	0.0024 (15)	0.0085 (14)	-0.0059 (15)
N1	0.0173 (18)	0.031 (2)	0.0176 (18)	0.0006 (14)	0.0026 (15)	0.0001 (14)
N2	0.0226 (19)	0.042 (2)	0.0131 (17)	-0.0025 (17)	0.0034 (15)	-0.0013 (16)
N3	0.0197 (18)	0.045 (2)	0.0129 (17)	0.0008 (17)	0.0016 (14)	0.0024 (16)
N4	0.0171 (18)	0.031 (2)	0.0158 (17)	0.0006 (14)	0.0029 (14)	0.0006 (14)
N5	0.0169 (18)	0.033 (2)	0.0168 (18)	-0.0014 (14)	0.0037 (15)	0.0019 (14)
N6	0.0200 (19)	0.042 (2)	0.016 (2)	0.0003 (16)	0.0012 (16)	0.0014 (15)
N7	0.0176 (18)	0.031 (2)	0.0143 (17)	-0.0007 (14)	0.0012 (14)	0.0000 (14)
N8	0.0243 (19)	0.036 (2)	0.0162 (19)	-0.0017 (16)	0.0040 (15)	-0.0003 (15)
C1	0.019 (2)	0.029 (2)	0.024 (2)	-0.0011 (17)	0.0101 (18)	-0.0002 (17)
C2	0.018 (2)	0.032 (2)	0.022 (2)	0.0017 (17)	0.0082 (18)	0.0025 (18)
C3	0.019 (2)	0.029 (2)	0.018 (2)	0.0004 (16)	0.0034 (17)	0.0014 (16)
C4	0.020 (2)	0.030 (2)	0.021 (2)	0.0011 (17)	0.0086 (18)	0.0002 (17)
C5	0.017 (2)	0.027 (2)	0.022 (2)	-0.0008 (16)	0.0062 (17)	-0.0011 (17)
C6	0.022 (2)	0.037 (3)	0.014 (2)	0.0008 (18)	0.0058 (17)	0.0023 (17)
C7	0.022 (2)	0.028 (2)	0.018 (2)	-0.0023 (17)	0.0067 (17)	-0.0004 (17)
C8	0.019 (2)	0.025 (2)	0.022 (2)	-0.0007 (16)	0.0079 (17)	0.0000 (17)
C9	0.023 (2)	0.032 (2)	0.023 (2)	-0.0018 (18)	0.0121 (18)	0.0025 (18)
C10	0.020 (2)	0.034 (2)	0.022 (2)	-0.0002 (18)	0.0090 (18)	0.0018 (18)
C11	0.018 (2)	0.035 (2)	0.021 (2)	0.0028 (17)	0.0081 (18)	0.0011 (18)
C12	0.017 (2)	0.034 (2)	0.020 (2)	0.0010 (17)	0.0073 (17)	0.0006 (18)
C13	0.023 (2)	0.031 (2)	0.021 (2)	0.0032 (17)	0.0100 (19)	0.0025 (17)
C14	0.018 (2)	0.031 (2)	0.027 (2)	0.0007 (17)	0.0101 (18)	0.0029 (18)
C15	0.019 (2)	0.027 (2)	0.017 (2)	-0.0004 (16)	0.0027 (17)	0.0005 (16)
C16	0.022 (2)	0.031 (2)	0.024 (2)	-0.0003 (17)	0.0107 (19)	0.0021 (18)
C17	0.021 (2)	0.030 (2)	0.025 (2)	-0.0002 (17)	0.0108 (19)	0.0012 (17)
C18	0.023 (2)	0.028 (2)	0.020 (2)	-0.0009 (17)	0.0070 (18)	0.0002 (17)
C19	0.023 (2)	0.032 (2)	0.021 (2)	-0.0026 (18)	0.0087 (18)	0.0023 (18)
C20	0.017 (2)	0.033 (2)	0.023 (2)	-0.0027 (17)	0.0047 (17)	0.0000 (18)
C21	0.020 (2)	0.024 (2)	0.022 (2)	-0.0012 (17)	0.0064 (17)	0.0012 (17)
C22	0.019 (2)	0.028 (2)	0.024 (2)	-0.0006 (17)	0.0100 (18)	0.0010 (17)
C23	0.021 (2)	0.028 (2)	0.024 (2)	-0.0007 (17)	0.0093 (18)	-0.0011 (17)

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C24	0.026 (2)	0.028 (2)	0.017 (2)	0.0024 (18)	0.0063 (18)	0.0034 (17)
C25	0.021 (2)	0.039 (3)	0.030 (2)	0.0001 (19)	0.0064 (19)	0.002 (2)
C26	0.020 (2)	0.033 (2)	0.025 (2)	0.0011 (18)	0.0032 (18)	0.0009 (19)

Geometric parameters (\AA , $^{\circ}$)

Ag1—N1	2.179 (4)	C6—H6	0.9500
Ag1—N5	2.177 (4)	C7—C8	1.471 (6)
Ag2—N4	2.165 (4)	C7—H7	0.9500
Ag2—N7	2.158 (4)	C8—C9	1.399 (6)
Ag1—Ag2 ⁱ	3.2088 (10)	C8—C12	1.402 (6)
Ag2—Ag1 ⁱ	3.2088 (10)	C9—C10	1.378 (6)
S1—O2	1.452 (3)	C9—H9	0.9500
S1—O3	1.457 (4)	C10—H10	0.9500
S1—O1	1.464 (3)	C11—C12	1.375 (6)
S1—C25	1.784 (5)	C11—H11	0.9500
S2—O6	1.450 (3)	C12—H12	0.9500
S2—O5	1.466 (3)	C13—C14	1.375 (7)
S2—O4	1.468 (3)	C13—H13	0.9500
S2—C26	1.790 (4)	C14—C15	1.404 (6)
N1—C5	1.341 (6)	C14—H14	0.9500
N1—C1	1.358 (6)	C15—C16	1.401 (6)
N2—C6	1.289 (6)	C15—C18	1.470 (6)
N2—N3	1.408 (5)	C16—C17	1.379 (7)
N3—C7	1.283 (6)	C16—H16	0.9500
N4—C10	1.352 (6)	C17—H17	0.9500
N4—C11	1.355 (6)	C18—H18	0.9500
N5—C13	1.350 (6)	C19—C20	1.384 (6)
N5—C17	1.351 (6)	C19—H19	0.9500
N6—C18	1.286 (6)	C20—C21	1.397 (6)
N6—N6 ⁱⁱ	1.412 (7)	C20—H20	0.9500
N7—C23	1.347 (6)	C21—C22	1.399 (6)
N7—C19	1.350 (6)	C21—C24	1.474 (6)
N8—C24	1.276 (6)	C22—C23	1.382 (6)
N8—N8 ⁱⁱⁱ	1.411 (7)	C22—H22	0.9500
C1—C2	1.379 (6)	C23—H23	0.9500
C1—H1	0.9500	C24—H24	0.9500
C2—C3	1.397 (6)	C25—H25A	0.9800
C2—H2	0.9500	C25—H25B	0.9800
C3—C4	1.410 (6)	C25—H25C	0.9800
C3—C6	1.466 (6)	C26—H26A	0.9800
C4—C5	1.381 (6)	C26—H26B	0.9800
C4—H4	0.9500	C26—H26C	0.9800
C5—H5	0.9500		
N1—Ag1—N5	169.88 (15)	C10—C9—H9	119.8
N5—Ag1—Ag2 ⁱ	95.02 (10)	C8—C9—H9	119.8
N1—Ag1—Ag2 ⁱ	91.85 (10)	N4—C10—C9	122.0 (4)
N4—Ag2—N7	169.32 (15)	N4—C10—H10	119.0

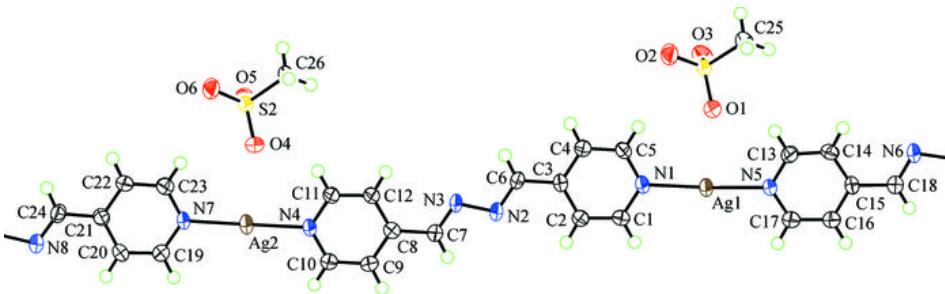
N7—Ag2—Ag1 ⁱ	92.34 (10)	C9—C10—H10	119.0
N4—Ag2—Ag1 ⁱ	96.46 (10)	N4—C11—C12	122.8 (4)
O2—S1—O3	112.8 (2)	N4—C11—H11	118.6
O2—S1—O1	113.1 (2)	C12—C11—H11	118.6
O3—S1—O1	112.2 (2)	C11—C12—C8	119.6 (4)
O2—S1—C25	106.1 (2)	C11—C12—H12	120.2
O3—S1—C25	106.3 (2)	C8—C12—H12	120.2
O1—S1—C25	105.7 (2)	N5—C13—C14	123.6 (4)
O6—S2—O5	113.1 (2)	N5—C13—H13	118.2
O6—S2—O4	113.3 (2)	C14—C13—H13	118.2
O5—S2—O4	111.8 (2)	C13—C14—C15	118.8 (4)
O6—S2—C26	106.5 (2)	C13—C14—H14	120.6
O5—S2—C26	105.7 (2)	C15—C14—H14	120.6
O4—S2—C26	105.7 (2)	C16—C15—C14	117.8 (4)
C5—N1—C1	118.5 (4)	C16—C15—C18	120.2 (4)
C5—N1—Ag1	122.2 (3)	C14—C15—C18	122.0 (4)
C1—N1—Ag1	119.2 (3)	C17—C16—C15	119.6 (4)
C6—N2—N3	111.9 (4)	C17—C16—H16	120.2
C7—N3—N2	111.3 (4)	C15—C16—H16	120.2
C10—N4—C11	118.1 (4)	N5—C17—C16	122.5 (4)
C10—N4—Ag2	120.9 (3)	N5—C17—H17	118.7
C11—N4—Ag2	120.9 (3)	C16—C17—H17	118.7
C13—N5—C17	117.7 (4)	N6—C18—C15	120.2 (4)
C13—N5—Ag1	121.1 (3)	N6—C18—H18	119.9
C17—N5—Ag1	121.0 (3)	C15—C18—H18	119.9
C18—N6—N6 ⁱⁱ	111.2 (5)	N7—C19—C20	123.4 (4)
C23—N7—C19	117.7 (4)	N7—C19—H19	118.3
C23—N7—Ag2	122.1 (3)	C20—C19—H19	118.3
C19—N7—Ag2	120.2 (3)	C19—C20—C21	119.0 (4)
C24—N8—N8 ⁱⁱⁱ	112.6 (4)	C19—C20—H20	120.5
N1—C1—C2	122.8 (4)	C21—C20—H20	120.5
N1—C1—H1	118.6	C20—C21—C22	117.5 (4)
C2—C1—H1	118.6	C20—C21—C24	123.2 (4)
C1—C2—C3	119.1 (4)	C22—C21—C24	119.3 (4)
C1—C2—H2	120.5	C23—C22—C21	120.1 (4)
C3—C2—H2	120.5	C23—C22—H22	120.0
C2—C3—C4	117.8 (4)	C21—C22—H22	120.0
C2—C3—C6	123.0 (4)	N7—C23—C22	122.3 (4)
C4—C3—C6	119.3 (4)	N7—C23—H23	118.8
C5—C4—C3	119.6 (4)	C22—C23—H23	118.8
C5—C4—H4	120.2	N8—C24—C21	121.3 (4)
C3—C4—H4	120.2	N8—C24—H24	119.4
N1—C5—C4	122.2 (4)	C21—C24—H24	119.4
N1—C5—H5	118.9	S1—C25—H25A	109.5
C4—C5—H5	118.9	S1—C25—H25B	109.5
N2—C6—C3	120.5 (4)	H25A—C25—H25B	109.5
N2—C6—H6	119.7	S1—C25—H25C	109.5
C3—C6—H6	119.7	H25A—C25—H25C	109.5

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N3—C7—C8	120.2 (4)	H25B—C25—H25C	109.5
N3—C7—H7	119.9	S2—C26—H26A	109.5
C8—C7—H7	119.9	S2—C26—H26B	109.5
C9—C8—C12	117.2 (4)	H26A—C26—H26B	109.5
C9—C8—C7	119.6 (4)	S2—C26—H26C	109.5
C12—C8—C7	123.2 (4)	H26A—C26—H26C	109.5
C10—C9—C8	120.4 (4)	H26B—C26—H26C	109.5
N5—Ag1—N1—C5	69.3 (9)	C11—N4—C10—C9	-0.6 (7)
Ag2 ⁱ —Ag1—N1—C5	-63.4 (3)	Ag2—N4—C10—C9	176.1 (4)
N5—Ag1—N1—C1	-114.5 (8)	C8—C9—C10—N4	0.4 (7)
Ag2 ⁱ —Ag1—N1—C1	112.7 (3)	C10—N4—C11—C12	-0.4 (7)
C6—N2—N3—C7	163.0 (4)	Ag2—N4—C11—C12	-177.1 (4)
N7—Ag2—N4—C10	106.9 (8)	N4—C11—C12—C8	1.7 (7)
Ag1 ⁱ —Ag2—N4—C10	-107.7 (3)	C9—C8—C12—C11	-1.8 (7)
N7—Ag2—N4—C11	-76.5 (9)	C7—C8—C12—C11	177.2 (4)
Ag1 ⁱ —Ag2—N4—C11	68.8 (3)	C17—N5—C13—C14	-0.6 (7)
N1—Ag1—N5—C13	-61.5 (9)	Ag1—N5—C13—C14	-175.7 (3)
Ag2 ⁱ —Ag1—N5—C13	71.0 (3)	N5—C13—C14—C15	1.6 (7)
N1—Ag1—N5—C17	123.6 (8)	C13—C14—C15—C16	-1.3 (7)
Ag2 ⁱ —Ag1—N5—C17	-103.9 (3)	C13—C14—C15—C18	178.4 (4)
N4—Ag2—N7—C23	79.9 (9)	C14—C15—C16—C17	0.2 (7)
Ag1 ⁱ —Ag2—N7—C23	-65.6 (3)	C18—C15—C16—C17	-179.5 (4)
N4—Ag2—N7—C19	-102.4 (8)	C13—N5—C17—C16	-0.6 (7)
Ag1 ⁱ —Ag2—N7—C19	112.1 (3)	Ag1—N5—C17—C16	174.4 (3)
C5—N1—C1—C2	-1.0 (7)	C15—C16—C17—N5	0.8 (7)
Ag1—N1—C1—C2	-177.3 (3)	N6 ⁱⁱ —N6—C18—C15	179.4 (3)
N1—C1—C2—C3	1.2 (7)	C16—C15—C18—N6	179.1 (4)
C1—C2—C3—C4	-0.1 (7)	C14—C15—C18—N6	-0.6 (7)
C1—C2—C3—C6	179.8 (4)	C23—N7—C19—C20	-0.4 (7)
C2—C3—C4—C5	-1.2 (6)	Ag2—N7—C19—C20	-178.1 (4)
C6—C3—C4—C5	179.0 (4)	N7—C19—C20—C21	0.9 (7)
C1—N1—C5—C4	-0.4 (6)	C19—C20—C21—C22	-0.2 (7)
Ag1—N1—C5—C4	175.8 (3)	C19—C20—C21—C24	178.9 (4)
C3—C4—C5—N1	1.4 (7)	C20—C21—C22—C23	-0.8 (7)
N3—N2—C6—C3	179.1 (4)	C24—C21—C22—C23	-180.0 (4)
C2—C3—C6—N2	6.5 (7)	C19—N7—C23—C22	-0.8 (7)
C4—C3—C6—N2	-173.6 (4)	Ag2—N7—C23—C22	177.0 (3)
N2—N3—C7—C8	-179.9 (4)	C21—C22—C23—N7	1.4 (7)
N3—C7—C8—C9	-176.2 (4)	N8 ⁱⁱⁱ —N8—C24—C21	179.8 (3)
N3—C7—C8—C12	4.8 (7)	C20—C21—C24—N8	8.0 (7)
C12—C8—C9—C10	0.8 (7)	C22—C21—C24—N8	-172.9 (4)
C7—C8—C9—C10	-178.3 (4)		

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x, y, -z-1/2$; (iii) $-x+2, y, -z+5/2$.

Fig. 1



supplementary materials

Fig. 2

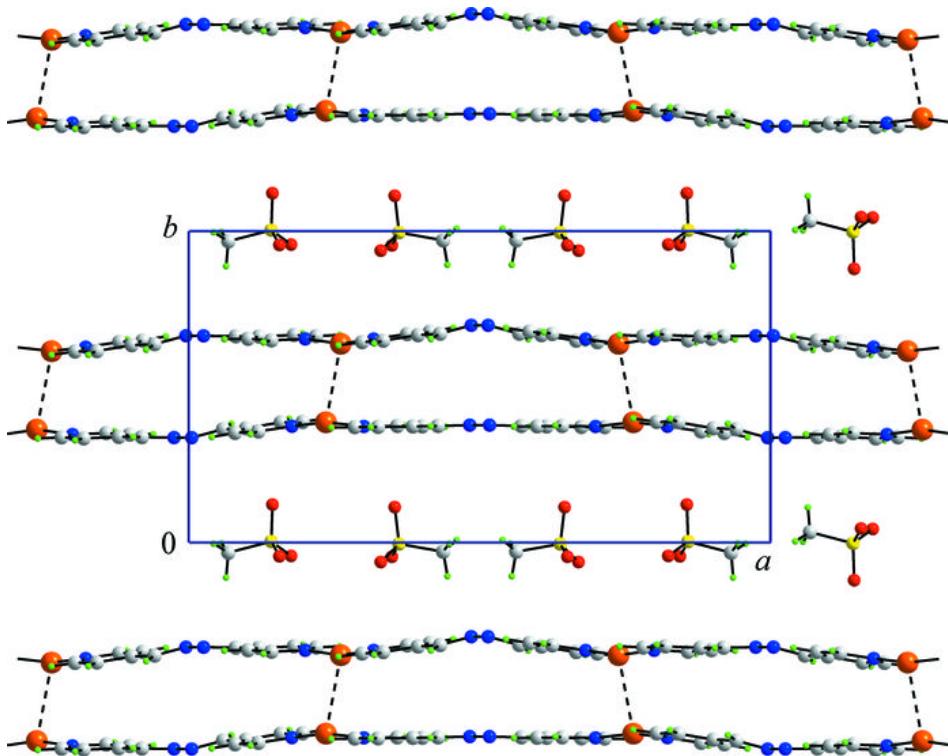


Fig. 3

