Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A one-dimensional Ag^{I} coordination polymer: *catena*-poly[[[[*N*′-(4-cyanobenzylidene)nicotinohydrazide]silver(I)]-*μ*-*N*′-(4-cyanobenzylidene)nicotinohydrazide] trifluoromethanesulfonate]

Cao-Yuan Niu,* Xin-Sheng Wan, Xiao-Wei Gui, Zhan-Guo Cao and Chun-Hong Kou

College of Sciences, Henan Agricultural University, Zhengzhou 450002, People's Republic of China
Correspondence e-mail: niu_cy2000@yahoo.com.cn

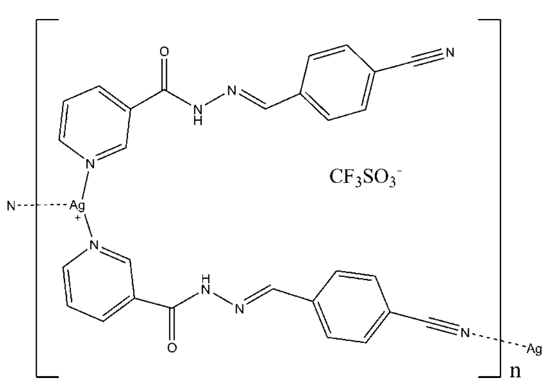
Received 10 October 2008; accepted 23 October 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.148; data-to-parameter ratio = 16.2.

In the title compound, $\{[Ag(C_{14}H_{10}N_4O)_2]CF_3SO_3\}_n$, the unique Ag^{I} ion is coordinated by two N atoms from two pyridine rings of two independent *N*′-(4-cyanobenzylidene)-nicotinohydrazide ligands and one N atom of a carbonitrile group of a symmetry-related *N*′-(4-cyanobenzylidene)-nicotinohydrazide ligand, forming a distorted T-shaped coordination environment. One of the independent ligands acts as a bridge connecting Ag^{I} ions, forming chains along the *a* axis. In the crystal structure, two neighbouring antiparallel chains are connected through N—H⋯O hydrogen bonds. In addition, there are relatively short Ag⋯O contacts of 2.723 (3) Å, which connect the chains into a three-dimensional structure.

Related literature

For a related structure, see: Niu *et al.* (2007).



Experimental

Crystal data

$[Ag(C_{14}H_{10}N_4O)_2]CF_3SO_3$
M_r = 757.46
Monoclinic, $C2/c$
a = 24.966 (2) Å
b = 13.9529 (13) Å
c = 17.6976 (16) Å
β = 98.437 (2)°
V = 6098.3 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 173 (2) K
0.51 × 0.32 × 0.27 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) T_{min} = 0.685, T_{max} = 0.813
19396 measured reflections
6990 independent reflections
5059 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.148
S = 1.03
6990 reflections
432 parameters
22 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.190 (3)	Ag1—N8^{i}	2.518 (3)
Ag1—N2	2.207 (3)		
N1—Ag1—N2	158.96 (11)	N2—Ag1—N8^{i}	96.76 (12)
N1—Ag1—N8^{i}	100.66 (12)		

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N3—H29⋯O2^{ii}	0.869 (14)	2.18 (2)	2.999 (4)	156 (4)
N6—H28⋯O3	0.852 (18)	2.07 (2)	2.911 (5)	171 (3)

Symmetry code: (ii) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

We are grateful to Mrs Li, Wuhan University, for her assistance with the X-ray crystallographic analysis. We also gratefully acknowledge financial support from the Natural Science Foundation of Henan Province (2008B150008) and the Science and Technology Key Task of Henan Province (0624040011).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2709).

References

Brandenburg, K. (2005). *DIAMOND*. Crystal Impact GbR. Bonn, Germany.
Niu, C.-Y., Wu, B.-L., Zheng, X.-F., Zhang, H.-Y., Li, Z.-J. & Hou, H.-W. (2007). *Dalton Trans.* pp. 5710–5713.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SAINT* and *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2008). E**64**, m1469-m1470 [**doi:10.1107/S1600536808034685**]

A one-dimensional Ag^{I} coordination polymer: *catena*-poly[[[*N'*-(4-cyanobenzylidene)nicotinohydrazide]silver(I)]-μ-*N'*-(4-cyanobenzylidene)nicotinohydrazide] trifluoromethanesulfonate]

C.-Y. Niu, X.-S. Wan, X.-W. Gui, Z.-G. Cao and C.-H. Kou

Comment

In the title compound, (I), the unique Ag^{I} ion is coordinated by two nitrogen atoms from two pyridyl rings of two different ligands (N1, N2) and one nitrogen atom from one carbonitrile group of another ligand [$N8^{i}$. symmetry code: (i) *x* - 1/2, -*y* + 1/2, *z* + 1/2,] forming a slightly distorted T-shaped coordination enviroment (Fig. 1). The N1—Ag1—N2 bond angle is 158.96 (11), indicating these three atoms are not exactly linear. Thus, the N1—Ag1—$N8^{i}$ and N2—Ag1—$N8^{i}$ bond angles are larger than 90°. The N—Ag bond distances involving the pyridine rings are in the range of 2.190 (3)–2.207 (3) Å, which are smaller than N—Ag bond distance involving the carbonitrile group, 2.518 (3) Å. This probably indicates that nitrogen atoms of carbonitrile groups possess a weaker coordinating ability with silver than the nitrogen atoms of the pyridine rings in one ligand. In the crystal structure, half of the 4-cyanobenzylidene nicotinohydrazide molecules act as bridging ligands, the other half coordinating only in the monodentate mode. Differences in bond distances between $N_{pyridine}$—Ag and $N_{carbonitrile}$—Ag bonds can also be found in {[Ag_2(1,6-Dihydro-2-methyl-6-oxo-(3,4'-bipyridine)-5-carbonitrile)$_3$] $_2(CH_3OH)_3(PF_6)_4$}$_n$ (Niu *et al.*, 2007), where the $N_{carbonitrile}$—Ag bond distance of 2.529 (3) Å (similar to that in the title compound), is larger than the $N_{pyridine}$—Ag bond distance of 2.151 (3) Å.

The ligands acting as μ_2-bridging ligands coordinate through pyridine and carbonitrile nitrogen atoms. Each of these bridging ligands connects two silver atoms together by one pyridine nitrogen atom N1 and one carbonitrile nitrogen atom $N8^{i}$ to form a one-dimensional chain along the *a* axis. The separation of two neighbouring silver atoms in one chain is ca. 16 Å, which means 4-cyanobenzylidene nicotinohydrazide acts as a moderately long bridging ligand. Interestingly, the other half of all ligands act only as monodentate terminal ligands and are coordinated to silver atoms in chains only through pyridine nitrogen atoms with the carbonitrile nitrogen atoms remaining uncoordinated. Two terminal ligands connecting to two adjacent silver atoms in one chain are located in opposite directions away from the chain. Thus, these chains possess a unusual 'saw-like' structure with the terminal ligands acting like 'saw-teeth' (Fig. 2).

In the crystal structure, the $CF_3SO_3^-$ counteranions are connected the ligands of chains by N—H···O hydrogen bonds (Table 2). In addition, there are also N—H···O hydrogen bondings between two neighbouring antiparallel chains (Fig. 3). Furthermore, there are weak Ag···O interactions between one oxygen atom [O1] of the terminal ligand in one chain and one silver atom in the neighbouring chain with the Ag···O separation of 2.8760 (21) Å (Fig. 4). These noncovalent interactions have large contributions to the supramolecular three-dimensional framework of the compound.

Experimental

A solution of $AgCF_3SO_3$ (0.026 g, 0.1 mmol) in CH_3OH (10 ml) was carefully layered on a $CH_3OH/CHCl_3$ solution (5 ml/10 ml) of 4-Cyanobenzylidene nicotinohydrazide (0.025 g, 0.1 mmol) in a straight glass tube. About ten days later, colourless single crystals suitable for X-ray analysis were obtained (yield about 35%). Elementary analysis, calculated for $C_{29}H_{20}AgN_8O_5F_3S$: C, 45.98, H, 2.66, N, 14.79%; found: C, 46.07, H, 2.53, N, 14.70%. One very strong bonds at 1262 cm^{-1} in the IR spectra were assigned to $CF_3SO_3^-$.

Refinement

C-bound H atoms were placed in calculated positions and refined using a riding model [C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The N-bound H atoms were first introduced in calculated positions, and then thier positions and displacement parameters were refined with the N—H bond distance to 0.88 (2) Å, the distances of H29 and N4, H29 and C6 to 1.93 (2) and 1.96 (2) Å, respectively. The final difference Fourier map had a highest peak at 0.90 Å from atom Ag1 and a deepest hole at 0.76 Å from atom Ag1, but were otherwise featureless.

Figures

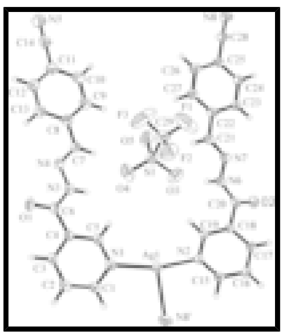


Fig. 1. A view of the Ag^I coordination environment in the polymeric structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) *x* - 1/2, -*y* + 1/2, *z* + 1/2.]

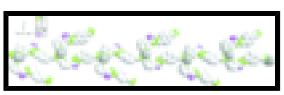


Fig. 2. A space-filling diagram showing the one-dimensional chain. All counteranions and H atoms have been omitted for clarity.

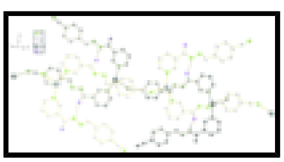


Fig. 3. A diagram showing the intermolecular hydrogen bonds indicated by dashed lines. All counteranions and H atoms not involved in hydrogen bonds have been omitted for clarity.

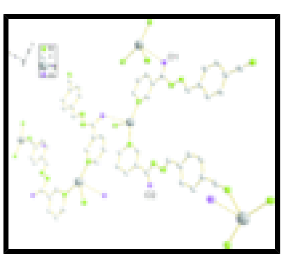


Fig. 4. A diagram showing the intermolecular Ag···O interactions indicated by dashed lines. All counteranions and H atoms have been omitted for clarity.

catena-poly[[[[N'-(4-cyanobenzylidene)nicotinohydrazide]silver(I)]-μ- N'-(4-cyanobenzylidene)nicotinohydrazide] trifluoromethanesulfonate]

Crystal data

$[Ag(C_{14}H_{10}N_4O)_2]CF_3SO_3$	F_{000} = 3040
M_r = 757.46	D_x = 1.650 Mg m^{-3}

Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 5153 reflections
$a = 24.966$ (2) Å	$\theta = 2.1–27.5°$
$b = 13.9529$ (13) Å	$\mu = 0.80$ mm^{-1}
$c = 17.6976$ (16) Å	$T = 173$ (2) K
$\beta = 98.437$ (2)°	Prism, colourless
$V = 6098.3$ (10) Å^3	0.51 × 0.32 × 0.27 mm
$Z = 8$	

Data collection

Siemens SMART CCD diffractometer	6990 independent reflections
Radiation source: fine-focus sealed tube	5059 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.031$
$T = 173(2)$ K	$\theta_{max} = 27.5°$
φ and ω scans	$\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -28 \rightarrow 32$
$T_{min} = 0.685$, $T_{max} = 0.813$	$k = -18 \rightarrow 17$
19396 measured reflections	$l = -22 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0766P)^2 + 8.964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
6990 reflections	$\Delta\rho_{max} = 1.47$ e Å^{-3}
432 parameters	$\Delta\rho_{min} = -0.79$ e Å^{-3}
22 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}
Ag1	0.177461 (13)	0.31617 (2)	0.21259 (2)	0.05965 (14)
N1	0.16489 (13)	0.4710 (2)	0.22045 (18)	0.0481 (7)
N2	0.19741 (12)	0.17730 (19)	0.16389 (17)	0.0421 (6)
N3	0.25625 (13)	0.6644 (2)	0.10836 (19)	0.0488 (7)
N4	0.29258 (12)	0.7215 (2)	0.07857 (19)	0.0497 (7)
N5	0.5169 (2)	0.9140 (4)	−0.1204 (3)	0.1027 (17)
N6	0.32032 (13)	0.1492 (2)	0.02428 (18)	0.0480 (7)
N7	0.35916 (12)	0.1432 (2)	−0.02381 (18)	0.0491 (7)
N8	0.60476 (14)	0.2456 (3)	−0.2154 (2)	0.0662 (10)
S1	0.35594 (5)	0.41766 (7)	0.11529 (6)	0.0575 (3)
O1	0.23222 (12)	0.78306 (19)	0.18438 (17)	0.0603 (7)
O2	0.28597 (11)	0.0026 (2)	−0.01063 (16)	0.0589 (7)
O3	0.33416 (17)	0.3230 (2)	0.1160 (2)	0.0852 (11)
O4	0.32654 (16)	0.4890 (3)	0.1495 (2)	0.0886 (11)
O5	0.37379 (17)	0.4448 (2)	0.04515 (19)	0.0852 (11)
F1	0.4489 (2)	0.3413 (5)	0.1600 (3)	0.180 (2)
F2	0.40950 (15)	0.3851 (3)	0.2507 (2)	0.1073 (11)
F3	0.4445 (2)	0.4874 (4)	0.1883 (3)	0.180 (2)
C1	0.12856 (16)	0.5082 (3)	0.2610 (2)	0.0548 (10)
H1	0.1059	0.4658	0.2839	0.066*
C2	0.12275 (17)	0.6049 (3)	0.2707 (3)	0.0611 (11)
H2	0.0966	0.6289	0.2998	0.073*
C3	0.15543 (18)	0.6664 (3)	0.2376 (3)	0.0562 (10)
H3	0.1524	0.7336	0.2444	0.067*
C4	0.19279 (14)	0.6307 (2)	0.19433 (19)	0.0410 (7)
C5	0.19597 (15)	0.5322 (3)	0.1878 (2)	0.0452 (8)
H5	0.2216	0.5065	0.1585	0.054*
C6	0.22824 (15)	0.6994 (2)	0.1618 (2)	0.0437 (8)
C7	0.32028 (16)	0.6787 (3)	0.0335 (2)	0.0497 (9)
H7	0.3143	0.6126	0.0226	0.060*
C8	0.36060 (15)	0.7304 (3)	−0.0009 (2)	0.0492 (9)
C9	0.39393 (18)	0.6808 (3)	−0.0440 (3)	0.0629 (11)
H9	0.3893	0.6137	−0.0514	0.075*
C10	0.43334 (18)	0.7280 (4)	−0.0756 (3)	0.0657 (11)
H10	0.4556	0.6936	−0.1054	0.079*
C11	0.44089 (18)	0.8263 (3)	−0.0643 (3)	0.0610 (11)
C12	0.40796 (18)	0.8751 (3)	−0.0220 (3)	0.0624 (11)
H12	0.4131	0.9420	−0.0139	0.075*
C13	0.36835 (17)	0.8298 (3)	0.0086 (2)	0.0549 (10)
H13	0.3455	0.8654	0.0367	0.066*
C14	0.4834 (2)	0.8750 (4)	−0.0962 (3)	0.0731 (13)
C15	0.18030 (14)	0.0956 (3)	0.1923 (2)	0.0434 (8)

H15	0.1556	0.0994	0.2283	0.052*
C16	0.19682 (16)	0.0068 (3)	0.1717 (2)	0.0496 (9)
H16	0.1842	−0.0494	0.1936	0.060*
C17	0.23172 (15)	0.0003 (2)	0.1192 (2)	0.0440 (8)
H17	0.2436	−0.0606	0.1042	0.053*
C18	0.24964 (13)	0.0833 (2)	0.08797 (19)	0.0390 (7)
C19	0.23178 (14)	0.1700 (2)	0.1127 (2)	0.0408 (7)
H19	0.2445	0.2273	0.0924	0.049*
C20	0.28677 (14)	0.0743 (2)	0.0289 (2)	0.0421 (8)
C21	0.38690 (16)	0.2191 (3)	−0.0263 (2)	0.0513 (9)
H21	0.3784	0.2739	0.0016	0.062*
C22	0.43167 (14)	0.2241 (3)	−0.0711 (2)	0.0470 (8)
C23	0.45139 (15)	0.1431 (3)	−0.1041 (2)	0.0496 (9)
H23	0.4343	0.0828	−0.1004	0.059*
C24	0.49545 (16)	0.1502 (3)	−0.1419 (2)	0.0516 (9)
H24	0.5091	0.0949	−0.1639	0.062*
C25	0.52007 (14)	0.2387 (3)	−0.1478 (2)	0.0481 (8)
C26	0.50079 (18)	0.3193 (3)	−0.1168 (3)	0.0615 (11)
H26	0.5176	0.3796	−0.1218	0.074*
C27	0.45664 (18)	0.3123 (3)	−0.0780 (3)	0.0590 (11)
H27	0.4433	0.3678	−0.0559	0.071*
C28	0.56767 (15)	0.2436 (3)	−0.1854 (2)	0.0524 (9)
C29	0.4169 (2)	0.4087 (4)	0.1813 (4)	0.0870 (16)
H28	0.3208 (14)	0.1991 (18)	0.0520 (17)	0.034 (9)*
H29	0.2522 (16)	0.6077 (15)	0.088 (2)	0.077 (15)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0648 (2)	0.03572 (18)	0.0846 (3)	0.00461 (12)	0.03151 (17)	−0.00623 (14)
N1	0.0518 (17)	0.0365 (16)	0.0593 (18)	0.0005 (13)	0.0199 (14)	−0.0055 (13)
N2	0.0429 (15)	0.0342 (15)	0.0533 (17)	0.0026 (12)	0.0204 (13)	0.0006 (12)
N3	0.0516 (18)	0.0351 (17)	0.062 (2)	−0.0037 (13)	0.0157 (15)	−0.0009 (14)
N4	0.0453 (17)	0.0426 (17)	0.0613 (19)	−0.0032 (13)	0.0087 (14)	0.0035 (15)
N5	0.097 (3)	0.080 (3)	0.145 (5)	0.001 (3)	0.067 (3)	0.018 (3)
N6	0.0516 (18)	0.0436 (17)	0.0556 (18)	−0.0025 (14)	0.0308 (14)	−0.0074 (15)
N7	0.0481 (17)	0.0516 (18)	0.0530 (17)	0.0022 (14)	0.0257 (14)	0.0003 (15)
N8	0.055 (2)	0.083 (3)	0.067 (2)	−0.0100 (19)	0.0293 (17)	−0.003 (2)
S1	0.0696 (6)	0.0462 (5)	0.0620 (6)	0.0057 (5)	0.0276 (5)	−0.0020 (5)
O1	0.0777 (19)	0.0316 (13)	0.0750 (19)	−0.0016 (13)	0.0223 (15)	−0.0033 (13)
O2	0.0707 (18)	0.0435 (15)	0.0692 (18)	−0.0031 (13)	0.0324 (14)	−0.0152 (13)
O3	0.116 (3)	0.066 (2)	0.081 (2)	−0.0313 (19)	0.039 (2)	−0.0132 (17)
O4	0.107 (3)	0.085 (3)	0.078 (2)	0.038 (2)	0.029 (2)	−0.0101 (19)
O5	0.129 (3)	0.063 (2)	0.073 (2)	0.010 (2)	0.048 (2)	0.0106 (17)
F1	0.107 (3)	0.242 (6)	0.198 (5)	0.086 (3)	0.042 (3)	0.023 (4)
F2	0.105 (2)	0.118 (3)	0.094 (2)	−0.018 (2)	0.0007 (19)	0.033 (2)
F3	0.157 (4)	0.179 (5)	0.188 (4)	−0.111 (4)	−0.028 (3)	0.067 (4)
C1	0.051 (2)	0.047 (2)	0.072 (3)	−0.0022 (17)	0.0272 (19)	−0.0071 (19)

C2	0.061 (2)	0.050 (2)	0.080 (3)	0.0048 (19)	0.034 (2)	−0.014 (2)
C3	0.063 (2)	0.038 (2)	0.073 (3)	0.0095 (17)	0.024 (2)	−0.0100 (18)
C4	0.0428 (18)	0.0347 (18)	0.0459 (18)	0.0056 (14)	0.0082 (14)	−0.0045 (14)
C5	0.0493 (19)	0.0372 (18)	0.052 (2)	0.0074 (15)	0.0164 (16)	−0.0047 (15)
C6	0.0469 (19)	0.0330 (18)	0.051 (2)	0.0038 (14)	0.0069 (16)	−0.0007 (14)
C7	0.048 (2)	0.043 (2)	0.058 (2)	0.0004 (16)	0.0065 (17)	0.0016 (17)
C8	0.0431 (19)	0.053 (2)	0.051 (2)	−0.0008 (16)	0.0067 (16)	0.0048 (17)
C9	0.060 (3)	0.059 (3)	0.073 (3)	−0.001 (2)	0.020 (2)	−0.010 (2)
C10	0.061 (3)	0.072 (3)	0.069 (3)	0.004 (2)	0.027 (2)	−0.005 (2)
C11	0.052 (2)	0.067 (3)	0.065 (3)	0.0033 (19)	0.012 (2)	0.012 (2)
C12	0.066 (3)	0.049 (2)	0.076 (3)	−0.0001 (19)	0.025 (2)	0.011 (2)
C13	0.056 (2)	0.047 (2)	0.064 (2)	0.0069 (17)	0.0162 (19)	0.0032 (18)
C14	0.065 (3)	0.070 (3)	0.091 (3)	0.006 (2)	0.032 (3)	0.012 (3)
C15	0.0481 (19)	0.0362 (18)	0.0500 (19)	−0.0016 (14)	0.0212 (16)	−0.0007 (15)
C16	0.063 (2)	0.0335 (18)	0.057 (2)	−0.0047 (16)	0.0237 (18)	0.0053 (16)
C17	0.054 (2)	0.0294 (16)	0.052 (2)	−0.0002 (14)	0.0169 (16)	−0.0006 (14)
C18	0.0390 (17)	0.0349 (17)	0.0456 (18)	0.0005 (13)	0.0141 (14)	−0.0002 (14)
C19	0.0425 (18)	0.0305 (17)	0.053 (2)	−0.0001 (13)	0.0196 (15)	0.0028 (14)
C20	0.0427 (18)	0.0383 (18)	0.0485 (19)	0.0036 (14)	0.0172 (15)	0.0025 (15)
C21	0.054 (2)	0.050 (2)	0.056 (2)	−0.0010 (17)	0.0284 (18)	−0.0037 (18)
C22	0.0435 (19)	0.051 (2)	0.050 (2)	−0.0004 (16)	0.0188 (16)	0.0042 (17)
C23	0.047 (2)	0.047 (2)	0.058 (2)	−0.0052 (16)	0.0204 (17)	0.0013 (18)
C24	0.052 (2)	0.051 (2)	0.056 (2)	0.0028 (17)	0.0228 (17)	0.0001 (18)
C25	0.0424 (19)	0.059 (2)	0.0463 (19)	−0.0018 (16)	0.0185 (15)	0.0042 (17)
C26	0.059 (2)	0.057 (3)	0.076 (3)	−0.0119 (19)	0.033 (2)	0.001 (2)
C27	0.060 (2)	0.050 (2)	0.074 (3)	−0.0063 (18)	0.034 (2)	−0.0062 (19)
C28	0.047 (2)	0.065 (3)	0.048 (2)	−0.0058 (18)	0.0171 (16)	−0.0006 (18)
C29	0.071 (3)	0.080 (4)	0.115 (4)	−0.009 (3)	0.032 (3)	0.026 (3)

Geometric parameters (Å, °)

Ag1—N1	2.190 (3)	C7—C8	1.444 (5)
Ag1—N2	2.207 (3)	C7—H7	0.9500
Ag1—N8^{i}	2.518 (3)	C8—C9	1.392 (6)
N1—C5	1.341 (5)	C8—C13	1.407 (6)
N1—C1	1.341 (5)	C9—C10	1.370 (6)
N2—C19	1.340 (4)	C9—H9	0.9500
N2—C15	1.340 (4)	C10—C11	1.396 (7)
N3—C6	1.348 (5)	C10—H10	0.9500
N3—N4	1.370 (4)	C11—C12	1.372 (6)
N3—H29	0.869 (14)	C11—C14	1.442 (6)
N4—C7	1.278 (5)	C12—C13	1.351 (6)
N5—C14	1.133 (6)	C12—H12	0.9500
N6—C20	1.348 (5)	C13—H13	0.9500
N6—N7	1.383 (4)	C15—C16	1.372 (5)
N6—H28	0.852 (18)	C15—H15	0.9500
N7—C21	1.270 (5)	C16—C17	1.367 (5)
N8—C28	1.134 (5)	C16—H16	0.9500
N8—Ag1^{ii}	2.518 (3)	C17—C18	1.385 (5)

S1—O4	1.424 (3)	C17—H17	0.9500
S1—O5	1.430 (3)	C18—C19	1.382 (5)
S1—O3	1.429 (3)	C18—C20	1.501 (4)
S1—C29	1.782 (6)	C19—H19	0.9500
O1—C6	1.232 (4)	C21—C22	1.464 (5)
O2—C20	1.220 (4)	C21—H21	0.9500
F1—C29	1.324 (8)	C22—C23	1.395 (6)
F2—C29	1.311 (6)	C22—C27	1.392 (5)
F3—C29	1.292 (7)	C23—C24	1.372 (5)
C1—C2	1.370 (6)	C23—H23	0.9500
C1—H1	0.9500	C24—C25	1.390 (6)
C2—C3	1.374 (6)	C24—H24	0.9500
C2—H2	0.9500	C25—C26	1.369 (6)
C3—C4	1.383 (5)	C25—C28	1.446 (5)
C3—H3	0.9500	C26—C27	1.385 (6)
C4—C5	1.382 (5)	C26—H26	0.9500
C4—C6	1.478 (5)	C27—H27	0.9500
C5—H5	0.9500		

N1—Ag1—N2	158.96 (11)	C12—C11—C14	121.0 (4)
N1—Ag1—N8[i]	100.66 (12)	C10—C11—C14	119.9 (4)
N2—Ag1—N8[i]	96.76 (12)	C13—C12—C11	121.3 (4)
C5—N1—C1	117.6 (3)	C13—C12—H12	119.4
C5—N1—Ag1	120.3 (2)	C11—C12—H12	119.4
C1—N1—Ag1	122.1 (3)	C12—C13—C8	120.6 (4)
C19—N2—C15	117.4 (3)	C12—C13—H13	119.7
C19—N2—Ag1	122.3 (2)	C8—C13—H13	119.7
C15—N2—Ag1	119.8 (2)	N5—C14—C11	179.1 (6)
C6—N3—N4	120.0 (3)	N2—C15—C16	122.9 (3)
C6—N3—H29	125.3 (15)	N2—C15—H15	118.5
N4—N3—H29	114.6 (15)	C16—C15—H15	118.5
C7—N4—N3	114.7 (3)	C17—C16—C15	119.2 (3)
C20—N6—N7	119.3 (3)	C17—C16—H16	120.4
C20—N6—H28	124 (2)	C15—C16—H16	120.4
N7—N6—H28	117 (2)	C16—C17—C18	119.4 (3)
C21—N7—N6	114.0 (3)	C16—C17—H17	120.3
C28—N8—Ag1[ii]	158.1 (4)	C18—C17—H17	120.3
O4—S1—O5	115.5 (2)	C19—C18—C17	117.8 (3)
O4—S1—O3	115.0 (2)	C19—C18—C20	123.7 (3)
O5—S1—O3	114.8 (2)	C17—C18—C20	118.5 (3)
O4—S1—C29	102.4 (3)	N2—C19—C18	123.3 (3)
O5—S1—C29	104.0 (3)	N2—C19—H19	118.3
O3—S1—C29	102.7 (3)	C18—C19—H19	118.3
N1—C1—C2	122.8 (4)	O2—C20—N6	124.0 (3)
N1—C1—H1	118.6	O2—C20—C18	120.5 (3)
C2—C1—H1	118.6	N6—C20—C18	115.5 (3)
C1—C2—C3	118.7 (4)	N7—C21—C22	121.4 (4)
C1—C2—H2	120.6	N7—C21—H21	119.3
C3—C2—H2	120.6	C22—C21—H21	119.3

C2—C3—C4	120.1 (3)	C23—C22—C27	119.3 (3)
C2—C3—H3	119.9	C23—C22—C21	122.2 (4)
C4—C3—H3	119.9	C27—C22—C21	118.4 (4)
C3—C4—C5	117.1 (3)	C24—C23—C22	120.2 (4)
C3—C4—C6	118.2 (3)	C24—C23—H23	119.9
C5—C4—C6	124.6 (3)	C22—C23—H23	119.9
N1—C5—C4	123.6 (3)	C23—C24—C25	119.7 (4)
N1—C5—H5	118.2	C23—C24—H24	120.1
C4—C5—H5	118.2	C25—C24—H24	120.1
O1—C6—N3	123.1 (4)	C26—C25—C24	120.9 (3)
O1—C6—C4	120.8 (3)	C26—C25—C28	120.5 (4)
N3—C6—C4	116.1 (3)	C24—C25—C28	118.6 (4)
N4—C7—C8	120.3 (4)	C25—C26—C27	119.5 (4)
N4—C7—H7	119.9	C25—C26—H26	120.2
C8—C7—H7	119.9	C27—C26—H26	120.2
C9—C8—C13	118.2 (4)	C26—C27—C22	120.3 (4)
C9—C8—C7	119.5 (4)	C26—C27—H27	119.8
C13—C8—C7	122.3 (4)	C22—C27—H27	119.8
C10—C9—C8	120.5 (4)	N8—C28—C25	178.6 (5)
C10—C9—H9	119.7	F3—C29—F2	105.7 (6)
C8—C9—H9	119.7	F3—C29—F1	107.3 (6)
C9—C10—C11	120.2 (4)	F2—C29—F1	105.2 (5)
C9—C10—H10	119.9	F3—C29—S1	113.3 (4)
C11—C10—H10	119.9	F2—C29—S1	114.0 (4)
C12—C11—C10	119.1 (4)	F1—C29—S1	110.8 (5)

N2—Ag1—N1—C5	−34.0 (5)	C19—N2—C15—C16	0.6 (5)
N8^{i}—Ag1—N1—C5	−179.4 (3)	Ag1—N2—C15—C16	−171.5 (3)
N2—Ag1—N1—C1	149.7 (3)	N2—C15—C16—C17	−0.9 (6)
N8^{i}—Ag1—N1—C1	4.4 (3)	C15—C16—C17—C18	0.0 (6)
N1—Ag1—N2—C19	27.7 (5)	C16—C17—C18—C19	1.0 (5)
N8^{i}—Ag1—N2—C19	173.4 (3)	C16—C17—C18—C20	−178.4 (3)
N1—Ag1—N2—C15	−160.7 (3)	C15—N2—C19—C18	0.6 (5)
N8^{i}—Ag1—N2—C15	−14.9 (3)	Ag1—N2—C19—C18	172.4 (3)
C6—N3—N4—C7	174.1 (3)	C17—C18—C19—N2	−1.4 (5)
C20—N6—N7—C21	177.1 (4)	C20—C18—C19—N2	178.0 (3)
C5—N1—C1—C2	−0.9 (6)	N7—N6—C20—O2	−4.8 (6)
Ag1—N1—C1—C2	175.5 (3)	N7—N6—C20—C18	174.3 (3)
N1—C1—C2—C3	0.1 (7)	C19—C18—C20—O2	−153.1 (4)
C1—C2—C3—C4	1.0 (7)	C17—C18—C20—O2	26.3 (5)
C2—C3—C4—C5	−1.2 (6)	C19—C18—C20—N6	27.7 (5)
C2—C3—C4—C6	−178.1 (4)	C17—C18—C20—N6	−152.9 (3)
C1—N1—C5—C4	0.6 (6)	N6—N7—C21—C22	176.8 (3)
Ag1—N1—C5—C4	−175.8 (3)	N7—C21—C22—C23	−9.6 (6)
C3—C4—C5—N1	0.4 (6)	N7—C21—C22—C27	173.2 (4)
C6—C4—C5—N1	177.1 (3)	C27—C22—C23—C24	1.0 (6)
N4—N3—C6—O1	2.4 (6)	C21—C22—C23—C24	−176.2 (4)
N4—N3—C6—C4	−176.0 (3)	C22—C23—C24—C25	−0.6 (6)
C3—C4—C6—O1	14.1 (5)	C23—C24—C25—C26	−0.4 (6)

C5—C4—C6—O1	−162.6 (4)	C23—C24—C25—C28	177.7 (4)
C3—C4—C6—N3	−167.4 (4)	C24—C25—C26—C27	1.0 (7)
C5—C4—C6—N3	15.9 (5)	C28—C25—C26—C27	−177.0 (4)
N3—N4—C7—C8	−179.1 (3)	C25—C26—C27—C22	−0.6 (7)
N4—C7—C8—C9	173.9 (4)	C23—C22—C27—C26	−0.4 (7)
N4—C7—C8—C13	−4.9 (6)	C21—C22—C27—C26	176.9 (4)
C13—C8—C9—C10	0.4 (6)	O4—S1—C29—F3	−62.1 (6)
C7—C8—C9—C10	−178.4 (4)	O5—S1—C29—F3	58.4 (6)
C8—C9—C10—C11	0.7 (7)	O3—S1—C29—F3	178.4 (5)
C9—C10—C11—C12	−0.8 (7)	O4—S1—C29—F2	58.8 (5)
C9—C10—C11—C14	178.4 (4)	O5—S1—C29—F2	179.4 (4)
C10—C11—C12—C13	−0.3 (7)	O3—S1—C29—F2	−60.7 (5)
C14—C11—C12—C13	−179.4 (4)	O4—S1—C29—F1	177.3 (4)
C11—C12—C13—C8	1.5 (7)	O5—S1—C29—F1	−62.2 (5)
C9—C8—C13—C12	−1.5 (6)	O3—S1—C29—F1	57.8 (5)
C7—C8—C13—C12	177.3 (4)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H29···O2^{iii}	0.869 (14)	2.18 (2)	2.999 (4)	156 (4)
N6—H28···O3	0.852 (18)	2.07 (2)	2.911 (5)	171 (3)

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

Fig. 1

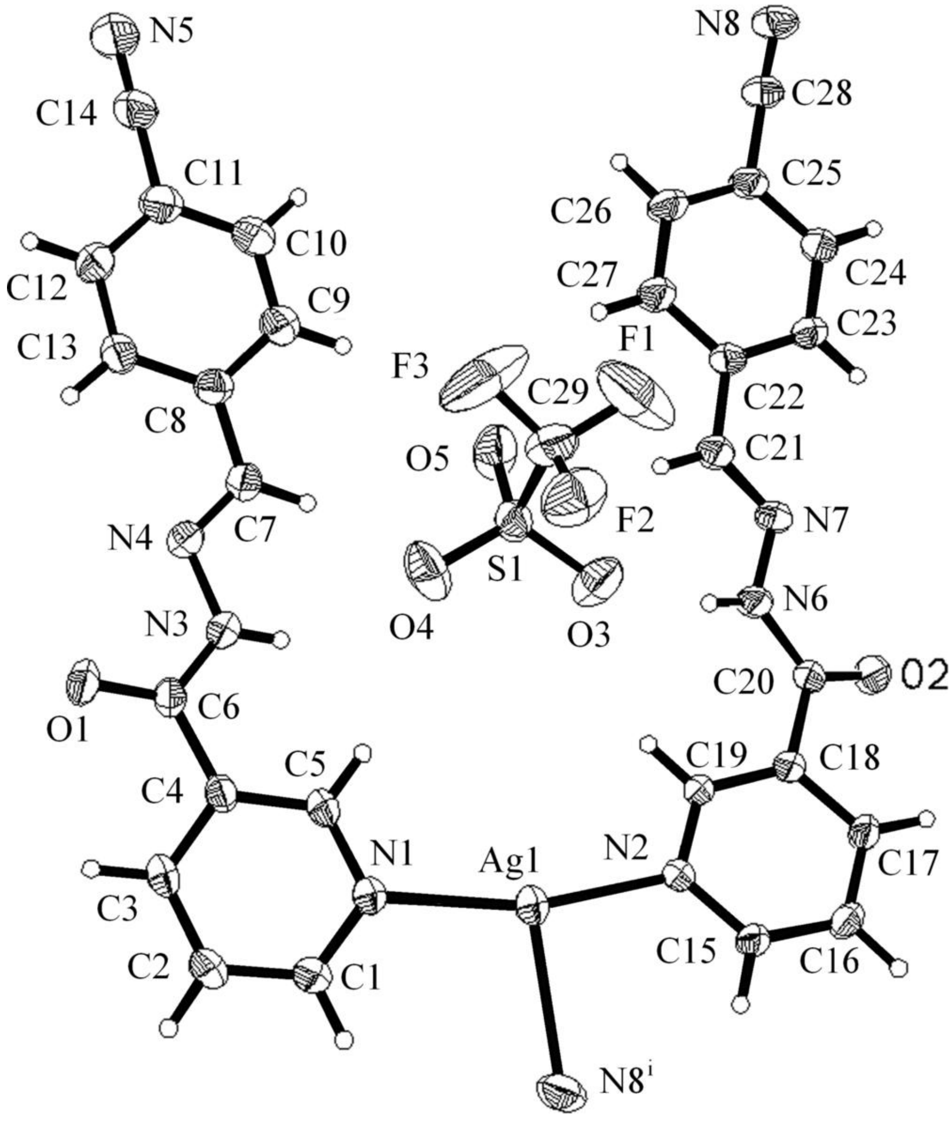

N5
C14
C11
C10
C12
C9
C13
C8
C7
N4
N3
O1
C6
C4
C5
N1
C3
C2
C1
Ag1
N8i
N2
C15
C16
C17
C19
C18
C20
O2
N6
N7
C21
C22
C23
C24
C27
C26
C25
C28
N8
F1
F3
C29
O5
F2
S1
O4
O3

Fig. 2

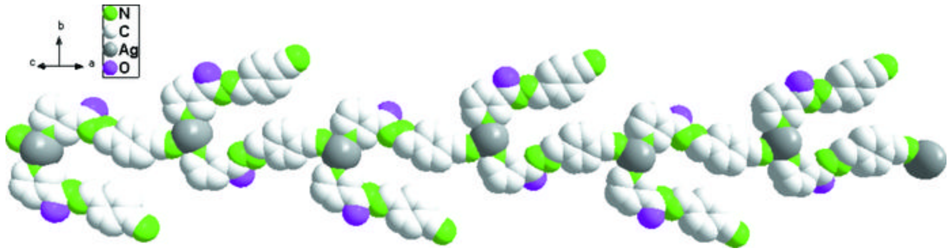


Fig. 3

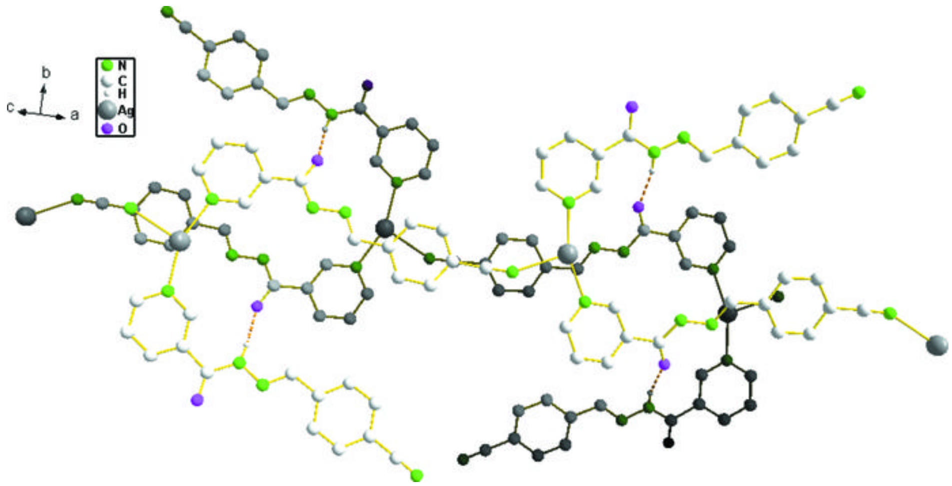


Fig. 4