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catena-Poly[silver(I)-μ-1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene hexafluoridophosphate–acetonitrile (1/1)]

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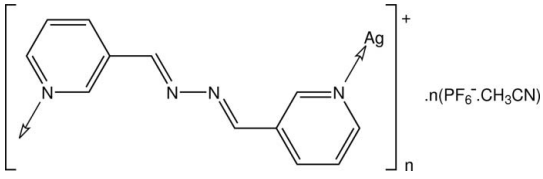
Key indicators: single-crystal X-ray study; T = 98 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.061; data-to-parameter ratio = 14.4.

The asymmetric unit in the polymeric title compound, $[Ag(C_{12}H_{10}N_4)]_n{\cdot}nPF_6{\cdot}nC_2H_3N$, comprises an Ag cation, two half 3-pyridinealdazine (3-PA) molecules, each disposed about a centre of inversion, a hexafluoridophosphate anion and an acetonitrile solvent molecule. The Ag atoms bond to two N atoms and the bridging 3-PA ligands lead to the formation of zigzag chains that are linked into a layer structure *via* weakly bridging acetonitrile molecules and argentophilic interactions [Ag···Ag = 3.2590 (15) Å]. The layers stack along the *b* axis and are interspersed by layers of hexafluoridophosphate anions. Various C—H···F and C—H···N interactions help to consolidate the structure.

Related literature

For related polymeric silver salts containing the 3-pyridinealdazine ligand, see: Kennedy *et al.* (2005); Broker & Tiekink (2007*c*). For related literature, see: Broker & Tiekink (2007*a*,*b*).



Experimental

Crystal data

$[Ag(C_{12}H_{10}N_4)]PF_6{\cdot}C_2H_3N$
M_r = 504.13
Triclinic, $P\overline{1}$
a = 7.917 (3) Å
b = 10.416 (3) Å
c = 11.357 (5) Å
α = 75.58 (5)°
β = 70.66 (3)°
γ = 81.11 (4)°
V = 853.2 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 98 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Rigaku AFC12κ/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.406, T_{max} = 1.000
(expected range = 0.355–0.874)
9571 measured reflections
3508 independent reflections
3404 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.061
S = 1.12
3508 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag—N1	2.1538 (19)	Ag—N3	2.160 (2)
N1—Ag—N3	168.86 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···F6^{i}	0.95	2.50	3.182 (3)	128
C1—H1···N5^{ii}	0.95	2.56	3.336 (3)	138
C2—H2···F2^{iii}	0.95	2.48	3.174 (3)	130
C5—H5···F1	0.95	2.46	3.291 (3)	146
C5—H5···F6	0.95	2.53	3.318 (3)	140
C9—H9···F3^{iv}	0.95	2.51	3.160 (3)	126
C11—H11···N5^{ii}	0.95	2.51	3.311 (3)	142

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

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: HB2531).

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supplementary materials

Acta Cryst. (2007). E**63**, m2485 [**doi:10.1107/S1600536807042912**]

catena-Poly[silver(I)-μ-1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene hexafluoridophosphate-acetonitrile (1/1)]

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

Comment

The structure of the title compound (I) was investigated as part of an on-going study of the structural chemistry of silver salts of the isomeric n-pyridinealdazine, n = 2, 3 and 4, molecules (Broker & Tiekink, 2007*a*-c).

Compound (I) features an Ag cation in a general position, two half 3-pyridinealdazine molecules, each disposed about a centre of inversion, an hexafluorophosphate anion and an acetonitrile solvent molecule, each in general positions (Fig. 1 & Table 1). The 3-pyridinealdazine molecule is bidentate bridging leading to a zigzag chain with a linear N_2 coordination geometry for Ag.

The chains thus formed are linked *via* weakly bridging acetonitrile molecules with Ag···N5 and N5···Ag^i of 2.800 (3) and 2.826 (2) Å, respectively, as well as Ag···Ag^i interactions of 3.2590 (15) Å for (i): −*x*, 2 − *y*, −*z*. The topology of the resulting layer in the *ac* plane resembles a brick wall (Fig. 2).

The layers stack along the *b* axis and are interspersed by layers of PF_6 anions. Various C—H···N and F interactions consolidate the structure (Fig. 3 & Table 2).

The zigzag topology found for the $[Ag(C_{12}H_{10}N_4)]_n$ chain in (I) has precedents in the perchlorate, tetrafluoroborate salts (each as acetonitrile solvates) (Kennedy *et al.*, 2005), and the methansulfonate salt (Broker & Tiekink, 2007*c*).

Experimental

$Ag(PF_6)$ (Aldrich, 0.05 g, 0.20 mmol) was dissolved in CH_3CN (20 ml) and layered on top of a CH_2Cl_2 solution (20 ml) containing 0.041 g (0.20 mmol) of 3-pyridinealdazine (Aldrich). After three days, yellow prisms of (I) were observed at the interface between the two layers; m.p. 579–581 K.

Refinement

All the H atoms were included in the riding-model approximation, with C–H = 0.95–98 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

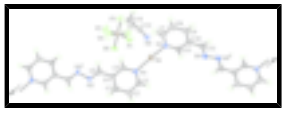


Fig. 1. Asymmetric unit of (I) expanded to show the polymeric connectivity. Displacement ellipsoids at the 70% probability level (arbitrary spheres for the H atoms). Symmetry operations (i): 1 − *x*, 2 − *y*, 1 − *z*, and (ii): −*x*, 2 − *y*, −1 − *z*.

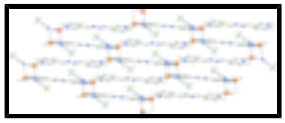


Fig. 2. View of the layers in (I) viewed down the *b* axis highlighting the brick wall topology. Weak Ag···N interactions involving the acetonitrile molecules are shown as dashed bonds. Colour code: orange (silver), yellow (sulfur), red (oxygen), blue (nitrogen), grey (carbon) and green (hydrogen).

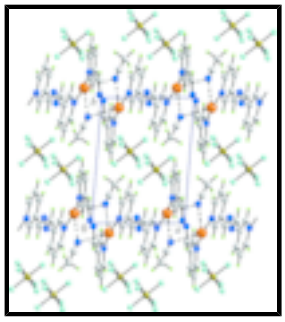


Fig. 3. View of the unit-cell contents of (I) highlighting the stacking of layers. Weak Ag···N interactions involving the acetonitrile molecules are shown as dashed bonds. Colour code as for Fig. 2.

catena-Poly[silver(I)-μ-1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene hexafluoridophosphate–acetonitrile (1/1)]

Crystal data

$[Ag(C_{12}H_{10}N_4)]PF_6·C_2H_3N$	$Z = 2$
$M_r = 504.13$	$F_{000} = 496$
Triclinic, $P\overline{1}$	$D_x = 1.962$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 7.917$ (3) Å	Cell parameters from 3181 reflections
$b = 10.416$ (3) Å	$\theta = 2.7$–$30.5°$
$c = 11.357$ (5) Å	$\mu = 1.35$ mm^{-1}
$\alpha = 75.58$ (5)°	$T = 98$ (2) K
$\beta = 70.66$ (3)°	Prism, yellow
$\gamma = 81.11$ (4)°	0.30 × 0.20 × 0.10 mm
$V = 853.2$ (5) Å^3	

Data collection

Rigaku AFC12κ/SATURN724 diffractometer	3508 independent reflections
Radiation source: fine-focus sealed tube	3404 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$
$T = 98(2)$ K	$\theta_{max} = 26.5°$
ω scans	$\theta_{min} = 2.5°$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -9 \rightarrow 9$
$T_{min} = 0.406$, $T_{max} = 1.000$	$k = -12 \rightarrow 13$
9571 measured reflections	$l = -12 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.061$

$S = 1.12$

3508 reflections

244 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0287P)^2 + 0.7535P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.58$ e Å^{-3}

$\Delta\rho_{min} = -0.42$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag	0.19529 (2)	0.921735 (16)	−0.001479 (15)	0.02331 (7)
P1	0.35231 (8)	0.57251 (5)	0.27956 (5)	0.02040 (12)
F1	0.2394 (2)	0.68371 (14)	0.20476 (16)	0.0373 (4)
F2	0.4462 (2)	0.51518 (15)	0.15379 (14)	0.0373 (3)
F3	0.1968 (2)	0.47507 (15)	0.32092 (16)	0.0406 (4)
F4	0.2591 (2)	0.63135 (17)	0.40388 (15)	0.0432 (4)
F5	0.46592 (19)	0.46138 (14)	0.35278 (14)	0.0344 (3)
F6	0.50926 (19)	0.66944 (14)	0.23800 (14)	0.0329 (3)
N1	0.2938 (2)	1.03785 (17)	0.09097 (16)	0.0170 (3)
N2	0.4846 (2)	1.04341 (17)	0.44581 (16)	0.0185 (4)
N3	0.1510 (2)	0.79723 (18)	−0.11309 (17)	0.0198 (4)
N4	0.0213 (2)	0.97670 (19)	−0.44279 (17)	0.0219 (4)
N5	−0.1325 (3)	0.84620 (19)	0.17805 (19)	0.0257 (4)
C1	0.3153 (3)	1.1678 (2)	0.0438 (2)	0.0198 (4)
H1	0.2888	1.2083	−0.0335	0.024*
C2	0.3746 (3)	1.2454 (2)	0.1027 (2)	0.0205 (4)
H2	0.3873	1.3373	0.0663	0.025*
C3	0.4149 (3)	1.1887 (2)	0.2139 (2)	0.0186 (4)
H3	0.4535	1.2406	0.2568	0.022*
C4	0.3977 (3)	1.0527 (2)	0.26239 (19)	0.0154 (4)
C5	0.3354 (3)	0.9823 (2)	0.19818 (19)	0.0168 (4)
H5	0.3218	0.8901	0.2322	0.020*

C6	0.4383 (3)	0.9820 (2)	0.37887 (19)	0.0168 (4)
H6	0.4301	0.8885	0.4054	0.020*
C7	0.1646 (3)	0.6635 (2)	−0.0804 (2)	0.0246 (5)
H7	0.1888	0.6218	−0.0025	0.030*
C8	0.1449 (3)	0.5847 (2)	−0.1553 (2)	0.0269 (5)
H8	0.1562	0.4906	−0.1294	0.032*
C9	0.1085 (3)	0.6436 (2)	−0.2681 (2)	0.0246 (5)
H9	0.0950	0.5910	−0.3213	0.030*
C10	0.0921 (3)	0.7817 (2)	−0.3023 (2)	0.0201 (4)
C11	0.1164 (3)	0.8541 (2)	−0.2224 (2)	0.0192 (4)
H11	0.1079	0.9484	−0.2468	0.023*
C12	0.0484 (3)	0.8502 (2)	−0.4185 (2)	0.0221 (4)
H12	0.0402	0.8008	−0.4761	0.027*
C13	−0.1674 (3)	0.7765 (2)	0.2742 (2)	0.0204 (4)
C14	−0.2150 (3)	0.6882 (2)	0.3989 (2)	0.0267 (5)
H14A	−0.2694	0.7407	0.4647	0.040*
H14B	−0.1068	0.6364	0.4137	0.040*
H14C	−0.3009	0.6278	0.4027	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag	0.02641 (11)	0.02883 (11)	0.02023 (10)	−0.00394 (7)	−0.01124 (7)	−0.00841 (7)
P1	0.0219 (3)	0.0189 (3)	0.0211 (3)	−0.0042 (2)	−0.0069 (2)	−0.0036 (2)
F1	0.0384 (8)	0.0276 (7)	0.0514 (10)	0.0002 (6)	−0.0285 (7)	0.0002 (7)
F2	0.0498 (9)	0.0342 (8)	0.0282 (8)	−0.0041 (7)	−0.0077 (7)	−0.0122 (6)
F3	0.0327 (8)	0.0354 (8)	0.0526 (10)	−0.0166 (6)	−0.0124 (7)	−0.0001 (7)
F4	0.0445 (9)	0.0501 (10)	0.0345 (9)	0.0053 (7)	−0.0059 (7)	−0.0223 (7)
F5	0.0321 (8)	0.0320 (8)	0.0303 (8)	0.0008 (6)	−0.0093 (6)	0.0064 (6)
F6	0.0310 (8)	0.0290 (7)	0.0415 (8)	−0.0117 (6)	−0.0157 (6)	−0.0002 (6)
N1	0.0176 (9)	0.0201 (9)	0.0137 (8)	−0.0017 (7)	−0.0056 (7)	−0.0030 (7)
N2	0.0208 (9)	0.0203 (9)	0.0146 (8)	−0.0032 (7)	−0.0075 (7)	−0.0004 (7)
N3	0.0189 (9)	0.0240 (9)	0.0175 (9)	−0.0042 (7)	−0.0057 (7)	−0.0045 (7)
N4	0.0173 (9)	0.0346 (11)	0.0155 (9)	−0.0034 (7)	−0.0039 (7)	−0.0090 (8)
N5	0.0295 (11)	0.0251 (10)	0.0236 (10)	−0.0050 (8)	−0.0094 (8)	−0.0035 (8)
C1	0.0200 (10)	0.0226 (10)	0.0160 (10)	−0.0041 (8)	−0.0057 (8)	−0.0007 (8)
C2	0.0219 (11)	0.0187 (10)	0.0188 (10)	−0.0027 (8)	−0.0048 (8)	−0.0012 (8)
C3	0.0154 (10)	0.0204 (10)	0.0203 (10)	−0.0034 (8)	−0.0044 (8)	−0.0054 (8)
C4	0.0121 (9)	0.0202 (10)	0.0136 (9)	−0.0002 (7)	−0.0030 (7)	−0.0047 (8)
C5	0.0168 (10)	0.0163 (9)	0.0166 (10)	−0.0004 (7)	−0.0046 (8)	−0.0033 (8)
C6	0.0157 (10)	0.0187 (10)	0.0156 (10)	−0.0014 (7)	−0.0047 (8)	−0.0030 (8)
C7	0.0206 (11)	0.0275 (11)	0.0251 (11)	−0.0037 (9)	−0.0079 (9)	−0.0021 (9)
C8	0.0240 (12)	0.0243 (11)	0.0330 (13)	−0.0006 (9)	−0.0094 (10)	−0.0071 (10)
C9	0.0189 (11)	0.0286 (11)	0.0313 (12)	−0.0019 (8)	−0.0073 (9)	−0.0157 (10)
C10	0.0123 (10)	0.0293 (11)	0.0187 (10)	−0.0030 (8)	−0.0020 (8)	−0.0081 (9)
C11	0.0147 (10)	0.0241 (10)	0.0187 (10)	−0.0040 (8)	−0.0032 (8)	−0.0056 (8)
C12	0.0168 (10)	0.0333 (12)	0.0191 (10)	−0.0023 (8)	−0.0041 (8)	−0.0123 (9)
C13	0.0195 (10)	0.0216 (10)	0.0225 (11)	−0.0014 (8)	−0.0080 (8)	−0.0070 (9)

C14	0.0327 (13)	0.0262 (12)	0.0196 (11)	−0.0036 (9)	−0.0085 (9)	−0.0005 (9)

Geometric parameters (Å, °)

Ag—N1	2.1538 (19)	C2—H2	0.9500
Ag—N3	2.160 (2)	C3—C4	1.397 (3)
Ag—N5	2.800 (2)	C3—H3	0.9500
Ag—Ag^{i}	3.2590 (15)	C4—C5	1.389 (3)
P1—F4	1.5858 (17)	C4—C6	1.455 (3)
P1—F3	1.5914 (16)	C5—H5	0.9500
P1—F2	1.5917 (17)	C6—H6	0.9500
P1—F5	1.5919 (16)	C7—C8	1.377 (3)
P1—F6	1.5964 (16)	C7—H7	0.9500
P1—F1	1.5984 (16)	C8—C9	1.377 (3)
N1—C5	1.335 (3)	C8—H8	0.9500
N1—C1	1.341 (3)	C9—C10	1.391 (3)
N2—C6	1.273 (3)	C9—H9	0.9500
N2—N2^{ii}	1.403 (3)	C10—C11	1.389 (3)
N3—C11	1.333 (3)	C10—C12	1.459 (3)
N3—C7	1.346 (3)	C11—H11	0.9500
N4—C12	1.276 (3)	C12—H12	0.9500
N4—N4^{iii}	1.401 (4)	C13—C14	1.448 (3)
N5—C13	1.124 (3)	C14—H14A	0.9800
C1—C2	1.384 (3)	C14—H14B	0.9800
C1—H1	0.9500	C14—H14C	0.9800
C2—C3	1.372 (3)		
N1—Ag—N3	168.86 (7)	C2—C3—H3	120.9
N1—Ag—N5	103.25 (7)	C4—C3—H3	120.9
N3—Ag—N5	86.67 (7)	C5—C4—C3	118.59 (19)
N1—Ag—Ag^{i}	101.63 (6)	C5—C4—C6	118.50 (18)
N3—Ag—Ag^{i}	88.15 (6)	C3—C4—C6	122.90 (19)
N5—Ag—Ag^{i}	54.97 (5)	N1—C5—C4	123.18 (19)
F4—P1—F3	90.61 (10)	N1—C5—H5	118.4
F4—P1—F2	179.32 (9)	C4—C5—H5	118.4
F3—P1—F2	89.86 (10)	N2—C6—C4	121.01 (19)
F4—P1—F5	91.01 (10)	N2—C6—H6	119.5
F3—P1—F5	90.18 (9)	C4—C6—H6	119.5
F2—P1—F5	89.48 (9)	N3—C7—C8	122.6 (2)
F4—P1—F6	89.61 (10)	N3—C7—H7	118.7
F3—P1—F6	179.63 (9)	C8—C7—H7	118.7
F2—P1—F6	89.93 (9)	C9—C8—C7	119.5 (2)
F5—P1—F6	89.52 (9)	C9—C8—H8	120.3
F4—P1—F1	89.54 (10)	C7—C8—H8	120.3
F3—P1—F1	89.92 (9)	C8—C9—C10	118.5 (2)
F2—P1—F1	89.98 (10)	C8—C9—H9	120.7
F5—P1—F1	179.44 (10)	C10—C9—H9	120.7
F6—P1—F1	90.38 (9)	C11—C10—C9	118.6 (2)
C5—N1—C1	117.55 (18)	C11—C10—C12	120.2 (2)

C5—N1—Ag	120.78 (14)	C9—C10—C12	121.2 (2)
C1—N1—Ag	121.66 (14)	N3—C11—C10	123.0 (2)
C6—N2—N2^{ii}	111.5 (2)	N3—C11—H11	118.5
C11—N3—C7	117.88 (19)	C10—C11—H11	118.5
C11—N3—Ag	119.05 (15)	N4—C12—C10	119.9 (2)
C7—N3—Ag	123.00 (15)	N4—C12—H12	120.1
C12—N4—N4^{iii}	111.3 (2)	C10—C12—H12	120.1
C13—N5—Ag	132.65 (18)	N5—C13—C14	179.0 (3)
N1—C1—C2	122.9 (2)	C13—C14—H14A	109.5
N1—C1—H1	118.6	C13—C14—H14B	109.5
C2—C1—H1	118.6	H14A—C14—H14B	109.5
C3—C2—C1	119.6 (2)	C13—C14—H14C	109.5
C3—C2—H2	120.2	H14A—C14—H14C	109.5
C1—C2—H2	120.2	H14B—C14—H14C	109.5
C2—C3—C4	118.2 (2)		
N3—Ag—N1—C5	−88.2 (4)	C1—N1—C5—C4	0.6 (3)
N5—Ag—N1—C5	64.29 (16)	Ag—N1—C5—C4	−179.35 (15)
Ag^{i}—Ag—N1—C5	120.67 (15)	C3—C4—C5—N1	1.1 (3)
N3—Ag—N1—C1	91.9 (4)	C6—C4—C5—N1	179.73 (18)
N5—Ag—N1—C1	−115.62 (17)	N2^{ii}—N2—C6—C4	179.41 (19)
Ag^{i}—Ag—N1—C1	−59.24 (16)	C5—C4—C6—N2	−175.40 (19)
N1—Ag—N3—C11	−95.7 (4)	C3—C4—C6—N2	3.1 (3)
N5—Ag—N3—C11	111.04 (16)	C11—N3—C7—C8	0.2 (3)
Ag^{i}—Ag—N3—C11	56.03 (15)	Ag—N3—C7—C8	−176.72 (17)
N1—Ag—N3—C7	81.2 (4)	N3—C7—C8—C9	−0.4 (3)
N5—Ag—N3—C7	−72.03 (18)	C7—C8—C9—C10	−0.3 (3)
Ag^{i}—Ag—N3—C7	−127.04 (17)	C8—C9—C10—C11	1.2 (3)
N1—Ag—N5—C13	−69.2 (2)	C8—C9—C10—C12	−178.1 (2)
N3—Ag—N5—C13	105.7 (2)	C7—N3—C11—C10	0.7 (3)
Ag^{i}—Ag—N5—C13	−164.3 (2)	Ag—N3—C11—C10	177.80 (15)
C5—N1—C1—C2	−1.4 (3)	C9—C10—C11—N3	−1.4 (3)
Ag—N1—C1—C2	178.55 (16)	C12—C10—C11—N3	177.89 (19)
N1—C1—C2—C3	0.4 (3)	N4^{iii}—N4—C12—C10	−179.1 (2)
C1—C2—C3—C4	1.3 (3)	C11—C10—C12—N4	−4.4 (3)
C2—C3—C4—C5	−2.0 (3)	C9—C10—C12—N4	174.9 (2)
C2—C3—C4—C6	179.45 (18)		

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

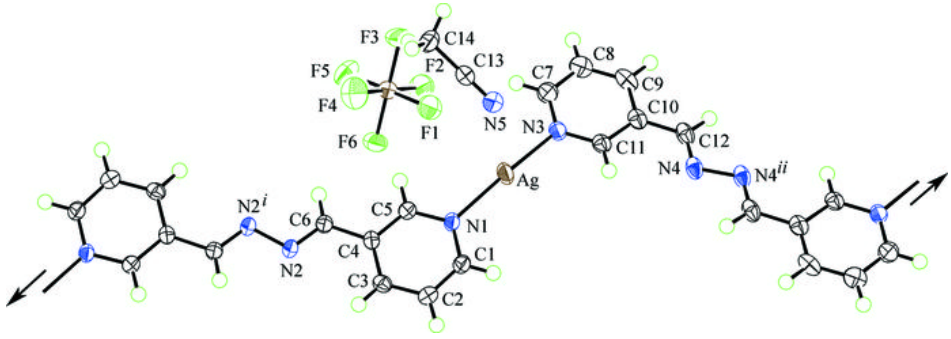
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···F6^{iv}	0.95	2.50	3.182 (3)	128
C1—H1···N5^{i}	0.95	2.56	3.336 (3)	138
C2—H2···F2^{v}	0.95	2.48	3.174 (3)	130
C5—H5···F1	0.95	2.46	3.291 (3)	146
C5—H5···F6	0.95	2.53	3.318 (3)	140

C9—H9···F3^{vi}	0.95	2.51	3.160 (3)	126
C11—H11···N5^{i}	0.95	2.51	3.311 (3)	142

Symmetry codes: (iv) −*x*+1, −*y*+2, −*z*; (i) −*x*, −*y*+2, −*z*; (v) *x*, *y*+1, *z*; (vi) −*x*, −*y*+1, −*z*.

Fig. 1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C4
C1
N2
C3
C2

Fig. 2

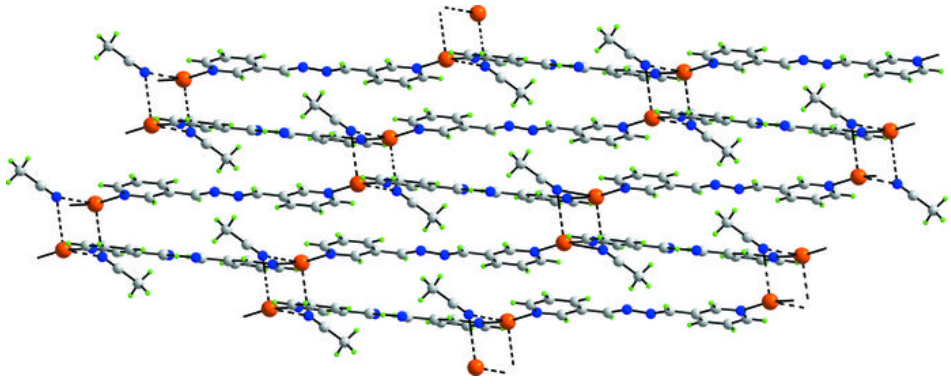

Fig. 3