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Crystal structure of an Ag^{I} intercalation compound: *catena*-poly[[silver(I)-μ-*N*-(pyridin-3-ylmethyl)-pyridin-3-amine-κ^2N:N'] hexafluoridophosphate acetonitrile disolvate]

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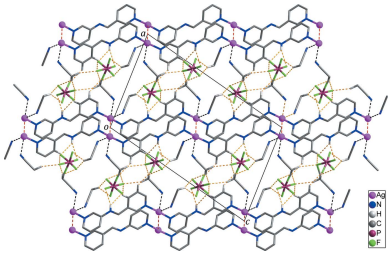
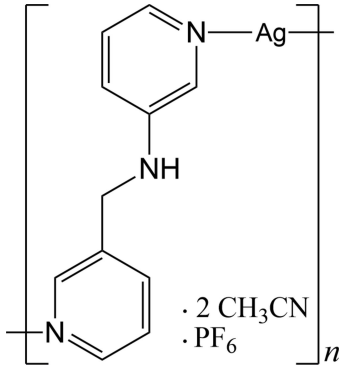
The asymmetric unit in the title compound, $[Ag(C_{11}H_{11}N_3)]PF_6{\cdot}2CH_3CN$ or $\{[AgL]{\cdot}PF_6{\cdot}2CH_3CN\}_n$, L = *N*-(pyridin-3-ylmethyl)pyridin-3-amine, comprises one Ag^{I} atom, one L ligand, two acetonitrile solvent molecules and one PF_6^- anion disordered over two orientations in a 0.567 (11):0.433 (11) ratio. Each Ag^{I} atom is coordinated by two pyridine N atoms from two L ligands in a slightly distorted linear coordination geometry [N—Ag—N = 170.55 (8)°]. Each L ligand bridges two Ag^{I} ions, resulting in the formation of a zigzag chain propagating along the [101] direction. In the crystal, Ag···Ag contacts [3.3023 (5) Å] and intermolecular π–π stacking interactions [centroid-to-centroid distance = 3.5922 (15) Å] between the pyridine rings link these chains into a corrugated layer parallel to the $(\bar{1}01)$ plane. The layers are stacked with a separation of 10.4532 (5) Å, and acetonitrile solvent molecules and PF_6^- anions as guests are intercalated between the layers. The layers are connected through several N/C—H···F hydrogen bonds and P—F···π interactions [F···ring centroid = 3.241 (8) Å] between the layer and the intercalated guests and between the intercalated guests, forming a three-dimensional supramolecular network.

1. Chemical context

Silver coordination polymers based on dipyridyl-type ligands have been widely exploited due to the intriguing topologies and the fascinating properties caused by a variety of coordination geometries and d^{10} electronic configurations of the Ag^{I} ion (Leong & Vittal, 2011; Moulton & Zaworotko, 2001; Wang *et al.*, 2012). In particular, Ag^{I} ions have a preference for a linear two-coordinate geometry and can serve to link bridging dipyridyl-type ligands to form polymeric chains. Based on this concept, we have focused our attention on the development of one-dimensional Ag^{I} coordination polymers with dipyridyl-type ligands. Up to date, we have reported several Ag^{I} coordination polymers with interesting topologies involving zigzag (Moon *et al.*, 2016), helical (Moon *et al.*, 2014, 2015) and double helical (Lee *et al.*, 2015) structures. In an extension of our research, the title compound was prepared by the reaction of silver(I) hexafluoridophosphate with a dipyridyl type-ligand, namely *N*-(pyridin-3-ylmethyl)pyridin-3-amine (*L*), synthesized according to a literature procedure (Lee *et al.*, 2013). Herein, we report on the crystal structure of the title compound in which lattice solvent molecules and anions as



guests are intercalated between the layers formed by intermolecular interactions between zigzag –(Ag–L)$_n$– chains.



2. Structural commentary

The molecular components of the title structure are shown in Fig. 1. The asymmetric unit comprises one Ag^{I} atom, one L ligand, two acetonitrile solvent molecules, and one hexafluoridophosphate anion disordered over two orientations in a 0.567 (11):0.433 (11) ratio. The silver(I) atom is coordinated by two pyridine N atoms (N1 and N2) from two symmetry-related L ligands, leading to the formation of an infinite zigzag chain propagating along the [101] direction. Thus, the Ag^{I} atom is two-coordinated in a slightly distorted linear coordination geometry [N1^{i}—Ag1—N2 = 170.55 (8)°; symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; Table 1]. This distortion from linear geometry may be caused by Ag···N interactions between the Ag^{I} ion and two acetonitrile N atoms [Ag1···N4 = 2.792 (4), Ag1···N5 = 2.815 (4) Å; black dashed lines in Fig. 1]. The two pyridine rings coordinated to the Ag^{I} center are tilted slightly, by 6.29 (15)° with respect to each other. In the chain, the Ag^{I} atoms are separated by 11.1009 (3) Å along the L linker which adopts a stretched *trans* conformation with the C2—N3—C6—C7 torsion angles being 174.7 (3)°.

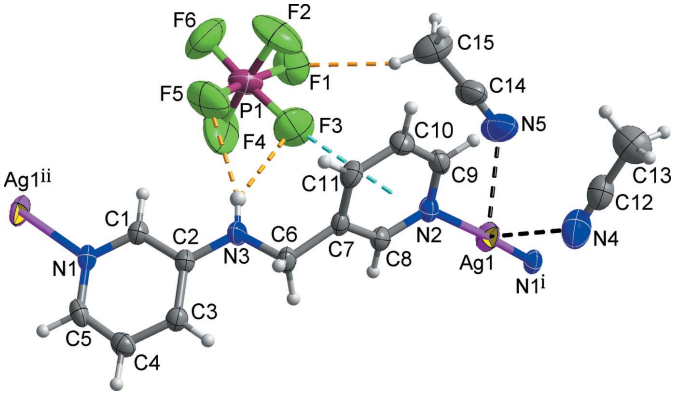


Figure 1
View of the molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Disordered F atoms of the PF_6^- anion have been omitted for clarity. Black and yellow dashed lines represent Ag···N interactions and intermolecular C/N—H···F hydrogen bonds, respectively. [Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.]

Table 1
Selected geometric parameters (Å, °).

Ag1—N1^{i}	2.163 (2)	Ag1—N2	2.166 (2)
N1^{i}—Ag1—N2	170.55 (8)		

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—H3A···F3	0.84 (3)	2.49 (3)	3.208 (8)	144 (3)
N3—H3A···F5	0.84 (3)	2.46 (3)	3.273 (10)	162 (3)
N3—H3A···F5′	0.84 (3)	2.18 (3)	2.999 (10)	167 (3)
C8—H8···N4^{ii}	0.95	2.63	3.478 (5)	149
C10—H10···F2^{iii}	0.95	2.39	3.176 (9)	140
C13—H13A···F2′^{iii}	0.98	2.54	3.487 (13)	163
C13—H13B···F6^{i}	0.98	2.53	3.365 (10)	144
C13—H13B···F1′^{i}	0.98	2.59	3.57 (2)	171
C15—H15A···F1	0.98	2.52	3.441 (9)	157
C15—H15A···F3′	0.98	2.42	3.356 (13)	160
C15—H15B···F2^{iv}	0.98	2.23	3.088 (10)	146
C15—H15B···F5′^{iv}	0.98	2.57	3.509 (11)	160
C15—H15C···F1^{iii}	0.98	2.36	3.329 (8)	168
C15—H15C···F1′^{iii}	0.98	2.09	3.037 (9)	161

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

3. Supramolecular features

The neighbouring zigzag chains are connected by Ag···Ag contacts [Ag1···Ag1 = 3.3023 (5) Å; red dashed lines in Fig. 2] and intermolecular π-π-stacking interactions between the pyridine rings [$Cg1\cdots Cg2^{ii}$ = 3.5922 (15) Å; yellow dashed lines in Fig. 2; $Cg1$ and $Cg2$ are the centroids of the N1/C1–C5 and N2/C7–C11 rings, respectively; symmetry code: (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$], resulting in the formation of a corrugated layer spreading out along the ($\bar{1}$01) plane (Fig. 2). Adjacent layers are stacked on each other with a separation of 10.4532 (5) Å. Acetonitrile molecules and PF_6^- anions as guests are intercalated between the layers (Fig. 3). The layers are further

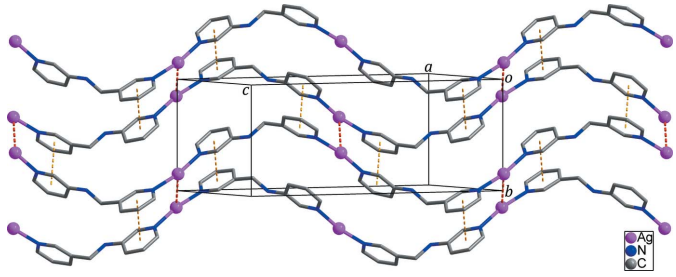


Figure 2
The two-dimensional network formed through Ag···Ag contacts (red dashed lines) and intermolecular π–π stacking interactions (yellow dashed lines). Acetonitrile solvent molecules, the PF_6^- anions and H atoms have been omitted for clarity.

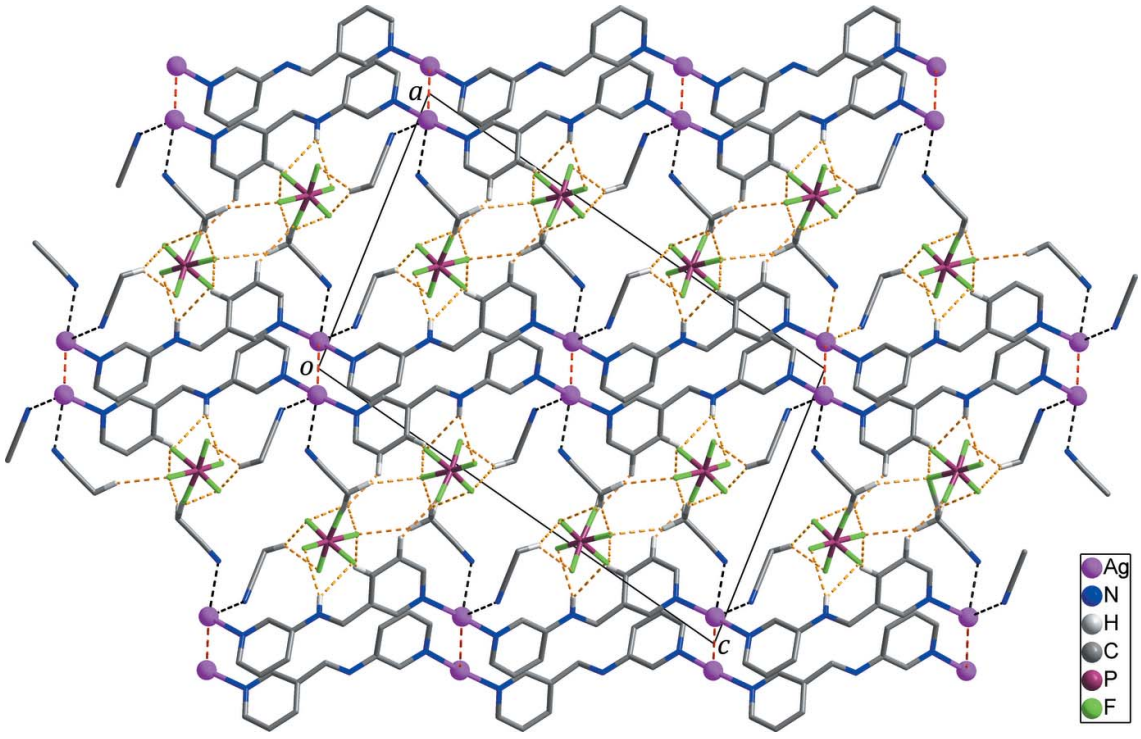


Figure 3
Interlayer stacking showing the intercalation of acetonitrile molecules and PF_6^- anions between the layers. Red, black and yellow dashed lines represent Ag···Ag contacts, Ag···N interactions and N/C—H···F hydrogen bonds, respectively. Disordered F atoms of the PF_6^- anions and H atoms not involved in intermolecular interactions have been omitted for clarity.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ag(C_{11}H_{11}N_3)]PF_6{\cdot}2C_2H_3N$
M_r	520.17
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	173
a, b, c (Å)	12.8997 (4), 7.5361 (3), 20.9747 (7)
β (°)	102.9900 (6)
V (Å^3)	1986.84 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.16
Crystal size (mm)	0.35 × 0.25 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.666, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11824, 4316, 3527
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.081, 1.10
No. of reflections	4316
No. of parameters	312
No. of restraints	18
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.12, −0.66

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010) and *publCIF* (Westrip, 2010).

connected by several intermolecular N/C—H···F hydrogen bonds (Table 2; yellow dashed lines in Figs. 1 and 3) and P—F···π interactions [F3···*Cg*2 = 3.241 (8) Å; sky-blue dashed line in Fig. 1] between the layer and the anions and between the acetonitrile solvent molecules and the anions, forming a three-dimensional supramolecular network.

4. Synthesis and crystallization

The *L* ligand was synthesized according to a literature method (Lee *et al.*, 2013). Slow evaporation of an acetonitrile solution of the *L* ligand with $AgPF_6$ in the molar ratio 1:1 afforded colourless block-like X-ray quality single crystals of the title compound.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The PF_6^- anion is disordered over two orientations in a 0.567 (11):0.433 (11) ratio. The amine H atom was located from a difference-Fourier map and freely refined [N—H = 0.84 (3) Å]. All other H atoms were positioned geometrically and refined as riding: C—H = 0.95 Å for Csp^2—H, 0.99 Å for methylene C—H and 0.98 Å for methyl C—H with U_{iso}(H) = 1.5U_{eq} (C-methyl) and 1.2U_{eq}(C) for other C-bound H atoms.

Funding information

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supporting information

Acta Cryst. (2017). E**73**, 1542-1545 [https://doi.org/10.1107/S2056989017013421]

Crystal structure of an Ag^{I} intercalation compound: *catena*-poly[[silver(I)-*μ*-*N*-(pyridin-3-ylmethyl)pyridin-3-amine-κ^2N:N'] hexafluoridophosphate acetonitrile disolvate]

Suk-Hee Moon, Youngjin Kang and Ki-Min Park

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

catena-Poly[[silver(I)-*μ*-*N*-(pyridin-3-ylmethyl)pyridine-3-amine-κ^2N:N'] hexafluoridophosphate acetonitrile disolvate]

Crystal data

$[Ag(C_{11}H_{11}N_3)]PF_6 \cdot 2C_2H_3N$
M_r = 520.17
Monoclinic, $P2_1/n$
a = 12.8997 (4) Å
b = 7.5361 (3) Å
c = 20.9747 (7) Å
β = 102.9900 (6)°
V = 1986.84 (12) Å^3
Z = 4
$F(000)$ = 1032
D_x = 1.739 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5825 reflections
θ = 2.9–28.0°
μ = 1.16 mm^{-1}
T = 173 K
Block, colorless
0.35 × 0.25 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.666, T_{max} = 0.746
11824 measured reflections
4316 independent reflections
3527 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.0°, θ_{min} = 1.7°
h = −10→16
k = −9→9
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.081
S = 1.10
4316 reflections
312 parameters
18 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 2.2488P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.66$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ag1	0.57809 (2)	0.34509 (3)	0.48065 (2)	0.04382 (9)	
N1	0.09170 (18)	0.3315 (3)	0.06343 (10)	0.0313 (5)	
N2	0.55270 (18)	0.4849 (3)	0.38820 (10)	0.0317 (5)	
N3	0.3023 (2)	0.4904 (4)	0.19724 (12)	0.0385 (6)	
H3A	0.352 (3)	0.439 (4)	0.1850 (15)	0.035 (8)*	
C1	0.1875 (2)	0.3614 (4)	0.10237 (12)	0.0305 (6)	
H1	0.2478	0.3053	0.0924	0.037*	
C2	0.2022 (2)	0.4724 (3)	0.15729 (12)	0.0282 (5)	
C3	0.1127 (2)	0.5557 (4)	0.17056 (13)	0.0315 (6)	
H3	0.1192	0.6331	0.2070	0.038*	
C4	0.0141 (2)	0.5233 (4)	0.12960 (13)	0.0347 (6)	
H4	−0.0477	0.5784	0.1379	0.042*	
C5	0.0059 (2)	0.4111 (4)	0.07669 (13)	0.0328 (6)	
H5	−0.0620	0.3897	0.0490	0.039*	
C6	0.3223 (2)	0.6106 (4)	0.25170 (13)	0.0363 (6)	
H6A	0.2721	0.5853	0.2800	0.044*	
H6B	0.3097	0.7338	0.2354	0.044*	
C7	0.4343 (2)	0.5940 (3)	0.29117 (12)	0.0288 (5)	
C8	0.4549 (2)	0.5027 (3)	0.34988 (12)	0.0294 (5)	
H8	0.3968	0.4500	0.3638	0.035*	
C9	0.6343 (2)	0.5596 (4)	0.36808 (14)	0.0355 (6)	
H9	0.7041	0.5474	0.3946	0.043*	
C10	0.6207 (2)	0.6531 (4)	0.31048 (14)	0.0400 (7)	
H10	0.6801	0.7041	0.2976	0.048*	
C11	0.5193 (2)	0.6720 (4)	0.27147 (13)	0.0374 (6)	
H11	0.5082	0.7374	0.2318	0.045*	
P1	0.52792 (8)	0.16310 (12)	0.15620 (5)	0.0532 (2)	
F1	0.6049 (5)	0.0241 (8)	0.2082 (3)	0.0812 (19)	0.567 (11)
F2	0.6355 (6)	0.2633 (12)	0.1590 (6)	0.106 (3)	0.567 (11)
F3	0.5178 (6)	0.2625 (10)	0.2228 (4)	0.106 (3)	0.567 (11)
F4	0.4273 (13)	0.060 (3)	0.1615 (8)	0.133 (6)	0.567 (11)
F5	0.4615 (6)	0.3036 (14)	0.1156 (4)	0.100 (3)	0.567 (11)
F6	0.5453 (8)	0.0508 (11)	0.0998 (4)	0.119 (3)	0.567 (11)
F1′	0.5583 (12)	−0.0286 (12)	0.1587 (9)	0.149 (7)	0.433 (11)
F2′	0.6253 (9)	0.2192 (19)	0.1252 (6)	0.106 (4)	0.433 (11)
F3′	0.5773 (14)	0.211 (2)	0.2223 (5)	0.184 (7)	0.433 (11)

F4′	0.4247 (14)	0.101 (3)	0.1739 (9)	0.128 (7)	0.433 (11)
F5′	0.4867 (8)	0.3671 (11)	0.1435 (6)	0.086 (3)	0.433 (11)
F6′	0.4650 (11)	0.1392 (17)	0.0770 (4)	0.125 (5)	0.433 (11)
N4	0.6922 (3)	0.6394 (5)	0.53962 (16)	0.0733 (10)	
C12	0.7722 (3)	0.6996 (5)	0.53960 (16)	0.0538 (9)	
C13	0.8750 (3)	0.7783 (6)	0.5397 (2)	0.0756 (12)	
H13A	0.8918	0.7604	0.4969	0.113*	
H13B	0.9298	0.7219	0.5736	0.113*	
H13C	0.8727	0.9057	0.5487	0.113*	
N5	0.7553 (3)	0.1622 (7)	0.45595 (18)	0.0922 (14)	
C14	0.7749 (3)	0.1581 (5)	0.40711 (19)	0.0566 (9)	
C15	0.7958 (4)	0.1556 (6)	0.3423 (2)	0.0749 (12)	
H15A	0.7287	0.1410	0.3098	0.112*	
H15B	0.8435	0.0566	0.3388	0.112*	
H15C	0.8295	0.2675	0.3343	0.112*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.05358 (16)	0.04805 (15)	0.02636 (12)	0.01328 (11)	0.00167 (9)	0.01001 (10)
N1	0.0354 (12)	0.0327 (12)	0.0226 (10)	−0.0052 (10)	−0.0003 (9)	0.0008 (9)
N2	0.0343 (12)	0.0324 (12)	0.0246 (11)	0.0031 (10)	−0.0010 (9)	0.0005 (9)
N3	0.0288 (12)	0.0498 (15)	0.0335 (12)	0.0031 (11)	0.0000 (10)	−0.0170 (11)
C1	0.0309 (14)	0.0348 (14)	0.0245 (12)	0.0000 (11)	0.0037 (10)	−0.0022 (10)
C2	0.0296 (13)	0.0307 (13)	0.0227 (12)	−0.0005 (11)	0.0026 (10)	0.0000 (10)
C3	0.0349 (14)	0.0309 (14)	0.0273 (13)	0.0024 (11)	0.0039 (11)	−0.0011 (10)
C4	0.0310 (14)	0.0341 (14)	0.0373 (15)	0.0061 (11)	0.0040 (11)	0.0072 (12)
C5	0.0276 (13)	0.0356 (14)	0.0295 (13)	−0.0035 (11)	−0.0055 (10)	0.0081 (11)
C6	0.0337 (15)	0.0436 (16)	0.0268 (13)	0.0037 (12)	−0.0034 (11)	−0.0095 (11)
C7	0.0325 (14)	0.0291 (13)	0.0221 (12)	0.0020 (11)	0.0005 (10)	−0.0053 (10)
C8	0.0316 (14)	0.0283 (13)	0.0273 (12)	−0.0023 (11)	0.0042 (10)	−0.0036 (10)
C9	0.0292 (14)	0.0393 (16)	0.0347 (14)	0.0019 (12)	0.0005 (11)	−0.0060 (12)
C10	0.0355 (15)	0.0484 (17)	0.0369 (15)	−0.0087 (13)	0.0101 (12)	−0.0023 (13)
C11	0.0451 (16)	0.0419 (16)	0.0246 (13)	−0.0021 (13)	0.0066 (11)	0.0027 (11)
P1	0.0471 (5)	0.0444 (5)	0.0736 (6)	0.0043 (4)	0.0254 (5)	−0.0012 (4)
F1	0.086 (4)	0.064 (3)	0.087 (4)	0.018 (3)	0.007 (3)	0.016 (3)
F2	0.052 (3)	0.092 (5)	0.175 (8)	−0.015 (3)	0.027 (5)	0.043 (5)
F3	0.103 (5)	0.094 (4)	0.119 (5)	0.022 (4)	0.022 (4)	−0.057 (4)
F4	0.115 (10)	0.173 (10)	0.102 (7)	−0.101 (9)	0.007 (6)	−0.010 (6)
F5	0.069 (4)	0.118 (6)	0.110 (6)	0.038 (4)	0.014 (4)	0.051 (5)
F6	0.159 (7)	0.143 (7)	0.065 (4)	0.024 (6)	0.044 (4)	−0.022 (4)
F1′	0.171 (11)	0.056 (5)	0.24 (2)	0.039 (6)	0.097 (12)	0.046 (7)
F2′	0.049 (5)	0.153 (10)	0.123 (8)	0.030 (6)	0.036 (5)	0.007 (7)
F3′	0.183 (14)	0.256 (18)	0.076 (7)	0.038 (13)	−0.048 (8)	−0.028 (8)
F4′	0.083 (9)	0.215 (18)	0.105 (10)	−0.012 (9)	0.063 (8)	0.054 (10)
F5′	0.077 (5)	0.063 (4)	0.129 (7)	0.016 (3)	0.047 (5)	−0.005 (4)
F6′	0.154 (10)	0.152 (10)	0.059 (4)	−0.049 (8)	0.002 (5)	−0.006 (5)
N4	0.084 (3)	0.080 (3)	0.0521 (19)	−0.026 (2)	0.0085 (17)	−0.0043 (17)

C12	0.067 (2)	0.051 (2)	0.0397 (18)	−0.0057 (18)	0.0052 (16)	−0.0009 (15)
C13	0.068 (3)	0.068 (3)	0.088 (3)	−0.002 (2)	0.013 (2)	0.013 (2)
N5	0.067 (2)	0.156 (4)	0.057 (2)	0.044 (3)	0.0217 (18)	0.025 (2)
C14	0.0406 (18)	0.071 (2)	0.060 (2)	0.0125 (17)	0.0159 (16)	0.0091 (19)
C15	0.092 (3)	0.071 (3)	0.074 (3)	−0.001 (2)	0.044 (3)	0.003 (2)

Geometric parameters (Å, º)

Ag1—N1^{i}	2.163 (2)	C9—H9	0.9500
Ag1—N2	2.166 (2)	C10—C11	1.385 (4)
Ag1—Ag1^{ii}	3.3023 (5)	C10—H10	0.9500
N1—C1	1.338 (3)	C11—H11	0.9500
N1—C5	1.341 (4)	P1—F3′	1.435 (10)
N1—Ag1^{iii}	2.163 (2)	P1—F1′	1.495 (8)
N2—C8	1.342 (3)	P1—F5	1.501 (6)
N2—C9	1.343 (4)	P1—F6	1.512 (5)
N3—C2	1.379 (3)	P1—F4′	1.532 (14)
N3—C6	1.435 (3)	P1—F4	1.539 (12)
N3—H3A	0.84 (3)	P1—F2	1.570 (7)
C1—C2	1.401 (3)	P1—F2′	1.596 (11)
C1—H1	0.9500	P1—F3	1.617 (6)
C2—C3	1.396 (4)	P1—F5′	1.629 (9)
C3—C4	1.387 (4)	P1—F1	1.669 (5)
C3—H3	0.9500	P1—F6′	1.687 (8)
C4—C5	1.380 (4)	N4—C12	1.127 (5)
C4—H4	0.9500	C12—C13	1.452 (6)
C5—H5	0.9500	C13—H13A	0.9800
C6—C7	1.500 (4)	C13—H13B	0.9800
C6—H6A	0.9900	C13—H13C	0.9800
C6—H6B	0.9900	N5—C14	1.110 (5)
C7—C8	1.383 (4)	C14—C15	1.445 (5)
C7—C11	1.387 (4)	C15—H15A	0.9800
C8—H8	0.9500	C15—H15B	0.9800
C9—C10	1.375 (4)	C15—H15C	0.9800
N1^{i}—Ag1—N2	170.55 (8)	C10—C11—H11	120.5
N1^{i}—Ag1—Ag1^{ii}	100.46 (6)	C7—C11—H11	120.5
N2—Ag1—Ag1^{ii}	84.17 (6)	F3′—P1—F1′	98.8 (9)
C1—N1—C5	119.3 (2)	F5—P1—F6	96.7 (5)
C1—N1—Ag1^{iii}	119.39 (18)	F3′—P1—F4′	93.7 (10)
C5—N1—Ag1^{iii}	121.31 (17)	F1′—P1—F4′	86.1 (10)
C8—N2—C9	117.9 (2)	F5—P1—F4	90.8 (9)
C8—N2—Ag1	121.18 (18)	F6—P1—F4	92.8 (7)
C9—N2—Ag1	120.91 (17)	F5—P1—F2	94.0 (5)
C2—N3—C6	121.4 (2)	F6—P1—F2	90.7 (5)
C2—N3—H3A	117 (2)	F4—P1—F2	173.7 (8)
C6—N3—H3A	121 (2)	F3′—P1—F2′	96.2 (8)
N1—C1—C2	122.6 (2)	F1′—P1—F2′	92.7 (6)

N1—C1—H1	118.7	F4′—P1—F2′	170.1 (8)
C2—C1—H1	118.7	F5—P1—F3	91.0 (4)
N3—C2—C3	122.6 (2)	F6—P1—F3	172.3 (4)
N3—C2—C1	119.6 (2)	F4—P1—F3	86.5 (6)
C3—C2—C1	117.8 (2)	F2—P1—F3	89.3 (5)
C4—C3—C2	118.8 (2)	F3′—P1—F5′	88.8 (8)
C4—C3—H3	120.6	F1′—P1—F5′	172.5 (8)
C2—C3—H3	120.6	F4′—P1—F5′	93.3 (11)
C5—C4—C3	120.0 (3)	F2′—P1—F5′	86.6 (6)
C5—C4—H4	120.0	F5—P1—F1	173.5 (4)
C3—C4—H4	120.0	F6—P1—F1	89.4 (4)
N1—C5—C4	121.5 (2)	F4—P1—F1	91.3 (9)
N1—C5—H5	119.2	F2—P1—F1	83.5 (4)
C4—C5—H5	119.2	F3—P1—F1	82.9 (3)
N3—C6—C7	111.4 (2)	F3′—P1—F6′	171.5 (8)
N3—C6—H6A	109.3	F1′—P1—F6′	89.8 (8)
C7—C6—H6A	109.3	F4′—P1—F6′	87.3 (8)
N3—C6—H6B	109.3	F2′—P1—F6′	82.9 (5)
C7—C6—H6B	109.3	F5′—P1—F6′	82.7 (5)
H6A—C6—H6B	108.0	N4—C12—C13	179.6 (5)
C8—C7—C11	118.0 (2)	C12—C13—H13A	109.5
C8—C7—C6	120.1 (3)	C12—C13—H13B	109.5
C11—C7—C6	121.9 (2)	H13A—C13—H13B	109.5
N2—C8—C7	123.4 (2)	C12—C13—H13C	109.5
N2—C8—H8	118.3	H13A—C13—H13C	109.5
C7—C8—H8	118.3	H13B—C13—H13C	109.5
N2—C9—C10	122.4 (3)	N5—C14—C15	177.5 (4)
N2—C9—H9	118.8	C14—C15—H15A	109.5
C10—C9—H9	118.8	C14—C15—H15B	109.5
C9—C10—C11	119.3 (3)	H15A—C15—H15B	109.5
C9—C10—H10	120.3	C14—C15—H15C	109.5
C11—C10—H10	120.3	H15A—C15—H15C	109.5
C10—C11—C7	119.0 (3)	H15B—C15—H15C	109.5

C5—N1—C1—C2	0.5 (4)	N3—C6—C7—C8	−102.6 (3)
Ag1^{iii}—N1—C1—C2	−179.21 (19)	N3—C6—C7—C11	79.0 (3)
C6—N3—C2—C3	−6.3 (4)	C9—N2—C8—C7	−0.1 (4)
C6—N3—C2—C1	176.2 (3)	Ag1—N2—C8—C7	178.53 (19)
N1—C1—C2—N3	176.7 (3)	C11—C7—C8—N2	−0.6 (4)
N1—C1—C2—C3	−0.9 (4)	C6—C7—C8—N2	−179.0 (2)
N3—C2—C3—C4	−176.8 (3)	C8—N2—C9—C10	0.3 (4)
C1—C2—C3—C4	0.7 (4)	Ag1—N2—C9—C10	−178.3 (2)
C2—C3—C4—C5	−0.3 (4)	N2—C9—C10—C11	0.1 (4)
C1—N1—C5—C4	0.0 (4)	C9—C10—C11—C7	−0.8 (4)
Ag1^{iii}—N1—C5—C4	179.7 (2)	C8—C7—C11—C10	1.0 (4)

C3—C4—C5—N1	−0.1 (4)	C6—C7—C11—C10	179.4 (3)
C2—N3—C6—C7	174.7 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···F3	0.84 (3)	2.49 (3)	3.208 (8)	144 (3)
N3—H3*A*···F5	0.84 (3)	2.46 (3)	3.273 (10)	162 (3)
N3—H3*A*···F5′	0.84 (3)	2.18 (3)	2.999 (10)	167 (3)
C8—H8···N4^{ii}	0.95	2.63	3.478 (5)	149
C10—H10···F2^{iv}	0.95	2.39	3.176 (9)	140
C13—H13*A*···F2′^{iv}	0.98	2.54	3.487 (13)	163
C13—H13*B*···F6^{i}	0.98	2.53	3.365 (10)	144
C13—H13*B*···F1′^{i}	0.98	2.59	3.57 (2)	171
C15—H15*A*···F1	0.98	2.52	3.441 (9)	157
C15—H15*A*···F3′	0.98	2.42	3.356 (13)	160
C15—H15*B*···F2^{v}	0.98	2.23	3.088 (10)	146
C15—H15*B*···F5′^{v}	0.98	2.57	3.509 (11)	160
C15—H15*C*···F1^{iv}	0.98	2.36	3.329 (8)	168
C15—H15*C*···F1′^{iv}	0.98	2.09	3.037 (9)	161

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+3/2, *y*+1/2, −*z*+1/2; (v) −*x*+3/2, *y*−1/2, −*z*+1/2.