

catena-Poly[[silver(I)- μ -1,1'-methylene-diimidazole] hexafluoridophosphate]

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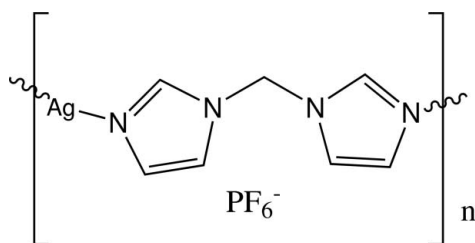
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.036; wR factor = 0.104; data-to-parameter ratio = 14.3.

The title compound, $\{[\text{Ag}(\text{C}_7\text{H}_8\text{N}_4)]\text{PF}_6\}_n$, has a one-dimensional zigzag chain structure. The Ag^+ cation and the PF_6^- anion reside on crystallographic inversion centres. The Ag^+ cation is coordinated by the unsubstituted N atoms of two separate 1,1'-methylene-diimidazole ligands. The closest $\text{Ag} \cdots \text{Ag}$ separation in the same cationic chain is 7.704 (2) Å and the dihedral angle between the two imidazole rings in the same ligand is 85.5 (1)°. A two-dimensional layer framework is formed by weak $\text{Ag} \cdots \text{N}$ interactions between adjacent chains, with an $\text{Ag} \cdots \text{N}$ distance of 3.472 (2) Å.

Related literature

For related literature, see: Barnett & Champness (2003); Batten & Robson (1998); Desiraju (1995); Hamilton & Ziegler (2004); Moulton & Zaworotko (2001); Leininger *et al.* (2000); Lobbia *et al.* (2002); Pschirer *et al.* (2002).



Experimental

Crystal data

$[\text{Ag}(\text{C}_7\text{H}_8\text{N}_4)]\text{PF}_6$
 $M_r = 401.01$
 Monoclinic, $P2_1/n$
 $a = 8.3966$ (10) Å
 $b = 5.1604$ (6) Å
 $c = 13.6211$ (16) Å
 $\beta = 94.666$ (2)°

$V = 588.24$ (12) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.92$ mm⁻¹
 $T = 293$ (2) K
 $0.23 \times 0.14 \times 0.12$ mm

Data collection

Bruker SMART APEX-CCD diffractometer
 Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
 $T_{\min} = 0.596$, $T_{\max} = 0.793$
 3264 measured reflections
 1285 independent reflections
 1073 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.080$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.104$
 $S = 1.07$
 1285 reflections
 90 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.81$ e Å⁻³
 $\Delta\rho_{\min} = -0.62$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{C3}-\text{H3} \cdots \text{F2}^i$	0.93	2.78	3.687 (5)	167
$\text{C3}-\text{H3} \cdots \text{F3}^i$	0.93	2.87	3.448 (5)	122
$\text{C4}-\text{H4A} \cdots \text{F2}^{ii}$	0.97	2.62	3.569 (4)	165
$\text{C4}-\text{H4A} \cdots \text{F3}^{iii}$	0.97	2.48	3.224 (3)	133
$\text{C2}-\text{H2} \cdots \text{F1}^{iv}$	0.93	2.81	3.628 (5)	148
$\text{C1}-\text{H1} \cdots \text{F3}^{iii}$	0.93	2.58	3.043 (4)	111

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2055).

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supplementary materials

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***catena*-Poly[[silver(I)- μ -1,1'-methylenediimidazole] hexafluoridophosphate]**

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Comment

The construction of solid-state architectures and crystal engineering has become rapidly developing areas of supramolecular chemistry in the past decade (Desiraju, 1995; Batten & Robson, 1998; Leininger *et al.*, 2000; Moulton & Zaworotko, 2001). Such molecular architectures have been successfully designed and synthesized by judicious combination of a metal 'node' and an organic ligand 'spacer'. The roles of counter anions and different solvent molecules are also of significant effect on supramolecular self-assembly. More recently, the molecular geometry and flexibility of multidentate N-donor spacer ligands play key roles in the development of the tailor-made molecular materials and supramolecular self-assemble crystal engineering. For example, 4, 4'-bipyridine, 1, 2-bis(4-pyridyl)ethane and *trans*-bis(4-pyridyl)ethene as ligands can form a lot of coordination polymers with different structure features (Barnett & Champness, 2003; Pschirer *et al.*, 2002). The coordination polymer frameworks which were built by methylene C-bridged bipyridine, bitriazole and bipyrazole ligands have also been described widely (Lobbia *et al.*, 2002; Hamilton & Ziegler, 2004). Bis(imidazol-1-yl)-methane (BIM) is flexibility V-shaped N-donor ligand which was built by methylene C-bridged two imidazole rings. The title compound, [Ag(BIM)PF₆]_n, (I), with a one-dimensional zigzag cationic chain structural motifs, was formed by the addition of a solution of BIM to AgPF₆.

Single crystal X-ray diffraction analysis reveals that complex (I) consist of one dimensional cationic polymeric chains and uncoordinated PF₆⁻. The Ag^I ion occupies a crystallographic inversion centre and is coordinated by two imidazolyl nitrogen atoms of independent BIM ligands, which act as bridges between silver(I) centers, generated one dimensional zigzag cationic chain polymeric structure (Fig. 1). Ag^I ion is a linear coordination mode with the bond angles of N—Ag—N being 180.0 (1)°, and the bond lengths of Ag—N is 2.097 (3) Å. The adjacent Ag·····Ag distance in the same cationic chain is 7.704 (2)Å and the dihedral angle of the two imidazole rings in the same ligand is 85.5 (1)°. The two-dimensional layer network was built by weak interactions between Ag^I ion and two nitrogen atoms from imidazole rings in the adjacent one-dimensional zigzag chain with the distance of Ag—N being 3.472 (2)Å (Fig. 2). The non-coordinated PF₆⁻ anions were filled in the void of each zigzag cationic chain through the weak C—H·····F hydrogen-bond interactions (Table 1).

Experimental

An acetone solution (5 ml) of BIM (74 mg, 0.5 mmol) was slowly diffused into an aqueous solution (5 ml) of AgPF₆(126 mg, 0.5 mmol) in test tube. Colorless crystals of [Ag(BIM) PF₆]_n were formed at the interface of solvent in two weeks and were obtained in 82% yield. Anal. Calcd for C₇H₈AgF₆N₄P: C, 20.97; H, 2.01; N, 13.97; Found (%): C, 21.04; H, 2.49; N, 13.92; IR (KBr, cm⁻¹): ν = 3150 s, 3114w, 3038w, 1712w, 1614w, 1530 s, 1411m, 1377w, 1355w, 1339w, 1291m, 1243 s, 1116 s, 1031w, 835 s, 747 s, 713w, 652m, 613w, 560 s.

Refinement

H atoms were positioned geometrically at distances of 0.93 (CH), 0.97 (CH₂) and 0.96 Å (CH₃) from the parent C atoms, a riding model was used during the refinement process. The U_{iso} values were constrained to be $1.2U_{\text{eq}}$ of the carrier atom, except for methyl H atoms that were constrained to $1.5U_{\text{eq}}$ of the C atom.

Figures

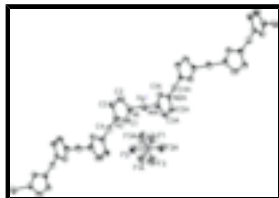


Fig. 1. The structure of (I) showing the atom-numbering of unsymmetry unit. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) $-x + 2, -y, -z + 1.$]



Fig. 2. Two-dimensional layer structure assembled by one-dimensional zigzag chains with weak Ag \cdots N interactions.

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Crystal data

[Ag(C₇H₈N₄)]PF₆

$M_r = 401.01$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1\ yac$

$a = 8.3966$ (10) Å

$b = 5.1604$ (6) Å

$c = 13.6211$ (16) Å

$\beta = 94.666$ (2)°

$V = 588.24$ (12) Å³

$Z = 2$

$F_{000} = 388$

$D_x = 2.264$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 1730 reflections

$\theta = 5.5\text{--}56.3^\circ$

$\mu = 1.92$ mm⁻¹

$T = 293$ (2) K

Prismatic, colorless

$0.23 \times 0.15 \times 0.12$ mm

Data collection

SMART APEX-CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

ϕ and ω scans

Absorption correction: multi-scan
SADABS (Sheldrick, 1996)

$T_{\text{min}} = 0.596, T_{\text{max}} = 0.793$

1285 independent reflections

1073 reflections with $> 2\sigma(I)$

$R_{\text{int}} = 0.080$

$\theta_{\text{max}} = 27.0^\circ$

$\theta_{\text{min}} = 2.8^\circ$

$h = -10 \rightarrow 10$

$k = -6 \rightarrow 6$

3264 measured reflections

$l = -17 \rightarrow 8$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.036$

H-atom parameters constrained

$wR(F^2) = 0.104$

$$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.0221P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.07$

$(\Delta/\sigma)_{\max} = 0.003$

1285 reflections

$\Delta\rho_{\max} = 0.81 \text{ e } \text{\AA}^{-3}$

90 parameters

$\Delta\rho_{\min} = -0.62 \text{ e } \text{\AA}^{-3}$

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>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ag1	1.0000	0.0000	0.5000	0.0467 (2)	
P1	0.5000	0.0000	0.5000	0.0395 (3)	
F1	0.6294 (4)	0.1949 (7)	0.5436 (2)	0.0925 (11)	
F2	0.4980 (3)	0.1377 (6)	0.39578 (17)	0.0719 (7)	
F3	0.3615 (4)	0.1824 (7)	0.5298 (2)	0.0900 (10)	
N1	0.9785 (3)	0.3049 (5)	0.39798 (19)	0.0421 (6)	
N2	0.8717 (3)	0.6069 (5)	0.30233 (19)	0.0356 (6)	
C1	0.8469 (4)	0.4306 (7)	0.3711 (3)	0.0397 (7)	
H1	0.7490	0.4010	0.3965	0.048*	
C2	1.0280 (4)	0.5957 (9)	0.2850 (3)	0.0547 (9)	
H2	1.0798	0.6969	0.2410	0.066*	
C3	1.0936 (4)	0.4092 (10)	0.3443 (3)	0.0592 (10)	
H3	1.2003	0.3590	0.3482	0.071*	
C4	0.7500	0.7683 (8)	0.2500	0.0403 (10)	
H4A	0.7007	0.8786	0.2966	0.048*	0.50
H4B	0.7993	0.8786	0.2034	0.048*	0.50

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0582 (3)	0.0379 (3)	0.0419 (3)	0.00042 (13)	-0.00903 (18)	0.00663 (14)
P1	0.0398 (7)	0.0396 (7)	0.0398 (7)	0.0011 (4)	0.0072 (5)	-0.0004 (5)
F1	0.104 (2)	0.103 (2)	0.088 (2)	-0.0565 (19)	-0.0051 (18)	-0.0118 (19)
F2	0.0843 (17)	0.0799 (19)	0.0524 (13)	0.0033 (13)	0.0112 (12)	0.0182 (13)
F3	0.103 (2)	0.101 (2)	0.086 (2)	0.0592 (18)	0.0278 (17)	0.0008 (19)
N1	0.0489 (14)	0.0392 (14)	0.0367 (14)	0.0002 (11)	-0.0051 (11)	0.0052 (12)
N2	0.0402 (13)	0.0338 (13)	0.0321 (13)	-0.0031 (10)	-0.0006 (10)	0.0002 (11)
C1	0.0439 (17)	0.0339 (14)	0.0411 (18)	-0.0017 (13)	0.0025 (14)	0.0024 (14)
C2	0.0441 (18)	0.072 (2)	0.049 (2)	-0.0050 (18)	0.0074 (16)	0.023 (2)
C3	0.0408 (18)	0.076 (2)	0.061 (2)	0.0030 (19)	0.0024 (17)	0.015 (2)
C4	0.050 (2)	0.029 (2)	0.041 (2)	0.000	-0.0025 (19)	0.000

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

Ag1—N1 ⁱ	2.097 (3)	N2—C1	1.334 (5)
Ag1—N1	2.097 (3)	N2—C2	1.354 (4)
P1—F1	1.562 (2)	N2—C4	1.459 (3)
P1—F1 ⁱⁱ	1.562 (2)	C1—H1	0.9300
P1—F3	1.575 (2)	C2—C3	1.345 (6)
P1—F3 ⁱⁱ	1.575 (2)	C2—H2	0.9300
P1—F2	1.586 (2)	C3—H3	0.9300
P1—F2 ⁱⁱ	1.586 (2)	C4—N2 ⁱⁱⁱ	1.459 (3)
N1—C1	1.308 (4)	C4—H4A	0.9700
N1—C3	1.369 (5)	C4—H4B	0.9700
N1 ⁱ —Ag1—N1	180.000 (1)	C1—N2—C2	107.6 (3)
F1—P1—F1 ⁱⁱ	180.00 (18)	C1—N2—C4	126.1 (2)
F1—P1—F3	91.3 (2)	C2—N2—C4	126.2 (3)
F1 ⁱⁱ —P1—F3	88.7 (2)	N1—C1—N2	111.0 (3)
F1—P1—F3 ⁱⁱ	88.7 (2)	N1—C1—H1	124.5
F1 ⁱⁱ —P1—F3 ⁱⁱ	91.3 (2)	N2—C1—H1	124.5
F3—P1—F3 ⁱⁱ	180.0 (2)	C3—C2—N2	106.4 (3)
F1—P1—F2	90.48 (15)	C3—C2—H2	126.8
F1 ⁱⁱ —P1—F2	89.52 (15)	N2—C2—H2	126.8
F3—P1—F2	90.52 (15)	C2—C3—N1	109.2 (3)
F3 ⁱⁱ —P1—F2	89.48 (15)	C2—C3—H3	125.4
F1—P1—F2 ⁱⁱ	89.52 (15)	N1—C3—H3	125.4
F1 ⁱⁱ —P1—F2 ⁱⁱ	90.48 (15)	N2 ⁱⁱⁱ —C4—N2	110.4 (3)
F3—P1—F2 ⁱⁱ	89.48 (15)	N2 ⁱⁱⁱ —C4—H4A	109.6
F3 ⁱⁱ —P1—F2 ⁱⁱ	90.52 (15)	N2—C4—H4A	109.6
F2—P1—F2 ⁱⁱ	180.000 (1)	N2 ⁱⁱⁱ —C4—H4B	109.6
C1—N1—C3	105.8 (3)	N2—C4—H4B	109.6

C1—N1—Ag1	125.7 (2)	H4A—C4—H4B	108.1
C3—N1—Ag1	128.5 (2)		
C3—N1—C1—N2	0.8 (4)	N2—C2—C3—N1	0.1 (6)
Ag1—N1—C1—N2	-177.7 (2)	C1—N1—C3—C2	-0.5 (5)
C2—N2—C1—N1	-0.7 (4)	Ag1—N1—C3—C2	177.8 (3)
C4—N2—C1—N1	175.0 (3)	C1—N2—C4—N2 ⁱⁱⁱ	-58.6 (3)
C1—N2—C2—C3	0.4 (5)	C2—N2—C4—N2 ⁱⁱⁱ	116.4 (4)
C4—N2—C2—C3	-175.4 (4)		

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $-x+3/2, y, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C3—H3 \cdots F2 ^{iv}	0.93	2.78	3.687 (5)	167
C3—H3 \cdots F3 ^{iv}	0.93	2.87	3.448 (5)	122
C4—H4A \cdots F2 ^v	0.97	2.62	3.569 (4)	165
C4—H4A \cdots F3 ^{vi}	0.97	2.48	3.224 (3)	133
C2—H2 \cdots F1 ^{vii}	0.93	2.81	3.628 (5)	148
C1—H1 \cdots F3 ^{vi}	0.93	2.58	3.043 (4)	111

Symmetry codes: (iv) $x+1, y, z$; (v) $x, y+1, z$; (vi) $-x+1, -y+1, -z+1$; (vii) $x+1/2, -y+1, z-1/2$.

Fig. 1

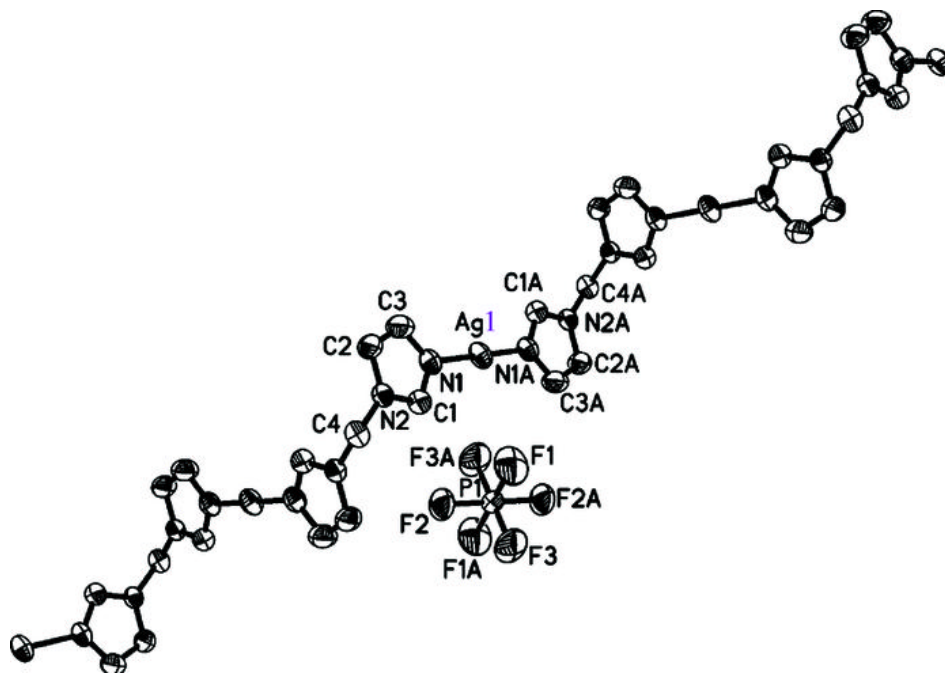


Fig. 2

