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catena-Poly[[[(2-pyridone-κO)silver(I)]-μ-2-pyridone-$\kappa^2 O$:O] hexafluoridophosphate]

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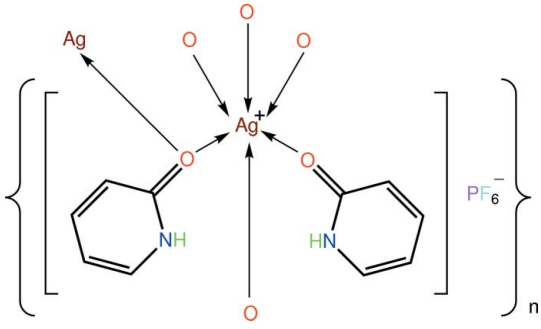
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.080; data-to-parameter ratio = 16.4.

The asymmetric unit of the polymeric title salt, $\{[Ag(C_5H_5NO)_2]PF_6\}_n$, comprises an Ag^I cation (located on a twofold axis), two 2-pyridone ligands (with distinct coordination modes), and half a PF_6^- anion (situated on a centre of inversion). The Ag^I atom is in an approximately octahedral AgO_6 coordination geometry, which is stabilized by intramolecular N—H···O hydrogen bonds. The result of the bridging mode of the 2-pyridone ligand is the formation of a supramolecular chain along the c axis; these are consolidated in the crystal by C—H···F interactions.

Related literature

For structural diversity in the supramolecular structures of silver salts, see: Kundu *et al.* (2010). For a related Ag structure, see: Arman *et al.* (2010).



Experimental

Crystal data

$[Ag(C_5H_5NO)_2]PF_6$
M_r = 633.24
Monoclinic, $C2/c$
a = 13.519 (5) Å
b = 24.187 (9) Å
c = 7.301 (3) Å
β = 96.918 (5)°
V = 2369.9 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 293 K
0.48 × 0.40 × 0.14 mm

Data collection

Rigaku AFC12/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.535, T_{max} = 1.000
8382 measured reflections
2703 independent reflections
2573 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.080
S = 1.14
2703 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag—O1	2.3543 (19)	Ag—O2^{i}	2.6278 (19)
Ag—O2	2.5055 (18)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	1.91	2.765 (2)	171
N2—H2···O1^{ii}	0.86	1.90	2.754 (3)	174
C3—H3···F1^{iii}	0.93	2.48	3.353 (3)	157
C5—H5···F3^{iv}	0.93	2.51	3.398 (3)	159

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5626).

References

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supplementary materials

Acta Cryst. (2010). E**66**, m1212 [**doi:10.1107/S1600536810035348**]

catena-Poly[[[(2-pyridone-κO)silver(I)]-μ-2-pyridone-$\kappa^2 O$:O] hexafluoridophosphate]

H. D. Arman, T. Miller and E. R. T. Tiekink

Comment

The structural diversity in the supramolecular structures of silver salts is well documented (Kundu *et al.*, 2010). The title compound, (I), was was isolated and characterized as a continuation of recent structural studies of such structures (Arman *et al.*, 2010).

The crystallographic asymmetric unit of (I) comprises half a Ag cation, situated on a crystallographic 2-fold axis, a monodentate 2-pyridone ligand, coordinating *via* the carbonyl-O atom, a bidentate 2-pyridone ligand, bridging two Ag cations *via* a carbonyl-O atom, and half a PF_6^- anion, situated about a crystallographic centre of inversion, Fig. 1. The resulting Ag^I atom coordination geomerty is based on a distorted octahedron defined by an O_6 donor set, with the Ag—O bond distances lying in the range 2.3543 (19) to 2.6278 (19) Å, Table 1. The coordination geometry is stabilized by intramolecular N—H···O hydrogen bonds, Table 2. As the carbonyl-O2 atom is bidentate bridging, a supramolecular chain along the *c* axis is generated, Fig. 2. The chains are consolidated in the 3-D structure by C—H···F interactions, Fig. 3.

Experimental

The title salt, (I), was isolated as colourless blocks from the 1:2 reaction of silver hexafluorophosphate (Aldrich) and 2-hydroxypyridine (Aldrich) in methanol solution; m. pt 393–399 K.

Refinement

The H-atoms were placed in calculated positions (N—H = 0.86 Å and C—H = 0.93 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2U_{eq}(carrier atom).

Figures

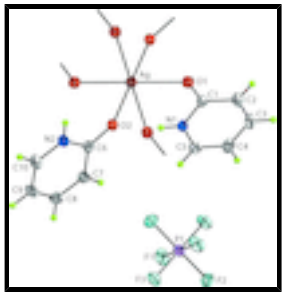

Fig. 1. Asymmetric unit in the structure of (I) showing displacement ellipsoids at the 50% probability level. The Ag (lying on a 2-fold axis of symmetry) and P (lying on a centre of inversion) atom environments have been expanded to show the respective coordination geometries.

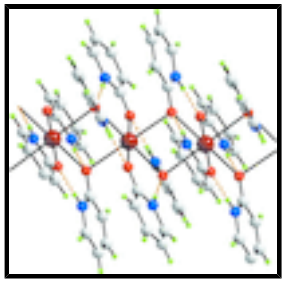

Fig. 2. Portion of the supramolecular chain aligned along the *c* axis in (I).

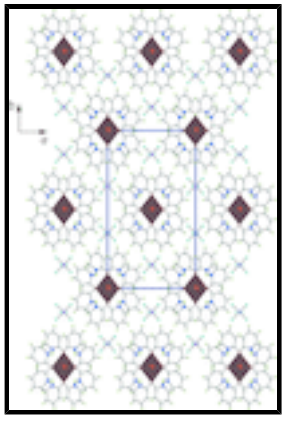

Fig. 3. A view in projection down the *c* axis of the crystal packing in (I), emphasizing the Ag octahedra and interspersing of the PF_6^- anions.

catena-Poly[[[(2-pyridone-κ*O*)silver(I)]-μ-2-pyridone- $\kappa^2 O$:*O*] hexafluoridophosphate]

Crystal data

$[Ag(C_5H_5NO)_2]PF_6$	$F(000) = 1264$
$M_r = 633.24$	$D_x = 1.775$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71069 Å
Hall symbol: -C 2yc	Cell parameters from 4745 reflections
a = 13.519 (5) Å	θ = 3.1–40.6°
b = 24.187 (9) Å	μ = 1.00 mm^{-1}
c = 7.301 (3) Å	*T* = 293 K
β = 96.918 (5)°	Block, colourless
V = 2369.9 (16) Å^3	0.48 × 0.40 × 0.14 mm
Z = 4	

Data collection

Rigaku AFC12K/SATURN724 diffractometer	2703 independent reflections
Radiation source: fine-focus sealed tube	2573 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.033$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	*h* = −14→17
$T_{min} = 0.535$, $T_{max} = 1.000$	*k* = −30→31
8382 measured reflections	*l* = −9→9

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.031$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.080$	H-atom parameters constrained
$S = 1.14$	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 3.3853P]$ where $P = (F_o^2 + 2F_c^2)/3$
2703 reflections	$(\Delta/\sigma)_{max} = 0.001$
165 parameters	$\Delta\rho_{max} = 0.78$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.47$ e Å^{-3}

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	0.0000	0.0000	0.0000	0.02327 (9)
P1	−0.5000	0.14921 (3)	0.2500	0.02229 (17)
O1	0.00398 (11)	0.09711 (7)	−0.0200 (2)	0.0243 (3)
N1	−0.13089 (13)	0.11598 (7)	0.1275 (2)	0.0206 (3)
H1	−0.1378	0.0811	0.1457	0.025*
F1	−0.52808 (12)	0.14954 (6)	0.4566 (2)	0.0349 (3)
O2	−0.13415 (13)	0.00438 (6)	0.2083 (2)	0.0239 (3)
C6	−0.19943 (16)	−0.03274 (9)	0.2224 (3)	0.0214 (4)
N2	−0.18133 (13)	−0.08533 (7)	0.1662 (2)	0.0223 (4)
H2	−0.1265	−0.0916	0.1210	0.027*
C1	−0.05410 (15)	0.13279 (8)	0.0342 (3)	0.0195 (4)
F2	−0.58219 (11)	0.19640 (6)	0.1951 (2)	0.0340 (3)
F3	−0.58231 (11)	0.10246 (6)	0.1955 (2)	0.0356 (3)
C5	−0.19677 (17)	0.15108 (9)	0.1932 (3)	0.0240 (4)
H5	−0.2478	0.1371	0.2544	0.029*
C10	−0.24535 (18)	−0.12841 (9)	0.1781 (3)	0.0261 (4)
H10	−0.2291	−0.1632	0.1369	0.031*
C2	−0.04687 (17)	0.19098 (9)	0.0059 (3)	0.0237 (4)

H2A	0.0028	0.2048	−0.0591	0.028*
C3	−0.11206 (18)	0.22646 (9)	0.0732 (3)	0.0279 (5)
H3	−0.1059	0.2643	0.0548	0.033*
C7	−0.29123 (17)	−0.02432 (10)	0.2950 (3)	0.0263 (5)
H7	−0.3080	0.0108	0.3333	0.032*
C9	−0.33255 (17)	−0.12096 (10)	0.2493 (3)	0.0293 (5)
H9	−0.3762	−0.1503	0.2585	0.035*
C4	−0.18849 (18)	0.20657 (9)	0.1700 (3)	0.0283 (5)
H4	−0.2324	0.2308	0.2171	0.034*
C8	−0.35494 (17)	−0.06760 (11)	0.3087 (3)	0.0296 (5)
H8	−0.4142	−0.0616	0.3584	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag	0.02195 (14)	0.01698 (14)	0.03202 (15)	0.00192 (7)	0.00785 (10)	0.00250 (8)
P1	0.0220 (4)	0.0201 (4)	0.0267 (4)	0.000	0.0106 (3)	0.000
O1	0.0232 (8)	0.0203 (8)	0.0304 (8)	0.0016 (5)	0.0076 (6)	0.0000 (6)
N1	0.0225 (8)	0.0173 (8)	0.0225 (8)	0.0008 (6)	0.0045 (7)	0.0029 (7)
F1	0.0418 (8)	0.0363 (8)	0.0298 (7)	0.0041 (7)	0.0174 (6)	0.0042 (6)
O2	0.0225 (8)	0.0191 (8)	0.0308 (9)	−0.0005 (5)	0.0063 (7)	0.0036 (6)
C6	0.0217 (10)	0.0204 (10)	0.0220 (10)	0.0003 (8)	0.0023 (8)	0.0040 (8)
N2	0.0218 (8)	0.0215 (9)	0.0244 (9)	−0.0021 (7)	0.0062 (7)	0.0015 (7)
C1	0.0198 (9)	0.0201 (10)	0.0186 (9)	−0.0001 (7)	0.0019 (7)	0.0017 (7)
F2	0.0328 (8)	0.0300 (7)	0.0408 (8)	0.0092 (6)	0.0106 (6)	0.0067 (6)
F3	0.0307 (7)	0.0292 (7)	0.0480 (9)	−0.0084 (6)	0.0086 (6)	−0.0009 (6)
C5	0.0239 (10)	0.0258 (11)	0.0228 (10)	0.0027 (8)	0.0055 (8)	0.0020 (8)
C10	0.0327 (11)	0.0213 (10)	0.0245 (10)	−0.0065 (9)	0.0043 (9)	0.0013 (8)
C2	0.0277 (11)	0.0197 (10)	0.0239 (10)	−0.0026 (8)	0.0039 (8)	0.0021 (8)
C3	0.0364 (12)	0.0165 (10)	0.0311 (11)	0.0019 (9)	0.0056 (10)	0.0018 (8)
C7	0.0234 (10)	0.0283 (12)	0.0278 (11)	0.0032 (8)	0.0048 (9)	0.0021 (9)
C9	0.0272 (11)	0.0320 (12)	0.0286 (11)	−0.0115 (9)	0.0025 (9)	0.0052 (9)
C4	0.0316 (12)	0.0234 (11)	0.0312 (11)	0.0070 (9)	0.0092 (9)	−0.0008 (9)
C8	0.0208 (10)	0.0406 (14)	0.0278 (11)	−0.0022 (9)	0.0042 (9)	0.0049 (10)

Geometric parameters (Å, °)

Ag—O1^{i}	2.3543 (19)	C6—C7	1.422 (3)
Ag—O1	2.3543 (19)	N2—C10	1.364 (3)
Ag—O2^{i}	2.5055 (18)	N2—H2	0.8600
Ag—O2	2.5055 (18)	C1—C2	1.427 (3)
Ag—O2^{ii}	2.6278 (19)	C5—C4	1.359 (3)
Ag—O2^{iii}	2.6278 (19)	C5—H5	0.9300
P1—F1	1.5993 (15)	C10—C9	1.356 (3)
P1—F1^{iv}	1.5993 (15)	C10—H10	0.9300
P1—F3^{iv}	1.6026 (15)	C2—C3	1.363 (3)
P1—F3	1.6026 (15)	C2—H2A	0.9300

P1—F2^{iv}	1.6095 (15)	C3—C4	1.405 (3)
P1—F2	1.6095 (15)	C3—H3	0.9300
O1—C1	1.262 (3)	C7—C8	1.367 (3)
N1—C5	1.359 (3)	C7—H7	0.9300
N1—C1	1.370 (3)	C9—C8	1.406 (4)
N1—H1	0.8600	C9—H9	0.9300
O2—C6	1.272 (3)	C4—H4	0.9300
C6—N2	1.368 (3)	C8—H8	0.9300
O1—Ag—O1^{i}	180	C6—O2—Ag	125.40 (14)
O1—Ag—O2	91.09 (5)	O2—C6—N2	118.79 (19)
O1—Ag—O2^{i}	88.91 (5)	O2—C6—C7	125.1 (2)
O1—Ag—O2^{ii}	89.50 (5)	N2—C6—C7	116.14 (19)
O1—Ag—O2^{iii}	90.50 (5)	C10—N2—C6	123.64 (19)
O1^{i}—Ag—O2	88.91 (5)	C10—N2—H2	118.2
O1^{i}—Ag—O2^{i}	91.09 (5)	C6—N2—H2	118.2
O1^{i}—Ag—O2^{ii}	90.50 (5)	O1—C1—N1	119.33 (19)
O1^{i}—Ag—O2^{iii}	89.50 (5)	O1—C1—C2	124.96 (19)
O2—Ag—O2^{i}	180	N1—C1—C2	115.70 (18)
O2—Ag—O2^{ii}	89.18 (5)	N1—C5—C4	120.4 (2)
O2—Ag—O2^{iii}	90.82 (5)	N1—C5—H5	119.8
O2^{i}—Ag—O2^{ii}	90.82 (5)	C4—C5—H5	119.8
O2^{i}—Ag—O2^{iii}	89.18 (5)	C9—C10—N2	120.7 (2)
O2^{ii}—Ag—O2^{iii}	180	C9—C10—H10	119.7
F1—P1—F1^{iv}	179.43 (13)	N2—C10—H10	119.7
F1—P1—F3^{iv}	90.33 (8)	C3—C2—C1	120.7 (2)
F1^{iv}—P1—F3^{iv}	90.07 (8)	C3—C2—H2A	119.7
F1—P1—F3	90.07 (8)	C1—C2—H2A	119.7
F1^{iv}—P1—F3	90.33 (8)	C2—C3—C4	120.8 (2)
F3^{iv}—P1—F3	90.26 (12)	C2—C3—H3	119.6
F1—P1—F2^{iv}	89.82 (8)	C4—C3—H3	119.6
F1^{iv}—P1—F2^{iv}	89.78 (8)	C8—C7—C6	120.3 (2)
F3^{iv}—P1—F2^{iv}	90.03 (8)	C8—C7—H7	119.9
F3—P1—F2^{iv}	179.68 (9)	C6—C7—H7	119.9
F1—P1—F2	89.78 (8)	C10—C9—C8	118.0 (2)
F1^{iv}—P1—F2	89.82 (8)	C10—C9—H9	121.0
F3^{iv}—P1—F2	179.69 (9)	C8—C9—H9	121.0
F3—P1—F2	90.03 (8)	C5—C4—C3	118.5 (2)
F2^{iv}—P1—F2	89.67 (12)	C5—C4—H4	120.7
C1—O1—Ag	130.04 (14)	C3—C4—H4	120.7
C5—N1—C1	123.91 (18)	C7—C8—C9	121.3 (2)
C5—N1—H1	118.0	C7—C8—H8	119.4
C1—N1—H1	118.0	C9—C8—H8	119.4
O2^{i}—Ag—O1—C1	170.23 (18)	C1—N1—C5—C4	−0.7 (3)

O2—Ag—O1—C1	−9.77 (18)	C6—N2—C10—C9	−0.4 (3)
O1^{i}—Ag—O2—C6	−28.01 (17)	O1—C1—C2—C3	−178.6 (2)
O1—Ag—O2—C6	151.99 (17)	N1—C1—C2—C3	1.5 (3)
Ag—O2—C6—N2	20.6 (3)	C1—C2—C3—C4	−0.7 (4)
Ag—O2—C6—C7	−160.21 (16)	O2—C6—C7—C8	−178.1 (2)
O2—C6—N2—C10	178.9 (2)	N2—C6—C7—C8	1.1 (3)
C7—C6—N2—C10	−0.4 (3)	N2—C10—C9—C8	0.5 (3)
Ag—O1—C1—N1	3.3 (3)	N1—C5—C4—C3	1.5 (3)
Ag—O1—C1—C2	−176.67 (15)	C2—C3—C4—C5	−0.8 (4)
C5—N1—C1—O1	179.28 (19)	C6—C7—C8—C9	−1.1 (4)
C5—N1—C1—C2	−0.8 (3)	C10—C9—C8—C7	0.2 (4)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	1.91	2.765 (2)	171
N2—H2···O1^{v}	0.86	1.90	2.754 (3)	174
C3—H3···F1^{vi}	0.93	2.48	3.353 (3)	157
C5—H5···F3^{iv}	0.93	2.51	3.398 (3)	159

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

Fig. 1

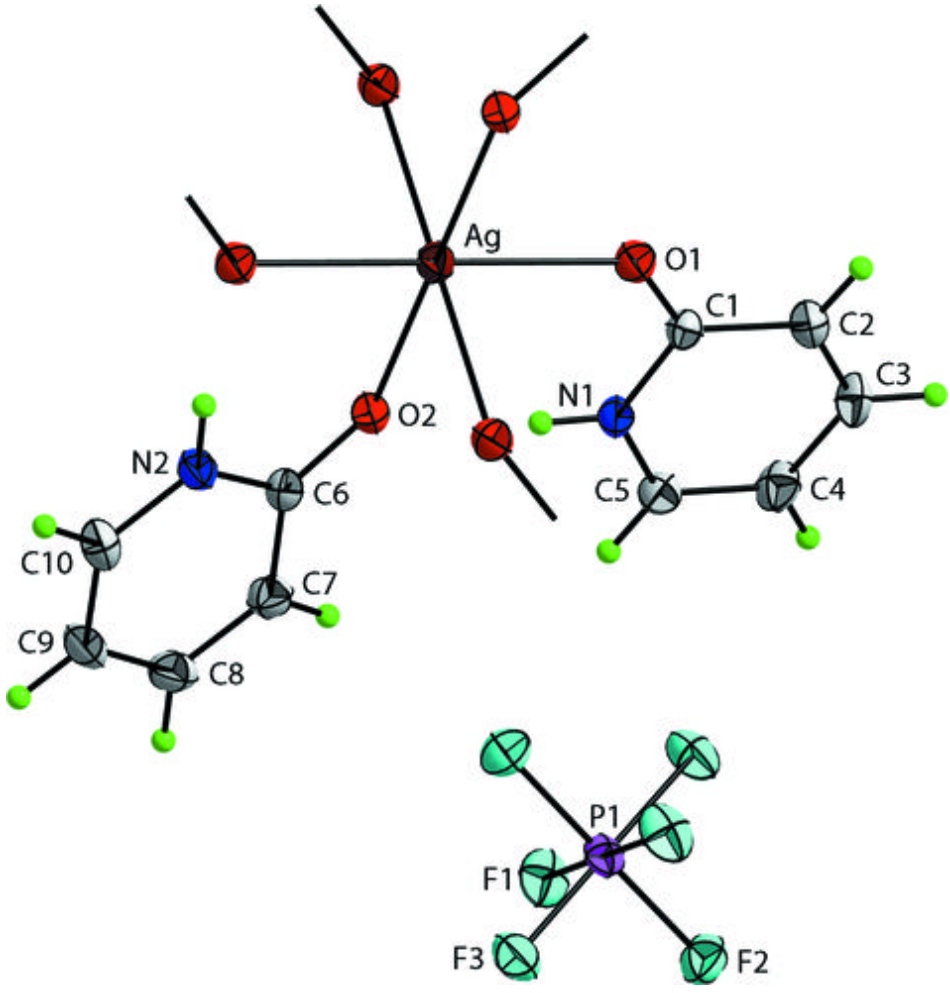

Fig. 2

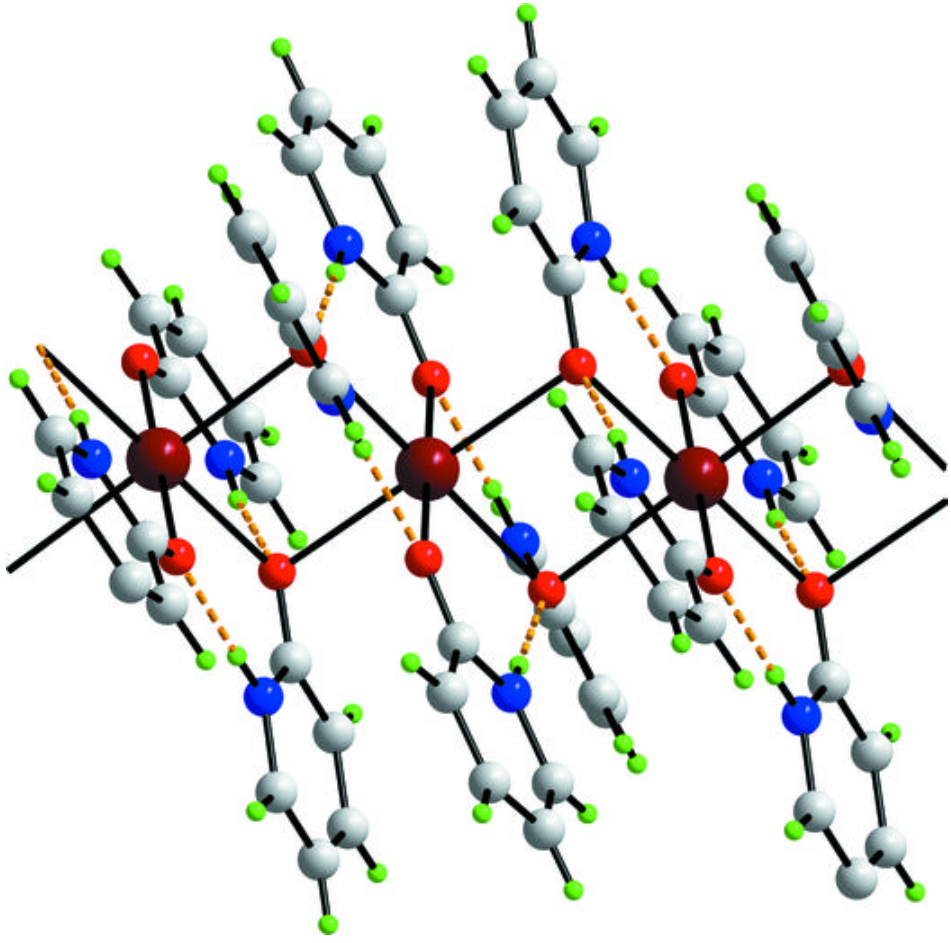

Fig. 3