

Bis(2-aminopyridine- κN^1)silver(I) hexafluoroarsenateHai-Lang Yang,^a Zhong-Lu You^b
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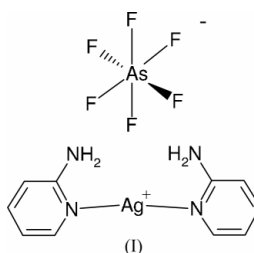
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(C-C) = 0.007$ Å
 R factor = 0.037
 wR factor = 0.098
Data-to-parameter ratio = 12.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, $[Ag(C_5H_6N_2)_2](AsF_6)$, is a mononuclear silver(I) compound. The Ag atom is bicoordinated in a distorted linear configuration by two N atoms from two symmetry-related 2-aminopyridine ligands. In the crystal structure, the molecules are linked by N—H...F intermolecular hydrogen bonds, forming layers parallel to the ac plane.

Comment

Recently, we have reported the structures of a few silver(I) complexes (You, Zhu & Liu, 2004; You, Yang *et al.*, 2004; Zhu *et al.*, 1999, 2000). As an extension of our work on the structural characterization of silver(I) complexes, the title complex, (I), is reported here.



The structure of (I), a mononuclear silver(I) complex, is illustrated in Fig. 1. The asymmetric unit contains one-half of the complex cation, with the other half generated by twofold rotation symmetry, and one-half of a hexafluoroarsenate anion, with the other half related by a crystallographic inversion centre. The Ag and As atoms lie on the crystallographic twofold axis and inversion centre, respectively.

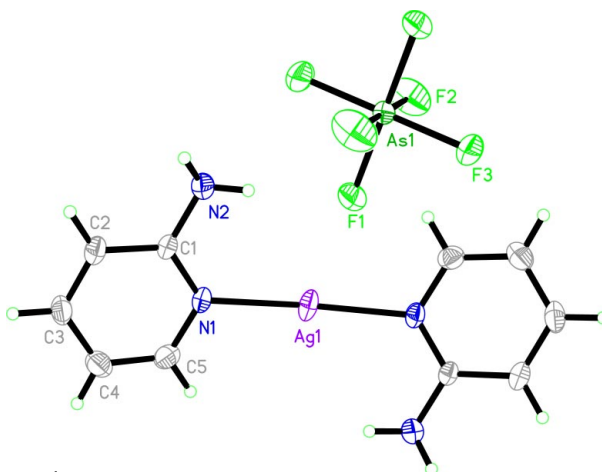


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

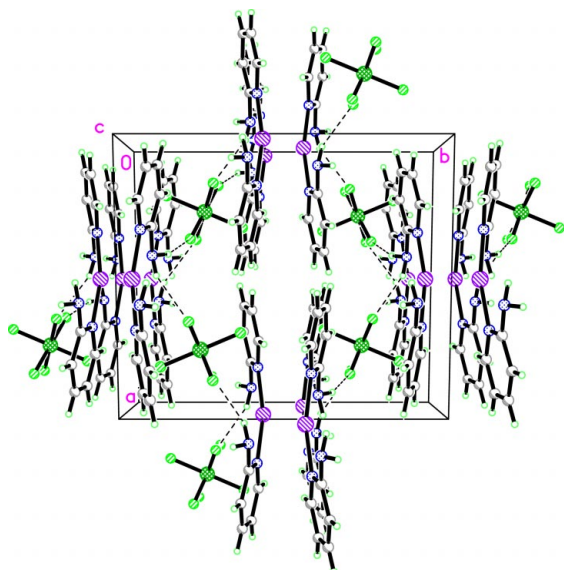


Figure 2
A packing diagram of (I), viewed along the c axis. Hydrogen bonds are shown as dashed lines.

In the cation, the Ag^{I} atom is in a roughly linear coordination environment and is bicoordinated by two N atoms from two symmetry-related 2-aminopyridine ligands. The $\text{N1}-\text{Ag1}-\text{N1}(1-x, y, \frac{1}{2}-z)$ angle is $167.40(17)^\circ$, indicating a significantly distorted linear geometry for atom Ag1 ; this value is comparable to that observed in a similar silver(I) complex [$172.37(8)^\circ$; Zhu *et al.*, 2003]. The $\text{Ag}-\text{N}$ bond length is $2.143(4) \text{ \AA}$, which is comparable to the value observed in another similar complex [$2.148(3) \text{ \AA}$; You, Yang *et al.*, 2004]. In the anion, the central As^{V} atom is coordinated by six F atoms in an octahedral geometry. The three *trans* angles are exactly equal to 180° by symmetry and all other angles around As1 are close to 90° , ranging from $89.4(2)$ to $90.6(2)^\circ$ (Table 1), indicating a very slightly distorted octahedral geometry for atom As1 .

In the crystal structure, the molecules are linked by $\text{N}-\text{H}\cdots\text{F}$ intermolecular hydrogen bonds (Table 2), forming layers parallel to the ac plane (Fig. 2).

Experimental

2-Aminopyridine (0.1 mmol, 9.4 mg) and silver hexafluoroarsenate (0.1 mmol, 29.7 mg) were dissolved in an ammonia solution (10 ml, 30%). The mixture was stirred for 10 min at room temperature to give a clear colourless solution. The resulting solution was kept in air and, after slow evaporation of the solvent over a period of 8 d, large colourless block-shaped crystals of (I) formed at the bottom of the vessel.

Crystal data

$[\text{Ag}(\text{C}_5\text{H}_6\text{N}_2)_2](\text{AsF}_6)$	$D_x = 2.214 \text{ Mg m}^{-3}$
$M_r = 485.03$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 872 reflections
$a = 11.379(2) \text{ \AA}$	$\theta = 2.1\text{--}23.2^\circ$
$b = 12.971(3) \text{ \AA}$	$\mu = 3.71 \text{ mm}^{-1}$
$c = 10.158(2) \text{ \AA}$	$T = 293(2) \text{ K}$
$\beta = 103.90(3)^\circ$	Block, colourless
$V = 1455.3(5) \text{ \AA}^3$	$0.18 \times 0.12 \times 0.11 \text{ mm}$
$Z = 4$	

Data collection

Siemens SMART CCD area-detector diffractometer	1353 independent reflections
ω scans	1210 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.041$
$T_{\text{min}} = 0.555, T_{\text{max}} = 0.686$	$\theta_{\text{max}} = 26.0^\circ$
2453 measured reflections	$h = -10 \rightarrow 14$
	$k = -10 \rightarrow 16$
	$l = -12 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.099$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.95 \text{ e \AA}^{-3}$
1353 reflections	$\Delta\rho_{\text{min}} = -0.76 \text{ e \AA}^{-3}$
111 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: $0.0051(7)$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

$\text{Ag1}-\text{N1}$	$2.143(4)$	$\text{As1}-\text{F3}$	$1.705(3)$
$\text{As1}-\text{F2}$	$1.689(3)$	$\text{As1}-\text{F1}$	$1.722(3)$
$\text{N1}^{\text{i}}-\text{Ag1}-\text{N1}$	$167.40(17)$	$\text{F2}-\text{As1}-\text{F1}^{\text{ii}}$	$89.84(17)$
$\text{F2}-\text{As1}-\text{F2}^{\text{ii}}$	180	$\text{F3}-\text{As1}-\text{F1}^{\text{ii}}$	$89.49(14)$
$\text{F2}-\text{As1}-\text{F3}^{\text{ii}}$	$90.6(2)$	$\text{F2}-\text{As1}-\text{F1}$	$90.16(17)$
$\text{F2}-\text{As1}-\text{F3}$	$89.4(2)$	$\text{F3}-\text{As1}-\text{F1}$	$90.51(14)$
$\text{F3}^{\text{ii}}-\text{As1}-\text{F3}$	180	$\text{F1}^{\text{ii}}-\text{As1}-\text{F1}$	180

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

Table 2

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2B}\cdots\text{F3}^{\text{iii}}$	$0.90(1)$	$2.23(2)$	$3.077(5)$	$158(4)$
$\text{N2}-\text{H2A}\cdots\text{F1}$	$0.90(1)$	$2.32(2)$	$3.163(5)$	$157(4)$

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

Atoms H2A and H2B were located in a difference Fourier map and refined isotropically, with the $\text{N}-\text{H}$ and $\text{H}\cdots\text{H}$ distances restrained to $0.90(1)$ and $1.43(2) \text{ \AA}$, respectively. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with $\text{C}-\text{H}$ distances of 0.93 \AA , and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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