

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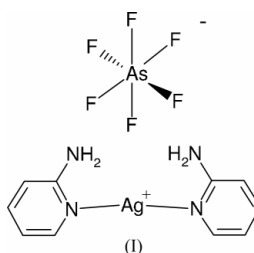
Key indicators

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.

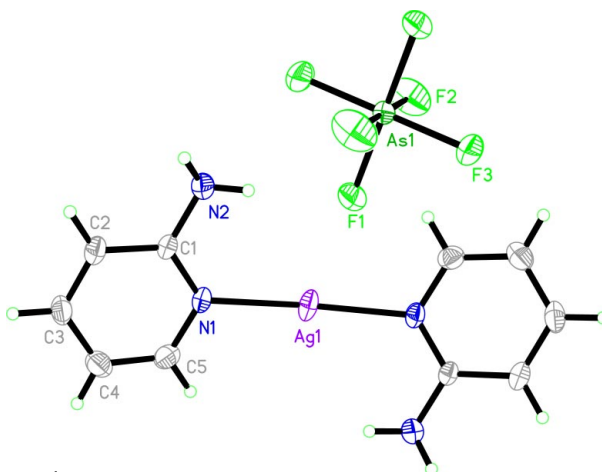


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

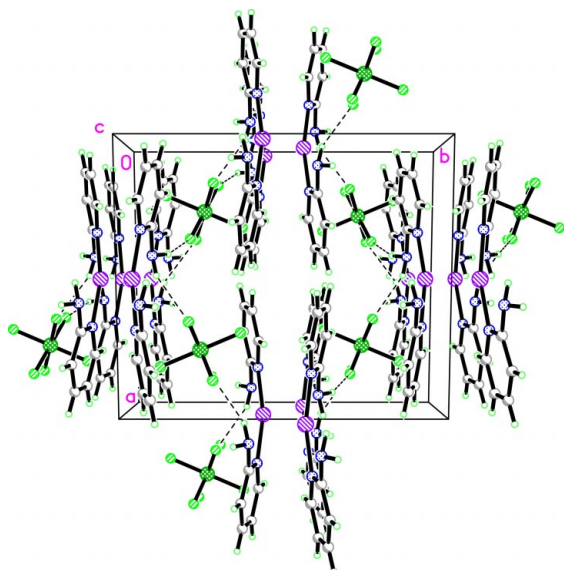


Figure 2
A packing diagram of (I), viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

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 N1—Ag1—N1(1 - *x*, *y*, $\frac{1}{2} - z$) angle is 167.40 (17)°, 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)°; Zhu *et al.*, 2003]. The Ag—N bond length is 2.143 (4) Å, which is comparable to the value observed in another similar complex [2.148 (3) Å; 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)° (Table 1), indicating a very slightly distorted octahedral geometry for atom As1.

In the crystal structure, the molecules are linked by N—H...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

[Ag(C ₅ H ₆ N ₂) ₂](AsF ₆)	<i>D_x</i> = 2.214 Mg m ⁻³
<i>M_r</i> = 485.03	Mo Kα radiation
Monoclinic, <i>C</i> 2/ <i>c</i>	Cell parameters from 872 reflections
<i>a</i> = 11.379 (2) Å	<i>θ</i> = 2.1–23.2°
<i>b</i> = 12.971 (3) Å	<i>μ</i> = 3.71 mm ⁻¹
<i>c</i> = 10.158 (2) Å	<i>T</i> = 293 (2) K
<i>β</i> = 103.90 (3)°	Block, colourless
<i>V</i> = 1455.3 (5) Å ³	0.18 × 0.12 × 0.11 mm
<i>Z</i> = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	1353 independent reflections
<i>ω</i> scans	1210 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R_{int}</i> = 0.041
<i>T_{min}</i> = 0.555, <i>T_{max}</i> = 0.686	<i>θ_{max}</i> = 26.0°
2453 measured reflections	<i>h</i> = -10 → 14
	<i>k</i> = -10 → 16
	<i>l</i> = -12 → 11

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.099$	(Δ/ <i>σ</i>) _{max} < 0.001
<i>S</i> = 1.08	Δ <i>ρ</i> _{max} = 0.95 e Å ⁻³
1353 reflections	Δ <i>ρ</i> _{min} = -0.76 e Å ⁻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 (Å, °).

Ag1—N1	2.143 (4)	As1—F3	1.705 (3)
As1—F2	1.689 (3)	As1—F1	1.722 (3)
N1 ⁱ —Ag1—N1	167.40 (17)	F2—As1—F1 ⁱⁱ	89.84 (17)
F2—As1—F2 ⁱⁱⁱ	180	F3—As1—F1 ⁱⁱ	89.49 (14)
F2—As1—F3 ⁱⁱ	90.6 (2)	F2—As1—F1	90.16 (17)
F2—As1—F3	89.4 (2)	F3—As1—F1	90.51 (14)
F3 ⁱⁱ —As1—F3	180	F1 ⁱⁱ —As1—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 (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2B...F3 ⁱⁱⁱ	0.90 (1)	2.23 (2)	3.077 (5)	158 (4)
N2—H2A...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 N—H and H...H distances restrained to 0.90 (1) and 1.43 (2) Å, respectively. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å, and with *U*_{iso}(H) = 1.2*U*_{eq}(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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