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**Key indicators**

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$   
 R factor = 0.057  
 wR factor = 0.178  
 Data-to-parameter ratio = 13.0

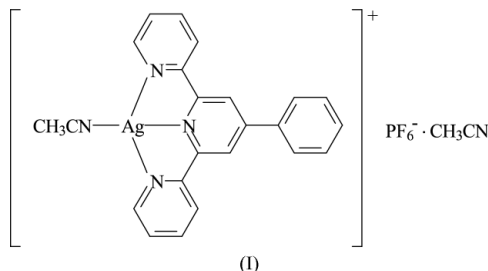
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

**(Acetonitrile- $\kappa N$ )(4'-phenyl-2,2':6',2''-terpyridine- $\kappa^3 N$ )silver(I) hexafluorophosphate acetonitrile solvate**

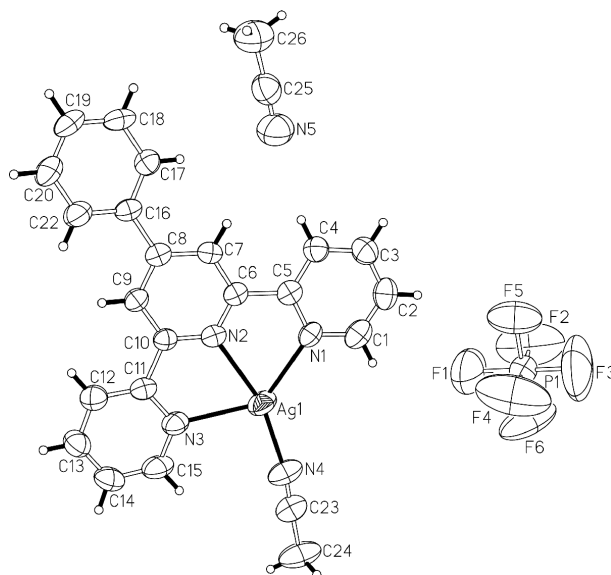
In the title complex,  $[\text{Ag}(\text{C}_2\text{H}_3\text{N})(\text{C}_{21}\text{H}_{15}\text{N}_3)]\text{PF}_6 \cdot \text{CH}_3\text{CN}$ , the  $\text{Ag}^{\text{I}}$  atom is coordinated by a tridentate chelating 4'-phenyl-2,2':6',2''-terpyridine ligand and an acetonitrile molecule, to form a distorted square-planar geometry.

**Comment**

We have previously demonstrated that 4'-phenyl-2,2':6',2''-terpyridine acts as a chelating tridentate ligand when coordinating to  $\text{Cu}^{\text{I}}$ , to form a five-coordinate copper complex (Feng *et al.*, 2002). In this work, the ligand is used to coordinate to  $\text{Ag}^{\text{I}}$ , giving the title complex, (I).



In complex (I) (Fig. 1), the Ag centre is coordinated by three N atoms from the 4'-phenyl-2,2':6',2''-terpyridine ligand and an N atom of the acetonitrile, showing an essentially square-planar geometry with constraints imposed by the



**Figure 1**  
 A view of the asymmetric unit of (I), showing the atom-labelling scheme and with 50% probability displacement ellipsoids. H atoms are drawn as small spheres of arbitrary radii.

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4'-phenyl-2,2':6',2''-terpyridyl ligand. The sum of the angles about the Ag atom is 360.0°.

It has been shown that 2,2':6',2''-terpyridine-analogue ligands and Ag<sup>I</sup> form a series of dinuclear and polynuclear molecules *via* Ag<sup>I</sup>··Ag interactions. The anions and solvents, and the additional steric constraints of the substituents, are some of the factors which influence the coordination and aggregation architecture of Ag<sup>I</sup>-terpyridine systems (Baum *et al.*, 1998; Constable *et al.*, 1998; Hannon *et al.*, 2002). In the present study, a donor solvent, CH<sub>3</sub>CN, was used. It is not surprising that only a mononuclear Ag<sup>I</sup> complex was obtained.

## Experimental

The 4'-phenyl-2,2':6',2''-terpyridine ligand was synthesized according to the method of Constable *et al.* (1990). To an acetone solution (10 ml) of AgPF<sub>6</sub> (0.0253 g, 0.1 mmol) was added 4'-phenyl-2,2':6',2''-terpyridine (0.0390 g, 0.1 mmol). A yellow precipitate was formed after stirring for 3 h and this was isolated by filtration. A solution of the resulting solid in acetonitrile was allowed to stand for 5 d and yellow prismatic crystals of (I) were obtained (yield 55%).

### Crystal data

[Ag(C <sub>2</sub> H <sub>3</sub> N)(C <sub>21</sub> H <sub>15</sub> N <sub>3</sub> )]PF <sub>6</sub> ·C <sub>2</sub> H <sub>3</sub> N	$D_x = 1.676 \text{ Mg m}^{-3}$
$M_r = 644.31$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 1971 reflections
$a = 16.777 (1) \text{ \AA}$	$\theta = 2.4\text{--}20.3^\circ$
$b = 7.8257 (6) \text{ \AA}$	$\mu = 0.92 \text{ mm}^{-1}$
$c = 19.447 (1) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 90.356 (2)^\circ$	Prism, yellow
$V = 2553.2 (3) \text{ \AA}^3$	$0.20 \times 0.18 \times 0.12 \text{ mm}$
$Z = 4$	

### Data collection

Bruker APEX CCD area-detector diffractometer	4488 independent reflections
$\varphi$ and $\omega$ scans	3262 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.038$
$T_{\text{min}} = 0.354$ , $T_{\text{max}} = 0.898$	$\theta_{\text{max}} = 25.0^\circ$
12 897 measured reflections	$h = -17 \rightarrow 19$
	$k = -9 \rightarrow 9$
	$l = -20 \rightarrow 23$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0996P)^2 + 1.6223P]$
$R[F^2 > 2\sigma(F^2)] = 0.057$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.178$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 1.06 \text{ e \AA}^{-3}$
4488 reflections	$\Delta\rho_{\text{min}} = -0.42 \text{ e \AA}^{-3}$
345 parameters	
H-atom parameters constrained	

**Table 1**

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

Ag1—N1	2.348 (5)	Ag1—N3	2.470 (5)
Ag1—N2	2.378 (4)	Ag1—N4	2.187 (6)
N1—Ag1—N2	69.3 (1)	N2—Ag1—N3	67.1 (2)
N1—Ag1—N3	136.4 (2)	N2—Ag1—N4	163.4 (2)
N1—Ag1—N4	127.2 (2)	N3—Ag1—N4	96.4 (2)

The reported transmission factors are those calculated by SADABS (Bruker, 2002), which treats other effects simultaneously with absorption as part of the interframe scaling process. H atoms were placed in calculated positions [ $\text{C—H} = 0.93 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for phenyl H atoms, and  $\text{C—H} = 0.96 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms], and were included in the refinement in the riding-model approximation. The methyl groups were allowed to rotate as rigid groups. The final difference map had a significant peak near atom F3, but was otherwise featureless.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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