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# *catena*-Poly[[[(dihydrogenphosphato)silver(I)]-$\mu$-4,4′-bipyridine] dihydrate]

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.020 Å
$R$ factor = 0.091
$wR$ factor = 0.328
Data-to-parameter ratio = 17.2

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

The crystal structure of the title complex, $\{[Ag(H_2PO_4)(C_{10}H_8N_2)]\cdot 2H_2O\}_n$, reveals a T-shaped geometry for the $Ag^I$ atom [N—Ag—N = 164.8 (5)°, and O—Ag—N = 100.0 (4) and 95.2 (2)°], coordinated by two N atoms from two 4,4′-bipyridine molecules and an O atom from a $H_2PO_4^-$ counter-ion. The silver–4,4′-bipyridine connectivity results in polymeric chains.

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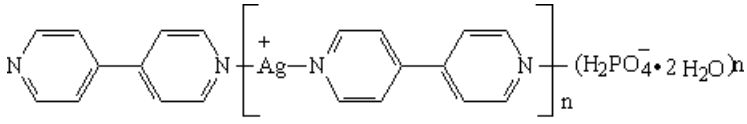
## Comment

The title compound, (I), has been prepared and characterized as part of our ongoing studies of complexes of silver(I) with 4,4′-bipyridine and related ligands (Wang *et al.*, 2004).




(I)

The Ag atom in (I) (Fig. 1) is coordinated by two N atoms from two 4,4′-bipyridine units and an O atom from a $H_2PO_4^-$ counter-ion in a T-shaped geometry (Table 1). The N—Ag—N and N—Ag—O angles are consistent with those in related compounds (Yang *et al.*, 2001). Each 4,4′-bipyridine unit is bonded to two Ag atoms, resulting in a polymeric chain (Fig. 2). The chains propagate along [201]. The bond lengths and angles in the pyridine rings are consistent with those in related compounds. The dihedral angle between the N1- and N2-containing rings is 2.6 (2)°, indicating approximate coplanarity.

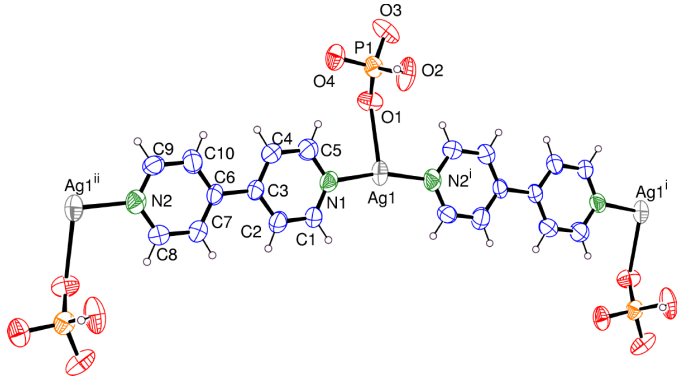



**Figure 1**
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms) and water molecules are omitted for clarity. Symmetry codes: (i) as in Table 1; (ii) $x-1, -y, z-\frac{1}{2}$.]

The shortest Ag···Ag distance between silver atoms in adjacent chains is 3.874 (4) Å. This value is longer than the sum of the van der Waals radii of two Ag atoms (3.44 Å; Bondi, 1964), indicating that no metal–metal interactions occur in (I).

## Experimental

A $CH_3CN$ solution (10 ml) of 4,4′-bipyridine (1 mmol, 0.156 g) was added dropwise to a stirred MeCN–$H_2O$ solution (10 ml) of $Ag(H_2PO_4)$ (0.205 g, 1 mmol). After 3 d at room temperature, the solution yielded colorless plate-shaped crystals of (I) in 75% yield.

*Crystal data*

$[Ag(H_2PO_4)(C_{10}H_8N_2)]\cdot 2H_2O$
$M_r$ = 397.07
Monoclinic, $P2/c$
$a$ = 8.566 (6) Å
$b$ = 8.807 (7) Å
$c$ = 18.729 (17) Å
$\beta$ = 101.37°
$V$ = 1385.2 (19) Å$^3$
$Z$ = 4
$D_x$ = 1.904 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 4–27°
$\mu$ = 1.60 mm$^{-1}$
$T$ = 293 (2) K
Plate, colorless
0.20 × 0.10 × 0.08 mm

*Data collection*

Siemens $R3m$ diffractometer
$\omega$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.843, $T_{max}$ = 0.880
3174 measured reflections
2939 independent reflections
1618 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 28.0°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 11$
$l = -24 \rightarrow 24$
2 standard reflections
every 118 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.091
$wR(F^2)$ = 0.328
$S$ = 1.09
2939 reflections
171 parameters
H-atom parameters constrained
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.08 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ag1—N1 | 2.148 (12) | Ag1—O1 | 2.639 (10) |
| Ag1—N2$^{i}$ | 2.168 (14) | | |
| N1—Ag1—N2$^{i}$ | 164.8 (5) | N2$^{i}$—Ag1—O1 | 95.2 (2) |
| N1—Ag1—O1 | 100.0 (4) | | |

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

Crystals of (I) were small and diffraction quality was very poor, resulting in high values for the refinement residuals. The percentage of unique data is also very low, at about 82%. The H atoms of the pyridine rings were positioned geometrically (C—H = 0.96 Å) and refined using the riding-model approximation, with $U_{iso}$(H) = 0.08 Å$^2$. One water H atom was positioned geometrically (O—H = 0.85 Å) and the other H atoms of water were found in Fourier maps and refined by riding in their as-found relative positions, with $U_{iso}$(H) = 0.05 Å$^2$. This led to some very short H···H intermolecular contacts ($d$ < 1.80 Å) and the positions of the water H atoms should be regarded as tentative. The maximum and minimum electron-density peaks were found at distances of 0.87 Å and 0.57 Å from atoms Ag1 and OW1, respectively.

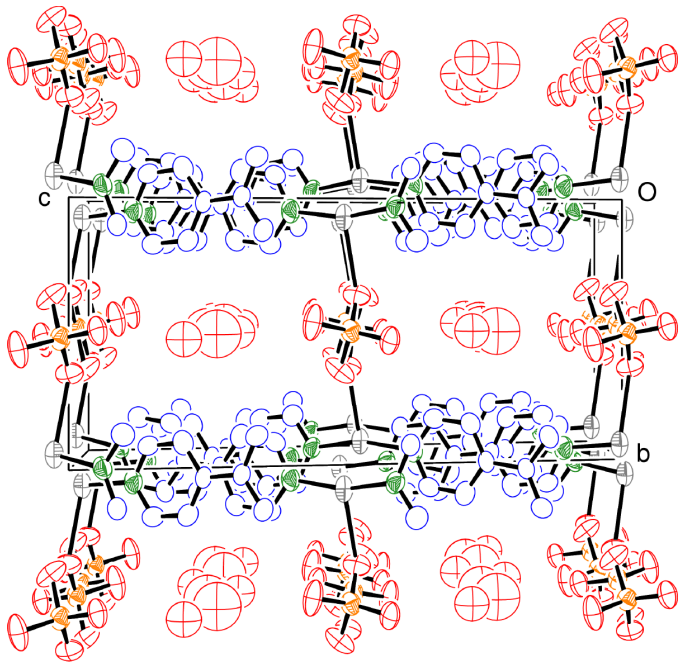



**Figure 2**
The packing in (I), viewed approximately down the $a$ axis, with H atoms omitted for clarity.

Data collection: *R3m Software* (Siemens, 1990); cell refinement: *R3m Software*; data reduction: *SHELXTL-Plus* (Sheldrick, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL*97.

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