

catena-Poly[[trifluoromethylphosphane- κP]-silver(I)- μ -4,4'-bipyridine- $\kappa^2 N:N'$ -[(trifluoromethylphosphane- κP)silver(I)]-di- μ -chlorido]

Xiao-Ming Song,^a Feng Hu,^b Hua-Tian Shi,^b Qun Chen^a and Qian-Feng Zhang^{b,a*}

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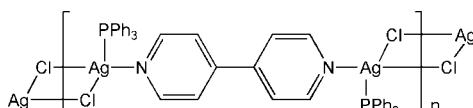
Received 8 May 2013; accepted 21 May 2013

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.039; wR factor = 0.092; data-to-parameter ratio = 19.7.

In the title coordination polymer, $[Ag_2Cl_2(C_{10}H_8N_2)-(C_{18}H_{15}P)_2]_n$, the Ag^I cation is coordinated by a 4,4'-bipyridine N atom, a trifluoromethylphosphane P atom and two Cl^- anions in a distorted tetrahedral geometry. The 4,4'-bipyridine and Cl^- anions bridge the Ag^I cations, forming polymeric chains running along [21̄]. In the crystal, weak C–H···Cl interactions link the polymeric chains into a three-dimensional supramolecular architecture.

Related literature

For background to silver coordination polymers, see: Hung-Low & Klausmeyer (2008); Mishra *et al.* (2007); Pyykkö (2004); Yam & Lo (1999); Zaworotko (1994). For related structures, see: Lu *et al.* (1997); Sampanthar & Vittal (2000); Sun *et al.* (2009).



Experimental

Crystal data

$[Ag_2Cl_2(C_{10}H_8N_2)(C_{18}H_{15}P)_2]$

$M_r = 967.36$

Triclinic, $P\bar{1}$

$a = 9.1042 (16)$ Å

$b = 13.887 (2)$ Å

$c = 17.826 (3)$ Å

$\alpha = 70.753 (3)^\circ$

$\beta = 79.332 (4)^\circ$

$\gamma = 75.190 (3)^\circ$

$V = 2044.5 (6)$ Å 3

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.20$ mm $^{-1}$
 $T = 296$ K

0.23 × 0.17 × 0.14 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
 $T_{min} = 0.770$, $T_{max} = 0.850$

14039 measured reflections
9594 independent reflections
6338 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.092$
 $S = 1.01$
9594 reflections

487 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.59$ e Å $^{-3}$
 $\Delta\rho_{\text{min}} = -0.44$ e Å $^{-3}$

Table 1
Selected bond lengths (Å).

Ag1—P1	2.4069 (9)	Ag2—P2	2.4162 (9)
Ag1—N1	2.430 (3)	Ag2—N2	2.386 (3)
Ag1—Cl1	2.5709 (10)	Ag2—Cl2	2.6111 (9)
Ag1—Cl1 ⁱ	2.6639 (10)	Ag2—Cl2 ⁱⁱ	2.6809 (10)

Symmetry codes: (i) $-x + 1$, $-y + 2$, $-z + 1$; (ii) $-x - 1$, $-y + 1$, $-z + 2$.

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C9—H9···Cl2 ⁱⁱⁱ	0.93	2.82	3.669 (4)	153

Symmetry code: (iii) $x + 1$, y , z .

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5704).

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supporting information

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S1. Comment

There has been an extensive interest in d^{10} metal complexes with phosphane ligands due to their potential application in luminescence (Yam & Lo, 1999), for this important reason, the study of d^{10} "closed-shell" interactions that exist between the monovalent elements of group 11 has been active for many years (Pyykko, 2004). Actually, these metal-metal interactions are typically associated with the ligand-bridged, hydrogen-bonded and pi-pi stacked effects, which may result in formation of supramolecular assemblies (Mishra *et al.*, 2007; Zaworotko, 1994). Metal coordination polymers with linear spacer ligands have been exploited by many research workers to construct a variety of network structures. Specifically silver(I) ion has been extensively used in inorganic crystal engineering using self-assembly of tailored building-blocks (Hung-Low & Klausmeyer, 2008). In recent decade, self-assembly of silver(I) salts with different aliphatic dinitrile ligands such as 4,4'-bipyridyl (4,4'-bpy) have also been successfully made resulting into novel coordination polymers (Sampanthar & Vittal, 2000). With this in mind, we have chosen a simple AgCl salt and a linear spacer 4,4'-bpy and allowed them to react separately with PPh_3 as an ancillary ligand. The results of this work are reported in this paper.

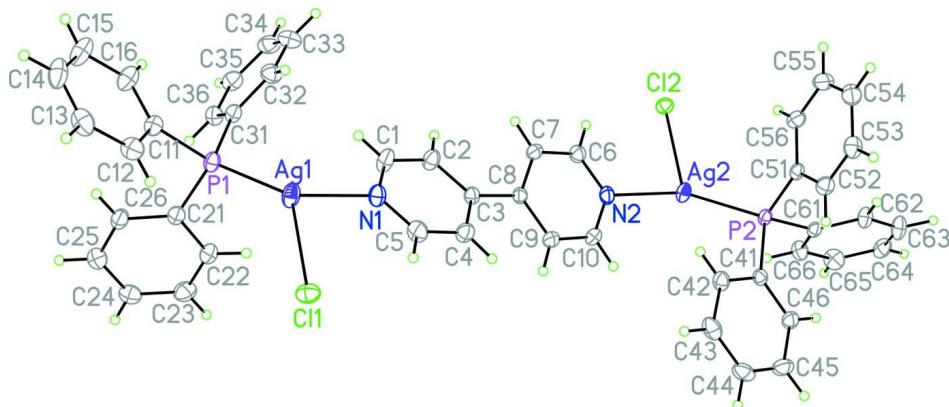
The title coordination polymer crystallizes in the triclinic centrosymmetric *P*-1 space group with $Z = 2$ as it contains one half molecule in an asymmetric unit. A view of the structure of building block in the title polymeric complex is depicted in Fig. 1. The structure consists of $\{(\mu\text{-Cl})(\text{AgPPh}_3)\}_2$ units bridged by 4,4'-bipy ligands to form a zig-zig infinite chain, as shown in Fig. 2. This structure is isostructural to $[(\mu\text{-4,4'-bipy})(\mu\text{-I})_2(\text{AgPPh}_3)_2]_n$ (Sampanthar & Vittal, 2000) and $[(\mu\text{-4,4'-bipy})(\mu\text{-Cl})_2(\text{CuPPh}_3)_2]_n$ (Lu *et al.*, 1997). The coordination polymer possesses to the crystallographic inversion center through the middle of Ag_2Cl_2 squares. Two pyridine rings in the 4,4'-bipy are non-planar with dihedral angle of 22.4 (3) $^\circ$. The average $\text{Ag}\cdots\text{Ag}$ distance in the Ag_2Cl_2 ring is 3.392 (1) Å, which is slightly longer than that of 3.139 (1) Å in $[(\mu\text{-4,4'-bipy})(\mu\text{-I})_2(\text{AgPPh}_3)_2]_n$ (Sampanthar & Vittal, 2000). Each silver(I) ion in the title coordination polymer is coordinated by one nitrogen atom of 4,4'-bipy ligand, one phosphorous atom of PPh_3 ligand and two chloride atoms, leading to the distorted tetrahedron with the angles around silver varying from 94.24 (7) $^\circ$ to 130.08 (3) $^\circ$. Two silver(I) ions are separated by 4,4'-bipy groups at a distances of 10.957 (1) Å along with axial direction. The average $\text{Ag}-\text{N}$ and $\text{Ag}-\text{P}$ bond lengths are 2.408 (3) Å and 2.4116 (9) Å, respectively, which almost similar to the values reported in the related other complexes (Sampanthar & Vittal, 2000, Sun *et al.*, 2009). The $\text{Ag}-\text{Cl}-\text{Ag}$ angles of 97.37 (3) $^\circ$ and 102.05 (2) $^\circ$ in the title coordination polymer are obviously larger than the $\text{Ag}-\text{I}-\text{Ag}$ angle of 66.27 (1) $^\circ$ in $[(\mu\text{-4,4'-bipy})(\mu\text{-I})_2(\text{AgPPh}_3)_2]_n$ (Sampanthar & Vittal, 2000).

S2. Experimental

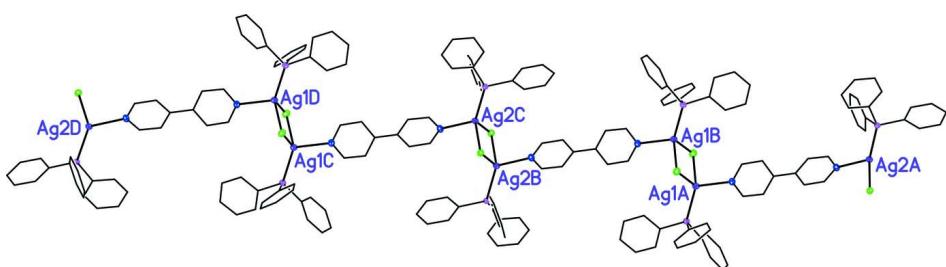
AgCl (0.080 g, 0.56 mmol) and PPh₃ (0.162 g, 0.62 mmol) were mixed together and stirred in a mixture of CH₂Cl₂ (15 mL) and MeCN (5 mL) for 45 min to get a clear solution. An MeCN solution (5 mL) of 4,4'-bipyridyl (0.043 g, 0.28 mmol) was added slowly to the above solution with stirring. The clear solution was filtered and left for slow evaporation. Colorless crystals were collected by decanting the solvent and washed with MeOH (5 mL) and Et₂O (5 x 2 mL) then air-dried. Yield: 157 mg, 58 %. Analysis for C₄₆H₃₈N₂Cl₂P₂Ag₂: calcd C 57.11, H 3.96, N 2.90 %; found C 57.07, H 4.03, N 2.88 %.

S3. Refinement

H atoms were placed in geometrically idealized positions and refined in riding model with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

The structure of the title coordination polymer, showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level.

**Figure 2**

A view the $[(\mu\text{-}4,4'\text{-bipy})(\mu\text{-Cl})_2(\text{AgPPh}_3)_2]_n$ chain, four unit cells along as drawn by ORTEP with 50% probability level.

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Crystal data

$M_r = 967.36$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 9.1042 (16)$ Å

$$b = 13.887 (2) \text{ Å}$$

$$c = 17.826 (3) \text{ Å}$$

$$\alpha = 70.753 (3)^\circ$$

$$\beta = 79.332 (4)^\circ$$

$$\gamma = 75.190 (3)^\circ$$

$V = 2044.5 (6) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 972$
 $D_x = 1.571 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Cell parameters from 4454 reflections

$\theta = 2.3\text{--}28.9^\circ$
 $\mu = 1.20 \text{ mm}^{-1}$
 $T = 296 \text{ K}$
Block, light yellow
 $0.23 \times 0.17 \times 0.14 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2001)
 $T_{\min} = 0.770$, $T_{\max} = 0.850$

14039 measured reflections
9594 independent reflections
6338 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 $\theta_{\max} = 29.2^\circ$, $\theta_{\min} = 1.6^\circ$
 $h = -10 \rightarrow 12$
 $k = -12 \rightarrow 19$
 $l = -15 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.092$
 $S = 1.01$
9594 reflections
487 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0251P)^2 + 1.3705P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.59 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.44 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.34094 (3)	1.07363 (2)	0.539814 (18)	0.05839 (9)
Ag2	-0.34478 (3)	0.431910 (18)	0.960631 (16)	0.05064 (8)
Cl1	0.59763 (10)	0.97839 (8)	0.59551 (5)	0.0607 (2)
Cl2	-0.60355 (9)	0.52295 (6)	0.90046 (5)	0.04829 (19)
P1	0.20766 (10)	1.25225 (6)	0.52007 (5)	0.0454 (2)
P2	-0.21810 (8)	0.25279 (6)	0.97259 (5)	0.03729 (17)
N1	0.1967 (3)	0.9471 (2)	0.62893 (17)	0.0524 (7)
N2	-0.2206 (3)	0.5717 (2)	0.88543 (16)	0.0469 (6)
C1	0.0440 (4)	0.9661 (3)	0.6366 (2)	0.0638 (10)
H1	-0.0076	1.0305	0.6071	0.077*
C2	-0.0412 (4)	0.8954 (3)	0.6859 (2)	0.0558 (9)

H2	-0.1473	0.9127	0.6886	0.067*
C3	0.0305 (3)	0.7994 (2)	0.73101 (18)	0.0416 (7)
C4	0.1897 (4)	0.7796 (3)	0.7233 (2)	0.0559 (9)
H4	0.2444	0.7161	0.7524	0.067*
C5	0.2660 (4)	0.8549 (3)	0.6722 (2)	0.0608 (10)
H5	0.3723	0.8397	0.6680	0.073*
C6	-0.2807 (4)	0.6486 (3)	0.8242 (2)	0.0490 (8)
H6	-0.3798	0.6521	0.8155	0.059*
C7	-0.2039 (4)	0.7233 (2)	0.77318 (19)	0.0468 (8)
H7	-0.2510	0.7751	0.7313	0.056*
C8	-0.0565 (3)	0.7208 (2)	0.78454 (18)	0.0391 (7)
C9	0.0055 (4)	0.6417 (3)	0.8484 (2)	0.0530 (9)
H9	0.1040	0.6365	0.8589	0.064*
C10	-0.0804 (4)	0.5706 (3)	0.8963 (2)	0.0555 (9)
H10	-0.0366	0.5184	0.9390	0.067*
C11	0.2506 (4)	1.3467 (3)	0.42354 (19)	0.0480 (8)
C12	0.4036 (4)	1.3413 (3)	0.3919 (2)	0.0631 (10)
H12	0.4798	1.2891	0.4181	0.076*
C13	0.4405 (5)	1.4153 (4)	0.3205 (2)	0.0745 (12)
H13	0.5423	1.4133	0.2995	0.089*
C14	0.3284 (7)	1.4907 (3)	0.2812 (3)	0.0820 (14)
H14	0.3544	1.5396	0.2336	0.098*
C15	0.1790 (6)	1.4946 (3)	0.3112 (2)	0.0799 (13)
H15	0.1029	1.5451	0.2835	0.096*
C16	0.1408 (5)	1.4234 (3)	0.3828 (2)	0.0637 (10)
H16	0.0387	1.4275	0.4037	0.076*
C21	0.2366 (3)	1.3116 (3)	0.5928 (2)	0.0460 (7)
C22	0.2340 (5)	1.2515 (3)	0.6731 (2)	0.0629 (10)
H22	0.2216	1.1830	0.6877	0.075*
C23	0.2498 (5)	1.2930 (4)	0.7306 (2)	0.0761 (12)
H23	0.2447	1.2530	0.7840	0.091*
C24	0.2731 (5)	1.3926 (4)	0.7100 (3)	0.0721 (11)
H24	0.2849	1.4200	0.7491	0.087*
C25	0.2789 (5)	1.4516 (3)	0.6310 (3)	0.0729 (11)
H25	0.2951	1.5191	0.6165	0.087*
C26	0.2608 (4)	1.4113 (3)	0.5732 (2)	0.0577 (9)
H26	0.2649	1.4520	0.5200	0.069*
C31	0.0001 (4)	1.2669 (2)	0.52947 (19)	0.0445 (7)
C32	-0.0577 (4)	1.2105 (3)	0.4944 (2)	0.0605 (9)
H32	0.0088	1.1696	0.4651	0.073*
C33	-0.2136 (5)	1.2147 (4)	0.5027 (3)	0.0779 (12)
H33	-0.2515	1.1756	0.4803	0.093*
C34	-0.3120 (5)	1.2778 (4)	0.5448 (2)	0.0697 (11)
H34	-0.4167	1.2810	0.5507	0.084*
C35	-0.2569 (4)	1.3350 (3)	0.5774 (2)	0.0602 (9)
H35	-0.3240	1.3783	0.6046	0.072*
C36	-0.1008 (4)	1.3293 (3)	0.5703 (2)	0.0510 (8)
H36	-0.0640	1.3682	0.5935	0.061*

C41	-0.0208 (3)	0.2281 (2)	0.99274 (19)	0.0405 (7)
C42	0.0690 (4)	0.2968 (3)	0.9441 (2)	0.0515 (8)
H42	0.0294	0.3501	0.9007	0.062*
C43	0.2169 (4)	0.2874 (3)	0.9591 (3)	0.0659 (11)
H43	0.2756	0.3344	0.9262	0.079*
C44	0.2764 (4)	0.2080 (3)	1.0228 (3)	0.0658 (11)
H44	0.3754	0.2015	1.0334	0.079*
C45	0.1892 (4)	0.1383 (3)	1.0709 (2)	0.0639 (10)
H45	0.2300	0.0839	1.1134	0.077*
C46	0.0410 (4)	0.1492 (3)	1.0561 (2)	0.0509 (8)
H46	-0.0177	0.1025	1.0894	0.061*
C51	-0.2043 (3)	0.2094 (2)	0.88489 (18)	0.0390 (7)
C52	-0.0742 (4)	0.1461 (3)	0.8581 (2)	0.0512 (8)
H52	0.0140	0.1270	0.8834	0.061*
C53	-0.0759 (4)	0.1116 (3)	0.7940 (2)	0.0590 (9)
H53	0.0108	0.0685	0.7769	0.071*
C54	-0.2042 (5)	0.1402 (3)	0.7555 (2)	0.0654 (10)
H54	-0.2037	0.1174	0.7119	0.078*
C55	-0.3335 (5)	0.2025 (3)	0.7812 (2)	0.0658 (10)
H55	-0.4212	0.2207	0.7556	0.079*
C56	-0.3337 (4)	0.2382 (3)	0.8448 (2)	0.0524 (8)
H56	-0.4209	0.2817	0.8611	0.063*
C61	-0.3002 (3)	0.1526 (2)	1.05223 (18)	0.0392 (7)
C62	-0.3049 (4)	0.0577 (3)	1.0440 (2)	0.0542 (9)
H62	-0.2648	0.0424	0.9963	0.065*
C63	-0.3694 (5)	-0.0147 (3)	1.1068 (2)	0.0696 (11)
H63	-0.3700	-0.0789	1.1015	0.084*
C64	-0.4319 (4)	0.0076 (3)	1.1765 (2)	0.0632 (10)
H64	-0.4768	-0.0406	1.2180	0.076*
C65	-0.4280 (5)	0.1006 (3)	1.1847 (2)	0.0688 (11)
H65	-0.4692	0.1153	1.2325	0.083*
C66	-0.3637 (4)	0.1737 (3)	1.1232 (2)	0.0551 (9)
H66	-0.3631	0.2374	1.1296	0.066*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.04979 (16)	0.03807 (14)	0.0748 (2)	-0.00268 (11)	0.00765 (13)	-0.01311 (13)
Ag2	0.04678 (15)	0.03340 (13)	0.06182 (17)	-0.00289 (10)	0.00090 (12)	-0.00901 (11)
Cl1	0.0483 (5)	0.0784 (6)	0.0510 (5)	-0.0104 (4)	-0.0062 (4)	-0.0153 (4)
Cl2	0.0403 (4)	0.0520 (5)	0.0485 (5)	-0.0089 (3)	-0.0058 (3)	-0.0095 (4)
P1	0.0429 (4)	0.0348 (4)	0.0514 (5)	-0.0040 (3)	0.0009 (4)	-0.0100 (4)
P2	0.0322 (4)	0.0296 (4)	0.0454 (5)	-0.0046 (3)	-0.0019 (3)	-0.0078 (3)
N1	0.0519 (17)	0.0442 (16)	0.0566 (18)	-0.0153 (13)	0.0060 (14)	-0.0115 (13)
N2	0.0563 (17)	0.0388 (14)	0.0472 (16)	-0.0181 (12)	-0.0025 (13)	-0.0104 (12)
C1	0.053 (2)	0.0410 (19)	0.077 (3)	-0.0055 (16)	0.0042 (19)	0.0007 (17)
C2	0.0427 (18)	0.0443 (19)	0.068 (2)	-0.0069 (15)	-0.0014 (16)	-0.0042 (16)
C3	0.0412 (16)	0.0386 (16)	0.0449 (18)	-0.0114 (13)	-0.0023 (14)	-0.0113 (13)

C4	0.0414 (18)	0.049 (2)	0.068 (2)	-0.0087 (15)	-0.0081 (17)	-0.0046 (17)
C5	0.0434 (19)	0.067 (2)	0.070 (2)	-0.0206 (18)	0.0038 (17)	-0.016 (2)
C6	0.0452 (18)	0.0458 (18)	0.056 (2)	-0.0146 (15)	-0.0048 (16)	-0.0110 (16)
C7	0.0448 (18)	0.0420 (17)	0.0492 (19)	-0.0092 (14)	-0.0151 (15)	-0.0024 (14)
C8	0.0414 (16)	0.0339 (15)	0.0425 (17)	-0.0083 (12)	-0.0048 (13)	-0.0115 (13)
C9	0.0489 (19)	0.0449 (19)	0.062 (2)	-0.0109 (15)	-0.0210 (17)	-0.0037 (16)
C10	0.068 (2)	0.0412 (18)	0.053 (2)	-0.0122 (17)	-0.0211 (18)	0.0005 (15)
C11	0.0536 (19)	0.0456 (18)	0.0419 (18)	-0.0091 (15)	0.0022 (15)	-0.0141 (14)
C12	0.058 (2)	0.078 (3)	0.055 (2)	-0.020 (2)	0.0035 (18)	-0.022 (2)
C13	0.079 (3)	0.093 (3)	0.063 (3)	-0.045 (3)	0.022 (2)	-0.034 (2)
C14	0.132 (4)	0.056 (3)	0.056 (3)	-0.036 (3)	0.020 (3)	-0.018 (2)
C15	0.111 (4)	0.051 (2)	0.053 (2)	0.002 (2)	0.008 (2)	-0.0067 (18)
C16	0.071 (2)	0.049 (2)	0.053 (2)	0.0042 (18)	0.0074 (18)	-0.0124 (17)
C21	0.0366 (16)	0.0446 (18)	0.052 (2)	-0.0065 (13)	-0.0017 (14)	-0.0108 (15)
C22	0.076 (3)	0.054 (2)	0.053 (2)	-0.0228 (19)	-0.0103 (19)	0.0001 (18)
C23	0.091 (3)	0.086 (3)	0.048 (2)	-0.024 (3)	-0.014 (2)	-0.007 (2)
C24	0.080 (3)	0.080 (3)	0.066 (3)	-0.019 (2)	-0.020 (2)	-0.026 (2)
C25	0.086 (3)	0.060 (2)	0.081 (3)	-0.020 (2)	-0.022 (2)	-0.020 (2)
C26	0.068 (2)	0.0422 (19)	0.057 (2)	-0.0104 (17)	-0.0109 (18)	-0.0065 (16)
C31	0.0426 (17)	0.0395 (17)	0.0458 (18)	-0.0078 (13)	-0.0025 (14)	-0.0072 (14)
C32	0.064 (2)	0.065 (2)	0.057 (2)	-0.0107 (19)	-0.0088 (19)	-0.0252 (19)
C33	0.075 (3)	0.089 (3)	0.081 (3)	-0.021 (3)	-0.033 (2)	-0.024 (3)
C34	0.049 (2)	0.088 (3)	0.065 (3)	-0.017 (2)	-0.0140 (19)	-0.007 (2)
C35	0.0456 (19)	0.065 (2)	0.059 (2)	-0.0056 (17)	-0.0021 (17)	-0.0114 (18)
C36	0.0433 (18)	0.0493 (19)	0.059 (2)	-0.0103 (15)	0.0003 (15)	-0.0168 (16)
C41	0.0366 (15)	0.0364 (15)	0.0501 (19)	-0.0047 (12)	-0.0034 (13)	-0.0181 (14)
C42	0.0432 (18)	0.0450 (18)	0.064 (2)	-0.0134 (14)	0.0007 (16)	-0.0131 (16)
C43	0.048 (2)	0.071 (3)	0.089 (3)	-0.0266 (19)	0.009 (2)	-0.035 (2)
C44	0.0371 (18)	0.085 (3)	0.089 (3)	-0.0070 (19)	-0.0128 (19)	-0.046 (3)
C45	0.050 (2)	0.068 (3)	0.070 (3)	0.0022 (18)	-0.0215 (19)	-0.019 (2)
C46	0.0411 (17)	0.0444 (18)	0.065 (2)	-0.0060 (14)	-0.0097 (16)	-0.0128 (16)
C51	0.0378 (15)	0.0311 (14)	0.0425 (17)	-0.0092 (12)	-0.0017 (13)	-0.0035 (12)
C52	0.0418 (17)	0.051 (2)	0.057 (2)	-0.0059 (15)	-0.0044 (15)	-0.0155 (16)
C53	0.067 (2)	0.052 (2)	0.056 (2)	-0.0120 (18)	0.0065 (19)	-0.0201 (17)
C54	0.092 (3)	0.060 (2)	0.047 (2)	-0.024 (2)	-0.004 (2)	-0.0149 (18)
C55	0.069 (3)	0.068 (3)	0.061 (2)	-0.018 (2)	-0.024 (2)	-0.008 (2)
C56	0.0443 (18)	0.052 (2)	0.053 (2)	-0.0082 (15)	-0.0091 (16)	-0.0051 (16)
C61	0.0295 (14)	0.0334 (15)	0.0488 (18)	-0.0060 (11)	-0.0051 (13)	-0.0046 (13)
C62	0.063 (2)	0.0381 (17)	0.055 (2)	-0.0130 (15)	0.0066 (17)	-0.0100 (15)
C63	0.081 (3)	0.0387 (19)	0.079 (3)	-0.0216 (19)	0.008 (2)	-0.0071 (18)
C64	0.058 (2)	0.054 (2)	0.061 (2)	-0.0197 (18)	-0.0008 (18)	0.0072 (18)
C65	0.072 (3)	0.083 (3)	0.049 (2)	-0.030 (2)	0.0130 (19)	-0.017 (2)
C66	0.061 (2)	0.054 (2)	0.052 (2)	-0.0216 (17)	0.0071 (17)	-0.0181 (16)

Geometric parameters (\AA , $^\circ$)

Ag1—P1	2.4069 (9)	C22—H22	0.9300
Ag1—N1	2.430 (3)	C23—C24	1.371 (6)

Ag1—Cl1	2.5709 (10)	C23—H23	0.9300
Ag1—Cl1 ⁱ	2.6639 (10)	C24—C25	1.376 (6)
Ag2—P2	2.4162 (9)	C24—H24	0.9300
Ag2—N2	2.386 (3)	C25—C26	1.376 (5)
Ag2—Cl2	2.6111 (9)	C25—H25	0.9300
Ag2—Cl2 ⁱⁱ	2.6809 (10)	C26—H26	0.9300
Ag2—Ag2 ⁱⁱ	3.3292 (6)	C31—C36	1.373 (4)
Cl1—Ag1 ⁱ	2.6639 (11)	C31—C32	1.392 (5)
Cl2—Ag2 ⁱⁱ	2.6809 (10)	C32—C33	1.387 (5)
P1—C31	1.830 (3)	C32—H32	0.9300
P1—C11	1.833 (3)	C33—C34	1.384 (6)
P1—C21	1.836 (4)	C33—H33	0.9300
P2—C41	1.821 (3)	C34—C35	1.355 (6)
P2—C51	1.825 (3)	C34—H34	0.9300
P2—C61	1.829 (3)	C35—C36	1.388 (5)
N1—C5	1.322 (5)	C35—H35	0.9300
N1—C1	1.336 (4)	C36—H36	0.9300
N2—C10	1.321 (4)	C41—C46	1.378 (4)
N2—C6	1.336 (4)	C41—C42	1.387 (4)
C1—C2	1.381 (5)	C42—C43	1.386 (5)
C1—H1	0.9300	C42—H42	0.9300
C2—C3	1.375 (4)	C43—C44	1.378 (6)
C2—H2	0.9300	C43—H43	0.9300
C3—C4	1.394 (4)	C44—C45	1.376 (5)
C3—C8	1.485 (4)	C44—H44	0.9300
C4—C5	1.384 (5)	C45—C46	1.384 (5)
C4—H4	0.9300	C45—H45	0.9300
C5—H5	0.9300	C46—H46	0.9300
C6—C7	1.381 (4)	C51—C56	1.393 (4)
C6—H6	0.9300	C51—C52	1.394 (4)
C7—C8	1.383 (4)	C52—C53	1.380 (5)
C7—H7	0.9300	C52—H52	0.9300
C8—C9	1.385 (4)	C53—C54	1.368 (5)
C9—C10	1.380 (5)	C53—H53	0.9300
C9—H9	0.9300	C54—C55	1.374 (6)
C10—H10	0.9300	C54—H54	0.9300
C11—C16	1.370 (5)	C55—C56	1.379 (5)
C11—C12	1.395 (5)	C55—H55	0.9300
C12—C13	1.396 (5)	C56—H56	0.9300
C12—H12	0.9300	C61—C66	1.382 (4)
C13—C14	1.364 (6)	C61—C62	1.385 (4)
C13—H13	0.9300	C62—C63	1.388 (5)
C14—C15	1.361 (6)	C62—H62	0.9300
C14—H14	0.9300	C63—C64	1.364 (5)
C15—C16	1.382 (5)	C63—H63	0.9300
C15—H15	0.9300	C64—C65	1.357 (6)
C16—H16	0.9300	C64—H64	0.9300
C21—C26	1.377 (5)	C65—C66	1.381 (5)

C21—C22	1.399 (5)	C65—H65	0.9300
C22—C23	1.374 (6)	C66—H66	0.9300
P1—Ag1—N1	114.03 (7)	C23—C22—C21	120.4 (4)
P1—Ag1—Cl1	130.08 (3)	C23—C22—H22	119.8
N1—Ag1—Cl1	95.47 (8)	C21—C22—H22	119.8
P1—Ag1—Cl1 ⁱ	112.23 (3)	C24—C23—C22	120.7 (4)
N1—Ag1—Cl1 ⁱ	103.72 (7)	C24—C23—H23	119.7
Cl1—Ag1—Cl1 ⁱ	97.37 (3)	C22—C23—H23	119.7
N2—Ag2—P2	120.95 (7)	C23—C24—C25	119.3 (4)
N2—Ag2—Cl2	94.24 (7)	C23—C24—H24	120.3
P2—Ag2—Cl2	124.50 (3)	C25—C24—H24	120.3
N2—Ag2—Cl2 ⁱⁱ	96.68 (7)	C26—C25—C24	120.4 (4)
P2—Ag2—Cl2 ⁱⁱ	113.34 (3)	C26—C25—H25	119.8
Cl2—Ag2—Cl2 ⁱⁱ	102.05 (2)	C24—C25—H25	119.8
N2—Ag2—Ag2 ⁱⁱ	98.72 (7)	C25—C26—C21	121.1 (4)
P2—Ag2—Ag2 ⁱⁱ	139.76 (2)	C25—C26—H26	119.5
Cl2—Ag2—Ag2 ⁱⁱ	51.96 (2)	C21—C26—H26	119.5
Cl2 ⁱⁱ —Ag2—Ag2 ⁱⁱ	50.090 (19)	C36—C31—C32	118.6 (3)
Ag1—Cl1—Ag1 ⁱ	82.63 (3)	C36—C31—P1	123.4 (3)
Ag2—Cl2—Ag2 ⁱⁱ	77.95 (2)	C32—C31—P1	118.1 (3)
C31—P1—C11	103.84 (15)	C33—C32—C31	120.7 (4)
C31—P1—C21	103.95 (15)	C33—C32—H32	119.7
C11—P1—C21	103.26 (15)	C31—C32—H32	119.7
C31—P1—Ag1	112.39 (11)	C34—C33—C32	119.3 (4)
C11—P1—Ag1	117.37 (11)	C34—C33—H33	120.4
C21—P1—Ag1	114.55 (11)	C32—C33—H33	120.4
C41—P2—C51	104.34 (14)	C35—C34—C33	120.4 (4)
C41—P2—C61	104.46 (14)	C35—C34—H34	119.8
C51—P2—C61	102.45 (14)	C33—C34—H34	119.8
C41—P2—Ag2	111.14 (10)	C34—C35—C36	120.3 (4)
C51—P2—Ag2	116.42 (10)	C34—C35—H35	119.8
C61—P2—Ag2	116.60 (10)	C36—C35—H35	119.8
C5—N1—C1	116.4 (3)	C31—C36—C35	120.7 (3)
C5—N1—Ag1	121.4 (2)	C31—C36—H36	119.6
C1—N1—Ag1	122.2 (2)	C35—C36—H36	119.6
C10—N2—C6	116.2 (3)	C46—C41—C42	118.4 (3)
C10—N2—Ag2	121.3 (2)	C46—C41—P2	123.8 (2)
C6—N2—Ag2	122.1 (2)	C42—C41—P2	117.7 (2)
N1—C1—C2	123.6 (3)	C43—C42—C41	121.0 (3)
N1—C1—H1	118.2	C43—C42—H42	119.5
C2—C1—H1	118.2	C41—C42—H42	119.5
C3—C2—C1	120.1 (3)	C44—C43—C42	119.6 (4)
C3—C2—H2	119.9	C44—C43—H43	120.2
C1—C2—H2	119.9	C42—C43—H43	120.2
C2—C3—C4	116.3 (3)	C45—C44—C43	119.9 (3)
C2—C3—C8	122.0 (3)	C45—C44—H44	120.0
C4—C3—C8	121.7 (3)	C43—C44—H44	120.0

C5—C4—C3	119.7 (3)	C44—C45—C46	120.0 (4)
C5—C4—H4	120.1	C44—C45—H45	120.0
C3—C4—H4	120.1	C46—C45—H45	120.0
N1—C5—C4	123.8 (3)	C41—C46—C45	121.0 (3)
N1—C5—H5	118.1	C41—C46—H46	119.5
C4—C5—H5	118.1	C45—C46—H46	119.5
N2—C6—C7	123.6 (3)	C56—C51—C52	118.6 (3)
N2—C6—H6	118.2	C56—C51—P2	117.7 (2)
C7—C6—H6	118.2	C52—C51—P2	123.7 (2)
C6—C7—C8	119.7 (3)	C53—C52—C51	120.1 (3)
C6—C7—H7	120.1	C53—C52—H52	120.0
C8—C7—H7	120.1	C51—C52—H52	120.0
C7—C8—C9	116.7 (3)	C54—C53—C52	120.6 (4)
C7—C8—C3	121.6 (3)	C54—C53—H53	119.7
C9—C8—C3	121.7 (3)	C52—C53—H53	119.7
C10—C9—C8	119.4 (3)	C53—C54—C55	120.1 (4)
C10—C9—H9	120.3	C53—C54—H54	120.0
C8—C9—H9	120.3	C55—C54—H54	120.0
N2—C10—C9	124.4 (3)	C54—C55—C56	120.2 (4)
N2—C10—H10	117.8	C54—C55—H55	119.9
C9—C10—H10	117.8	C56—C55—H55	119.9
C16—C11—C12	119.1 (3)	C55—C56—C51	120.5 (3)
C16—C11—P1	123.2 (3)	C55—C56—H56	119.8
C12—C11—P1	117.7 (3)	C51—C56—H56	119.8
C11—C12—C13	119.0 (4)	C66—C61—C62	118.5 (3)
C11—C12—H12	120.5	C66—C61—P2	118.3 (2)
C13—C12—H12	120.5	C62—C61—P2	123.1 (3)
C14—C13—C12	120.5 (4)	C61—C62—C63	120.1 (3)
C14—C13—H13	119.7	C61—C62—H62	120.0
C12—C13—H13	119.7	C63—C62—H62	120.0
C15—C14—C13	120.5 (4)	C64—C63—C62	120.6 (4)
C15—C14—H14	119.8	C64—C63—H63	119.7
C13—C14—H14	119.8	C62—C63—H63	119.7
C14—C15—C16	119.7 (4)	C65—C64—C63	119.6 (3)
C14—C15—H15	120.1	C65—C64—H64	120.2
C16—C15—H15	120.1	C63—C64—H64	120.2
C11—C16—C15	121.2 (4)	C64—C65—C66	121.0 (4)
C11—C16—H16	119.4	C64—C65—H65	119.5
C15—C16—H16	119.4	C66—C65—H65	119.5
C26—C21—C22	118.1 (3)	C65—C66—C61	120.3 (3)
C26—C21—P1	124.1 (3)	C65—C66—H66	119.9
C22—C21—P1	117.8 (3)	C61—C66—H66	119.9

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x-1, -y+1, -z+2$.

Hydrogen-bond geometry (\AA , $^\circ$)

D—H···A	D—H	H···A	D···A	D—H···A

supporting information

C9—H9…Cl2 ⁱⁱⁱ	0.93	2.82	3.669 (4)	153
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Symmetry code: (iii) $x+1, y, z$.