

Poly[[(μ_3 -isonicotinato- κ^3 O:O:N)- (triphenylphosphine- κ P)silver(I)] ethanol solvate]

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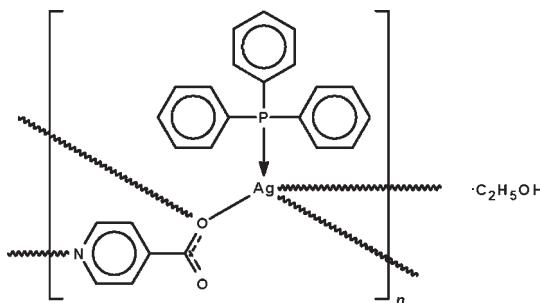
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(C-C) = 0.005$ Å; disorder in solvent or counterion; R factor = 0.030; wR factor = 0.078; data-to-parameter ratio = 18.2.

In the crystal structure of $\{[\text{Ag}(\text{C}_6\text{H}_4\text{NO}_2)(\text{C}_{18}\text{H}_{15}\text{P})]\cdot\text{C}_2\text{H}_6\text{O}\}_n$, the 4-pyridylcarboxylate ion binds to the phosphine-coordinated silver atoms through one of the two oxygen atoms of the carboxyl unit, and to a third phosphine-coordinate silver atom through the nitrogen atom of the aromatic ring, giving a distorted tetrahedral coordination at the metal atom. The μ_3 -bridging mode leads to a layer motif; the disordered ethanol molecules are linked to the free carboxyl oxygen atom by O—H···O hydrogen bonds.

Related literature

For the crystal structure of polymeric 4-pyridylcarboxylatosilver, see: Yang *et al.* (2004). For the synthesis of the reactant used in the metathetical reaction, see: Ng & Othman (1995, 1997).



Experimental

Crystal data

| | |
|---|-----------------------------------|
| $[\text{Ag}(\text{C}_6\text{H}_4\text{NO}_2)(\text{C}_{18}\text{H}_{15}\text{P})]\cdot\text{C}_2\text{H}_6\text{O}$ | $V = 2448.4(3)$ Å ³ |
| $M_r = 538.31$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 15.8026(10)$ Å | $\mu = 0.92$ mm ⁻¹ |
| $b = 13.2430(9)$ Å | $T = 295$ K |
| $c = 12.5483(8)$ Å | $0.40 \times 0.20 \times 0.05$ mm |
| $\beta = 111.1937(9)^\circ$ | |

Data collection

| | |
|-----------------------------------|--|
| Bruker SMART APEX | 22818 measured reflections |
| diffractometer | 5615 independent reflections |
| Absorption correction: multi-scan | 4111 reflections with $I > 2\sigma(I)$ |
| (SADABS; Sheldrick, 1996) | $R_{\text{int}} = 0.039$ |
| | |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.030$ | H atoms treated by a mixture of |
| $wR(F^2) = 0.078$ | independent and constrained |
| $S = 1.06$ | refinement |
| 5615 reflections | $\Delta\rho_{\text{max}} = 0.41$ e Å ⁻³ |
| 308 parameters | $\Delta\rho_{\text{min}} = -0.31$ e Å ⁻³ |
| 29 restraints | |

Table 1
Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|----------------------|--------------|--------------------|-------------|----------------------|
| O3—H3···O2 | 0.84 (5) | 1.92 (5) | 2.749 (4) | 172 (6) |

Data collection: *APEX2* software (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *PLATON* (Spek, 200) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2530).

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supporting information

Acta Cryst. (2010). E66, m285 [doi:10.1107/S1600536810004733]

Poly[[(μ_3 -isonicotinato- κ^3 O:O:N)(triphenylphosphine- κ P)silver(I)] ethanol solvate]

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S1. Comment

Silver carboxylates form adducts with triphenylphosphine; silver acetate itself furnishes silver acetate:2triphenylphosphine hemihydrate (Ng & Othman, 1995; Ng & Othman, 1997). The carboxylate unit in this adduct can be exchanged for a pyridylcarboxylate unit reacting the compound with the pyridylcarboxylic acid as the silver pyridylcarboxylate cannot be readily synthesized by condensing silver oxide with the pyridylcarboxylic acid.

In the crystal structure of $\text{Ag}(\text{C}_6\text{H}_4\text{NO}_2)(\text{C}_{18}\text{H}_{15}\text{P})\text{C}_2\text{H}_6\text{O}$ (Scheme I, Fig. 1), the anion binds through to phosphine-coordinated silver atoms through one of the two oxygen atoms of the carboxyl unit and to a third phosphine-coordinate silver atom through the nitrogen atom of the aromatic ring to render tetrahedral coordination at the metal atom. The μ_3 -bridging model leads to a layer motif (Fig. 2); the disordered ethanol molecules bind to the free carboxyl oxygen atom by hydrogen bonds.

S2. Experimental

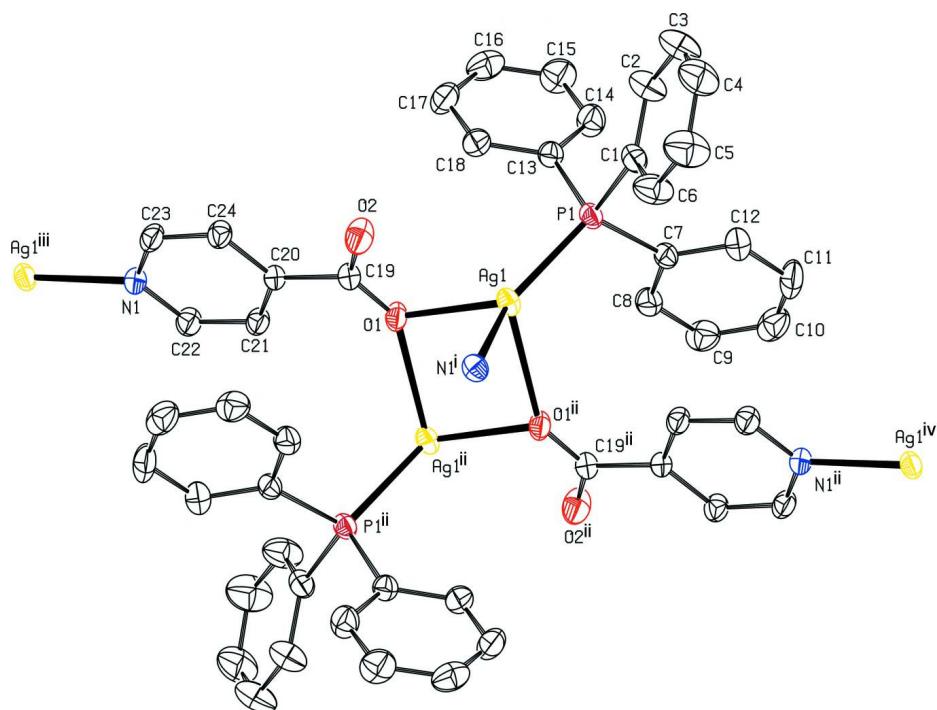
The bis-adduct, silver acetate:2triphenylphosphine hemihydrate, was first synthesized by reacting silver acetate (1 mmol, 0.17 g) and triphenylphosphine (2 mmol, 0.53 g) in ethanol (50 ml) (Ng & Othman, 1995; Ng & Othman, 1997). The adduct was isolated as colorless crystals. The adduct, (1 mmol, 0.69 g) was reacted with 4-pyridinecarboxylic acid (1 mmol, 0.13 g) in ethanol (50 ml). Slow evaporation of solvent afford suitable crystals (m.p. 408–409 K). The crystals rapidly turned opaque when taken out of solution. A specimen was coated in glue for the diffraction measurements.

S3. Refinement

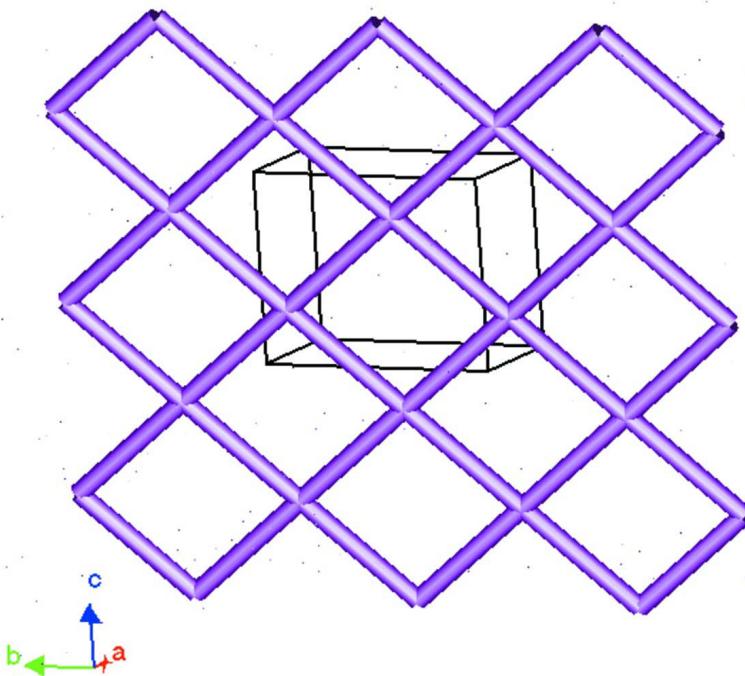
Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to 1.2 to 1.5 $U(\text{C})$.

The hydroxy H-atom was located in a difference Fourier map, and was refined with a distance restraint of O—H 0.84±0.01 Å; its temperature factor was freely refined.

The ethyl chain of the ethanol molecule is disordered over two positions; the occupancies refined to a 60:40 ratio. The oxygen-carbon distances were tightly restrained to 1.440±0.005 Å and the carbon-carbon distances to 1.54±0.005 Å. The anisotropic temperature factors of the carbon atoms were restrained to be nearly isotropic.

**Figure 1**

ORTEP view showing the coordination mode of the silver with the atom labeling scheme. Ellipsoids are shown at the 30% probability level. Hydrogen atoms and the disordered solvate have been omitted for clarity. [Symmetry codes: (i) - $x+1, -y+1, -z+1$; (ii) $-x+1, y-1/2, -z+3/2$; (iii) $-x+1, y+1/2, -z+3/2$; (iv) $x, 1/2-y, z-1/2$].

**Figure 2**

OLEX (Dolomanov *et al.*, 2003) representation of the layer structure.

Poly[[(μ_3 -isonicotinato- κ^3 O:O:N)(triphenylphosphine- κ P)silver(I)] ethanol solvate]

Crystal data



$M_r = 538.31$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 15.8026 (10)$ Å

$b = 13.2430 (9)$ Å

$c = 12.5483 (8)$ Å

$\beta = 111.1937 (9)^\circ$

$V = 2448.4 (3)$ Å³

$Z = 4$

$F(000) = 1096$

$D_x = 1.460$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6635 reflections

$\theta = 2.4\text{--}28.1^\circ$

$\mu = 0.92$ mm⁻¹

$T = 295$ K

Block coated in glue, colorless

0.40 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

$T_{\min} = 0.711$, $T_{\max} = 0.956$

22818 measured reflections

5615 independent reflections

4111 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -20 \rightarrow 20$

$k = -17 \rightarrow 17$

$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.078$
 $S = 1.06$
 5615 reflections
 308 parameters
 29 restraints
 Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: inferred from neighbouring sites
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 1.2212P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.41 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.31 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|---------------|---------------|---------------|----------------------------------|-----------|
| Ag1 | 0.614660 (14) | 0.443563 (16) | 0.564182 (18) | 0.03977 (8) | |
| P1 | 0.73287 (5) | 0.49413 (6) | 0.50219 (6) | 0.03698 (17) | |
| O1 | 0.53235 (13) | 0.57005 (15) | 0.61834 (16) | 0.0421 (5) | |
| O2 | 0.63385 (16) | 0.54142 (18) | 0.79082 (19) | 0.0636 (7) | |
| O3 | 0.7823 (2) | 0.4374 (3) | 0.9329 (3) | 0.1018 (11) | |
| H3 | 0.738 (3) | 0.473 (4) | 0.895 (4) | 0.16 (3)* | |
| N1 | 0.44392 (15) | 0.81511 (17) | 0.8642 (2) | 0.0396 (5) | |
| C1 | 0.83757 (19) | 0.4219 (2) | 0.5607 (3) | 0.0444 (7) | |
| C2 | 0.9230 (2) | 0.4634 (3) | 0.5938 (3) | 0.0674 (10) | |
| H2 | 0.9296 | 0.5324 | 0.5854 | 0.081* | |
| C3 | 0.9994 (2) | 0.4033 (4) | 0.6393 (4) | 0.0864 (13) | |
| H3A | 1.0568 | 0.4322 | 0.6616 | 0.104* | |
| C4 | 0.9907 (3) | 0.3027 (4) | 0.6516 (4) | 0.0881 (14) | |
| H4 | 1.0422 | 0.2629 | 0.6832 | 0.106* | |
| C5 | 0.9073 (3) | 0.2598 (3) | 0.6181 (4) | 0.0944 (15) | |
| H5 | 0.9015 | 0.1904 | 0.6243 | 0.113* | |
| C6 | 0.8307 (2) | 0.3198 (3) | 0.5748 (4) | 0.0725 (11) | |
| H6 | 0.7736 | 0.2904 | 0.5548 | 0.087* | |
| C7 | 0.70310 (19) | 0.4873 (2) | 0.3475 (2) | 0.0392 (6) | |
| C8 | 0.6256 (2) | 0.5381 (2) | 0.2796 (3) | 0.0491 (8) | |
| H8 | 0.5923 | 0.5752 | 0.3137 | 0.059* | |
| C9 | 0.5973 (2) | 0.5339 (3) | 0.1614 (3) | 0.0621 (9) | |
| H9 | 0.5457 | 0.5688 | 0.1165 | 0.075* | |
| C10 | 0.6454 (3) | 0.4787 (3) | 0.1113 (3) | 0.0681 (10) | |
| H10 | 0.6262 | 0.4755 | 0.0320 | 0.082* | |
| C11 | 0.7216 (3) | 0.4281 (3) | 0.1764 (3) | 0.0686 (11) | |
| H11 | 0.7538 | 0.3905 | 0.1413 | 0.082* | |
| C12 | 0.7516 (2) | 0.4323 (3) | 0.2954 (3) | 0.0550 (8) | |
| H12 | 0.8040 | 0.3982 | 0.3394 | 0.066* | |
| C13 | 0.76577 (18) | 0.6258 (2) | 0.5340 (2) | 0.0401 (6) | |
| C14 | 0.8048 (2) | 0.6813 (3) | 0.4702 (3) | 0.0565 (8) | |
| H14 | 0.8170 | 0.6506 | 0.4107 | 0.068* | |
| C15 | 0.8260 (3) | 0.7820 (3) | 0.4944 (3) | 0.0705 (10) | |

| | | | | | |
|------|--------------|------------|-------------|-------------|------------|
| H15 | 0.8528 | 0.8183 | 0.4515 | 0.085* | |
| C16 | 0.8079 (3) | 0.8284 (3) | 0.5804 (3) | 0.0680 (10) | |
| H16 | 0.8214 | 0.8965 | 0.5955 | 0.082* | |
| C17 | 0.7698 (2) | 0.7747 (3) | 0.6445 (3) | 0.0633 (10) | |
| H17 | 0.7578 | 0.8065 | 0.7036 | 0.076* | |
| C18 | 0.7487 (2) | 0.6734 (3) | 0.6226 (3) | 0.0500 (8) | |
| H18 | 0.7232 | 0.6374 | 0.6672 | 0.060* | |
| C19 | 0.56739 (18) | 0.5860 (2) | 0.7242 (2) | 0.0368 (6) | |
| C20 | 0.52434 (17) | 0.6678 (2) | 0.7719 (2) | 0.0329 (6) | |
| C21 | 0.44917 (19) | 0.7210 (2) | 0.7046 (2) | 0.0408 (7) | |
| H21 | 0.4240 | 0.7083 | 0.6265 | 0.049* | |
| C22 | 0.41135 (19) | 0.7928 (2) | 0.7527 (3) | 0.0451 (7) | |
| H22 | 0.3606 | 0.8277 | 0.7053 | 0.054* | |
| C23 | 0.5173 (2) | 0.7646 (2) | 0.9290 (2) | 0.0442 (7) | |
| H23 | 0.5416 | 0.7792 | 1.0067 | 0.053* | |
| C24 | 0.55900 (19) | 0.6919 (2) | 0.8871 (2) | 0.0421 (7) | |
| H24 | 0.6104 | 0.6590 | 0.9359 | 0.051* | |
| C25 | 0.8216 (4) | 0.4024 (7) | 0.8541 (5) | 0.075 (3) | 0.596 (11) |
| H25A | 0.7898 | 0.4300 | 0.7785 | 0.090* | 0.596 (11) |
| H25B | 0.8197 | 0.3293 | 0.8494 | 0.090* | 0.596 (11) |
| C26 | 0.9193 (4) | 0.4398 (7) | 0.9016 (7) | 0.166 (6) | 0.596 (11) |
| H26A | 0.9505 | 0.4179 | 0.8528 | 0.248* | 0.596 (11) |
| H26B | 0.9492 | 0.4129 | 0.9770 | 0.248* | 0.596 (11) |
| H26C | 0.9198 | 0.5122 | 0.9051 | 0.248* | 0.596 (11) |
| C25' | 0.8433 (5) | 0.4584 (7) | 0.8721 (8) | 0.118 (6) | 0.404 (11) |
| H25C | 0.8087 | 0.4779 | 0.7939 | 0.142* | 0.404 (11) |
| H25D | 0.8839 | 0.5134 | 0.9089 | 0.142* | 0.404 (11) |
| C26' | 0.8952 (4) | 0.3674 (7) | 0.8736 (11) | 0.172 (9) | 0.404 (11) |
| H26D | 0.9253 | 0.3456 | 0.9512 | 0.259* | 0.404 (11) |
| H26E | 0.9396 | 0.3814 | 0.8398 | 0.259* | 0.404 (11) |
| H26F | 0.8551 | 0.3152 | 0.8310 | 0.259* | 0.404 (11) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Ag1 | 0.04098 (12) | 0.04309 (13) | 0.04407 (13) | 0.00077 (10) | 0.02597 (10) | 0.00367 (10) |
| P1 | 0.0358 (3) | 0.0432 (4) | 0.0369 (4) | -0.0001 (3) | 0.0191 (3) | 0.0016 (3) |
| O1 | 0.0466 (11) | 0.0507 (13) | 0.0322 (11) | 0.0068 (9) | 0.0181 (9) | -0.0047 (9) |
| O2 | 0.0622 (14) | 0.0722 (16) | 0.0456 (13) | 0.0335 (12) | 0.0066 (11) | -0.0037 (11) |
| O3 | 0.095 (2) | 0.137 (3) | 0.0668 (19) | 0.046 (2) | 0.0219 (18) | 0.0116 (19) |
| N1 | 0.0423 (13) | 0.0414 (14) | 0.0388 (13) | -0.0001 (10) | 0.0189 (11) | -0.0078 (11) |
| C1 | 0.0389 (15) | 0.054 (2) | 0.0441 (17) | 0.0064 (13) | 0.0191 (13) | 0.0031 (14) |
| C2 | 0.0427 (18) | 0.077 (3) | 0.084 (3) | 0.0021 (17) | 0.0237 (18) | 0.014 (2) |
| C3 | 0.0393 (19) | 0.108 (4) | 0.111 (4) | 0.004 (2) | 0.025 (2) | 0.011 (3) |
| C4 | 0.052 (2) | 0.099 (4) | 0.106 (4) | 0.027 (2) | 0.019 (2) | 0.011 (3) |
| C5 | 0.069 (3) | 0.066 (3) | 0.136 (4) | 0.015 (2) | 0.021 (3) | 0.013 (3) |
| C6 | 0.0487 (19) | 0.058 (2) | 0.101 (3) | 0.0035 (17) | 0.016 (2) | 0.006 (2) |
| C7 | 0.0427 (15) | 0.0412 (16) | 0.0409 (16) | -0.0083 (12) | 0.0238 (13) | -0.0022 (13) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|-------------|--------------|
| C8 | 0.0466 (16) | 0.060 (2) | 0.0435 (18) | -0.0016 (14) | 0.0200 (14) | -0.0002 (15) |
| C9 | 0.061 (2) | 0.075 (3) | 0.046 (2) | -0.0075 (18) | 0.0134 (17) | 0.0058 (17) |
| C10 | 0.089 (3) | 0.075 (3) | 0.043 (2) | -0.022 (2) | 0.027 (2) | -0.0057 (19) |
| C11 | 0.094 (3) | 0.073 (3) | 0.055 (2) | 0.000 (2) | 0.047 (2) | -0.0152 (19) |
| C12 | 0.060 (2) | 0.059 (2) | 0.055 (2) | 0.0043 (16) | 0.0310 (17) | -0.0039 (16) |
| C13 | 0.0395 (15) | 0.0447 (17) | 0.0369 (15) | -0.0006 (12) | 0.0148 (12) | 0.0000 (13) |
| C14 | 0.071 (2) | 0.052 (2) | 0.056 (2) | -0.0092 (17) | 0.0343 (18) | -0.0025 (16) |
| C15 | 0.085 (3) | 0.057 (2) | 0.074 (3) | -0.018 (2) | 0.034 (2) | 0.001 (2) |
| C16 | 0.067 (2) | 0.051 (2) | 0.072 (3) | -0.0088 (18) | 0.008 (2) | -0.0078 (19) |
| C17 | 0.062 (2) | 0.070 (2) | 0.050 (2) | 0.0034 (18) | 0.0113 (17) | -0.0216 (18) |
| C18 | 0.0452 (17) | 0.061 (2) | 0.0399 (17) | 0.0009 (15) | 0.0113 (14) | -0.0038 (15) |
| C19 | 0.0396 (15) | 0.0380 (15) | 0.0366 (16) | 0.0031 (12) | 0.0182 (13) | -0.0003 (12) |
| C20 | 0.0352 (13) | 0.0352 (14) | 0.0310 (14) | 0.0009 (11) | 0.0152 (11) | -0.0012 (11) |
| C21 | 0.0433 (15) | 0.0465 (17) | 0.0308 (15) | 0.0056 (13) | 0.0113 (12) | -0.0043 (12) |
| C22 | 0.0417 (15) | 0.0503 (18) | 0.0394 (17) | 0.0118 (13) | 0.0101 (13) | -0.0030 (14) |
| C23 | 0.0508 (17) | 0.0498 (18) | 0.0311 (15) | -0.0003 (14) | 0.0137 (13) | -0.0085 (13) |
| C24 | 0.0417 (15) | 0.0491 (18) | 0.0329 (15) | 0.0093 (13) | 0.0103 (12) | -0.0016 (13) |
| C25 | 0.067 (4) | 0.092 (6) | 0.068 (4) | 0.020 (4) | 0.025 (3) | -0.011 (4) |
| C26 | 0.146 (8) | 0.201 (10) | 0.167 (9) | -0.028 (7) | 0.078 (7) | -0.039 (7) |
| C25' | 0.121 (10) | 0.111 (9) | 0.106 (9) | 0.028 (7) | 0.020 (7) | -0.031 (7) |
| C26' | 0.187 (13) | 0.184 (13) | 0.151 (11) | 0.003 (9) | 0.068 (9) | -0.019 (9) |

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

| | | | |
|-----------------------|-------------|----------|-----------|
| Ag1—P1 | 2.3651 (7) | C11—H11 | 0.9300 |
| Ag1—O1 | 2.3662 (18) | C12—H12 | 0.9300 |
| Ag1—O1 ⁱ | 2.6131 (19) | C13—C14 | 1.386 (4) |
| Ag1—N1 ⁱⁱ | 2.271 (2) | C13—C18 | 1.387 (4) |
| P1—C1 | 1.820 (3) | C14—C15 | 1.381 (5) |
| P1—C13 | 1.822 (3) | C14—H14 | 0.9300 |
| P1—C7 | 1.827 (3) | C15—C16 | 1.359 (5) |
| O1—C19 | 1.259 (3) | C15—H15 | 0.9300 |
| O2—C19 | 1.231 (3) | C16—C17 | 1.366 (5) |
| O3—C25 | 1.423 (4) | C16—H16 | 0.9300 |
| O3—C25' | 1.457 (5) | C17—C18 | 1.386 (5) |
| O3—H3 | 0.84 (5) | C17—H17 | 0.9300 |
| N1—C23 | 1.331 (4) | C18—H18 | 0.9300 |
| N1—C22 | 1.338 (3) | C19—C20 | 1.512 (4) |
| N1—Ag1 ⁱⁱⁱ | 2.271 (2) | C20—C21 | 1.377 (4) |
| C1—C6 | 1.373 (5) | C20—C24 | 1.385 (4) |
| C1—C2 | 1.375 (4) | C21—C22 | 1.374 (4) |
| C2—C3 | 1.384 (5) | C21—H21 | 0.9300 |
| C2—H2 | 0.9300 | C22—H22 | 0.9300 |
| C3—C4 | 1.354 (6) | C23—C24 | 1.374 (4) |
| C3—H3A | 0.9300 | C23—H23 | 0.9300 |
| C4—C5 | 1.356 (6) | C24—H24 | 0.9300 |
| C4—H4 | 0.9300 | C25—C26 | 1.523 (5) |
| C5—C6 | 1.383 (5) | C25—H25A | 0.9700 |

| | | | |
|---------------------------------------|-------------|-------------|-----------|
| C5—H5 | 0.9300 | C25—H25B | 0.9700 |
| C6—H6 | 0.9300 | C26—H26A | 0.9600 |
| C7—C12 | 1.381 (4) | C26—H26B | 0.9600 |
| C7—C8 | 1.387 (4) | C26—H26C | 0.9600 |
| C8—C9 | 1.387 (5) | C25'—C26' | 1.4538 |
| C8—H8 | 0.9300 | C25'—H25C | 0.9700 |
| C9—C10 | 1.361 (5) | C25'—H25D | 0.9700 |
| C9—H9 | 0.9300 | C26'—H26D | 0.9600 |
| C10—C11 | 1.362 (5) | C26'—H26E | 0.9600 |
| C10—H10 | 0.9300 | C26'—H26F | 0.9600 |
| C11—C12 | 1.394 (5) | | |
| | | | |
| N1 ⁱⁱ —Ag1—P1 | 145.63 (6) | C14—C13—C18 | 118.6 (3) |
| N1 ⁱⁱ —Ag1—O1 | 94.11 (8) | C14—C13—P1 | 122.2 (2) |
| P1—Ag1—O1 | 118.40 (5) | C18—C13—P1 | 119.2 (2) |
| N1 ⁱⁱ —Ag1—O1 ⁱ | 86.25 (7) | C15—C14—C13 | 120.6 (3) |
| P1—Ag1—O1 ⁱ | 106.79 (5) | C15—C14—H14 | 119.7 |
| O1—Ag1—O1 ⁱ | 83.90 (6) | C13—C14—H14 | 119.7 |
| C1—P1—C13 | 105.57 (14) | C16—C15—C14 | 120.5 (4) |
| C1—P1—C7 | 104.47 (13) | C16—C15—H15 | 119.8 |
| C13—P1—C7 | 102.95 (13) | C14—C15—H15 | 119.8 |
| C1—P1—Ag1 | 115.44 (10) | C15—C16—C17 | 119.7 (4) |
| C13—P1—Ag1 | 113.30 (9) | C15—C16—H16 | 120.1 |
| C7—P1—Ag1 | 113.88 (9) | C17—C16—H16 | 120.1 |
| C19—O1—Ag1 | 110.15 (16) | C16—C17—C18 | 120.9 (3) |
| C25—O3—H3 | 106 (4) | C16—C17—H17 | 119.6 |
| C25'—O3—H3 | 100 (4) | C18—C17—H17 | 119.6 |
| C23—N1—C22 | 116.7 (2) | C17—C18—C13 | 119.8 (3) |
| C23—N1—Ag1 ⁱⁱⁱ | 121.66 (18) | C17—C18—H18 | 120.1 |
| C22—N1—Ag1 ⁱⁱⁱ | 121.41 (19) | C13—C18—H18 | 120.1 |
| C6—C1—C2 | 117.9 (3) | O2—C19—O1 | 125.3 (3) |
| C6—C1—P1 | 117.8 (2) | O2—C19—C20 | 118.1 (2) |
| C2—C1—P1 | 124.2 (3) | O1—C19—C20 | 116.7 (2) |
| C1—C2—C3 | 120.6 (4) | C21—C20—C24 | 116.8 (2) |
| C1—C2—H2 | 119.7 | C21—C20—C19 | 122.3 (2) |
| C3—C2—H2 | 119.7 | C24—C20—C19 | 120.9 (2) |
| C4—C3—C2 | 120.2 (4) | C22—C21—C20 | 120.0 (3) |
| C4—C3—H3A | 119.9 | C22—C21—H21 | 120.0 |
| C2—C3—H3A | 119.9 | C20—C21—H21 | 120.0 |
| C3—C4—C5 | 120.3 (4) | N1—C22—C21 | 123.2 (3) |
| C3—C4—H4 | 119.9 | N1—C22—H22 | 118.4 |
| C5—C4—H4 | 119.9 | C21—C22—H22 | 118.4 |
| C4—C5—C6 | 119.7 (4) | N1—C23—C24 | 123.4 (3) |
| C4—C5—H5 | 120.2 | N1—C23—H23 | 118.3 |
| C6—C5—H5 | 120.2 | C24—C23—H23 | 118.3 |
| C1—C6—C5 | 121.2 (4) | C23—C24—C20 | 119.8 (3) |
| C1—C6—H6 | 119.4 | C23—C24—H24 | 120.1 |
| C5—C6—H6 | 119.4 | C20—C24—H24 | 120.1 |

| | | | |
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| C12—C7—C8 | 118.9 (3) | O3—C25—C26 | 104.9 (5) |
| C12—C7—P1 | 123.7 (2) | O3—C25—H25A | 110.8 |
| C8—C7—P1 | 117.4 (2) | C26—C25—H25A | 110.8 |
| C7—C8—C9 | 120.6 (3) | O3—C25—H25B | 110.8 |
| C7—C8—H8 | 119.7 | C26—C25—H25B | 110.8 |
| C9—C8—H8 | 119.7 | H25A—C25—H25B | 108.8 |
| C10—C9—C8 | 119.8 (4) | C26'—C25'—O3 | 108.2 (7) |
| C10—C9—H9 | 120.1 | C26'—C25'—H25C | 110.1 |
| C8—C9—H9 | 120.1 | O3—C25'—H25C | 110.1 |
| C9—C10—C11 | 120.4 (3) | C26'—C25'—H25D | 110.1 |
| C9—C10—H10 | 119.8 | O3—C25'—H25D | 110.1 |
| C11—C10—H10 | 119.8 | H25C—C25'—H25D | 108.4 |
| C10—C11—C12 | 120.6 (3) | C25'—C26'—H26D | 109.5 |
| C10—C11—H11 | 119.7 | C25'—C26'—H26E | 109.5 |
| C12—C11—H11 | 119.7 | H26D—C26'—H26E | 109.5 |
| C7—C12—C11 | 119.7 (3) | C25'—C26'—H26F | 109.5 |
| C7—C12—H12 | 120.2 | H26D—C26'—H26F | 109.5 |
| C11—C12—H12 | 120.2 | H26E—C26'—H26F | 109.5 |
| | | | |
| N1 ⁱⁱ —Ag1—P1—C1 | -23.79 (16) | C9—C10—C11—C12 | -0.2 (6) |
| O1—Ag1—P1—C1 | 135.40 (12) | C8—C7—C12—C11 | -0.6 (5) |
| O1 ⁱ —Ag1—P1—C1 | -132.48 (12) | P1—C7—C12—C11 | 177.4 (3) |
| N1 ⁱⁱ —Ag1—P1—C13 | -145.70 (14) | C10—C11—C12—C7 | 0.7 (6) |
| O1—Ag1—P1—C13 | 13.50 (11) | C1—P1—C13—C14 | 78.6 (3) |
| O1 ⁱ —Ag1—P1—C13 | 105.62 (11) | C7—P1—C13—C14 | -30.7 (3) |
| N1 ⁱⁱ —Ag1—P1—C7 | 97.08 (15) | Ag1—P1—C13—C14 | -154.1 (2) |
| O1—Ag1—P1—C7 | -103.72 (12) | C1—P1—C13—C18 | -103.5 (2) |
| O1 ⁱ —Ag1—P1—C7 | -11.60 (12) | C7—P1—C13—C18 | 147.2 (2) |
| N1 ⁱⁱ —Ag1—O1—C19 | 75.80 (19) | Ag1—P1—C13—C18 | 23.8 (3) |
| P1—Ag1—O1—C19 | -92.60 (18) | C18—C13—C14—C15 | -0.2 (5) |
| O1 ⁱ —Ag1—O1—C19 | 161.6 (2) | P1—C13—C14—C15 | 177.7 (3) |
| C13—P1—C1—C6 | 163.9 (3) | C13—C14—C15—C16 | -0.7 (6) |
| C7—P1—C1—C6 | -87.9 (3) | C14—C15—C16—C17 | 1.0 (6) |
| Ag1—P1—C1—C6 | 37.9 (3) | C15—C16—C17—C18 | -0.4 (6) |
| C13—P1—C1—C2 | -14.8 (3) | C16—C17—C18—C13 | -0.5 (5) |
| C7—P1—C1—C2 | 93.4 (3) | C14—C13—C18—C17 | 0.8 (4) |
| Ag1—P1—C1—C2 | -140.8 (3) | P1—C13—C18—C17 | -177.2 (2) |
| C6—C1—C2—C3 | 0.2 (6) | Ag1—O1—C19—O2 | -1.2 (4) |
| P1—C1—C2—C3 | 178.9 (3) | Ag1—O1—C19—C20 | 177.99 (18) |
| C1—C2—C3—C4 | 0.2 (7) | O2—C19—C20—C21 | -179.2 (3) |
| C2—C3—C4—C5 | 0.8 (8) | O1—C19—C20—C21 | 1.6 (4) |
| C3—C4—C5—C6 | -2.2 (8) | O2—C19—C20—C24 | 0.3 (4) |
| C2—C1—C6—C5 | -1.6 (6) | O1—C19—C20—C24 | -179.0 (3) |
| P1—C1—C6—C5 | 179.6 (4) | C24—C20—C21—C22 | -1.0 (4) |
| C4—C5—C6—C1 | 2.6 (7) | C19—C20—C21—C22 | 178.4 (3) |
| C1—P1—C7—C12 | 3.2 (3) | C23—N1—C22—C21 | 0.8 (4) |
| C13—P1—C7—C12 | 113.3 (3) | Ag1 ⁱⁱⁱ —N1—C22—C21 | 174.9 (2) |
| Ag1—P1—C7—C12 | -123.6 (2) | C20—C21—C22—N1 | 0.0 (5) |

| | | | |
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| C1—P1—C7—C8 | −178.8 (2) | C22—N1—C23—C24 | −0.7 (4) |
| C13—P1—C7—C8 | −68.7 (2) | Ag1 ⁱⁱⁱ —N1—C23—C24 | −174.7 (2) |
| Ag1—P1—C7—C8 | 54.3 (2) | N1—C23—C24—C20 | −0.4 (5) |
| C12—C7—C8—C9 | −0.1 (5) | C21—C20—C24—C23 | 1.2 (4) |
| P1—C7—C8—C9 | −178.2 (2) | C19—C20—C24—C23 | −178.3 (3) |
| C7—C8—C9—C10 | 0.7 (5) | C25'—O3—C25—C26 | 38.5 (4) |
| C8—C9—C10—C11 | −0.5 (6) | C25—O3—C25'—C26' | −41.6 (7) |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, y-1/2, -z+3/2$; (iii) $-x+1, y+1/2, -z+3/2$.

Hydrogen-bond geometry (\AA , °)

| $D\cdots H\cdots A$ | $D—H$ | $H\cdots A$ | $D\cdots A$ | $D—H\cdots A$ |
|---------------------|----------|-------------|-------------|---------------|
| O3—H3 \cdots O2 | 0.84 (5) | 1.92 (5) | 2.749 (4) | 172 (6) |