Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{4-[(Diphenylphosphino)methylamino]-pyridinium-κ*P*}bis(nitrato-κ*O*)silver(I)

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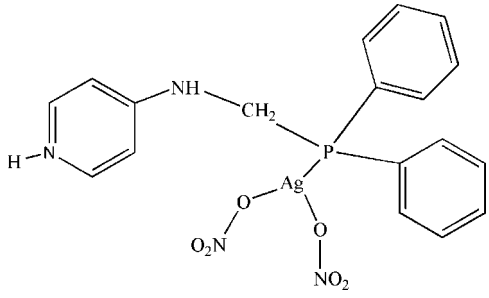
Received 30 June 2009; accepted 12 August 2009

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.029; wR factor = 0.109; data-to-parameter ratio = 16.1.

In the title mononuclear complex, $[Ag(C_{18}H_{18}N_2P)(NO_3)_2]$, the metal centre is coordinated in a slightly distorted trigonal–planar geometry by the P atom of the phosphine ligand and the O atoms of the two monodentate nitrate anions. In the crystal structure, complex molecules are connected by intermolecular N—H···O hydrogen bonds, forming chains running parallel to the b axis.

Related literature

For related structures, see: Song *et al.* (2002); Durran *et al.* (2006); Jiang *et al.* (2009); Wang *et al.* (2008).



Experimental

Crystal data

$[Ag(C_{18}H_{18}N_2P)(NO_3)_2]$
M_r = 525.20
Triclinic, $P\overline{1}$
a = 7.9760 (9) Å
b = 9.6895 (11) Å
c = 14.1207 (16) Å
α = 86.170 (2)°
β = 89.170 (2)°
γ = 69.439 (2)°
V = 1019.5 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 173 K
0.47 × 0.33 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.699, T_{max} = 0.838
8623 measured reflections
4367 independent reflections
3802 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.109
S = 1.15
4367 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O5^{i}	0.88	1.93	2.807 (3)	172
N2—H2A···O4^{ii}	0.88	2.16	3.013 (3)	162
N2—H2A···O5^{ii}	0.88	2.47	3.075 (3)	127

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of Guangxi Province (grant No. 0832100) and the Programme for Excellent Talents in Guangxi Higher Education Institutions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2347).

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supporting information

Acta Cryst. (2009). E**65**, m1087 [doi:10.1107/S160053680903178X]

{4-[(Diphenylphosphino)methylamino]pyridinium-*κP*}bis(nitrato-*κO*)silver(I)

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S1. Comment

Silver(I) metal complexes with pyridine-phosphine ligands which contain a soft Lewis base (P) and a hard Lewis acid (N) had been extensively studied so far (Song *et al.*, 2002; Durran *et al.*, 2006; Jiang *et al.*, 2009; Wang *et al.* 2008). Herein, we report the crystal structure of the title complex.

In the title complex (Fig. 1), the silver(I) metal centre adopts a slightly distorted trigonal-planar geometry provided by the P atom of the phosphine ligand and by the O atoms of two monodentate nitrate anions. The metal is displaced by 0.0629 (3) Å from the plane of the donor atoms. In the crystal structure, the complex molecules are linked by intermolecular N—H···O hydrogen bonds (Table 1, Fig. 2) to form chains running parallel to the *b* axis.

S2. Experimental

Silver nitrate (0.0168 g, 1 mmol) was dissolved in CH_3CN (2 ml) and a solution of *N*-diphenylphosphinomethyl-4-amino-pyridinium (0.0292 g, 1 mmol) in CH_3OH (4 ml) was added with stirring for three hours at room temperature. Subsequent diethyl ether diffusion into the solution afforded colourless crystal of the title compound suitable for X-ray analysis.

S3. Refinement

All H atoms were located geometrically and treated as riding atoms, with N—H= 0.88 Å, C—H = 0.95–0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C, N).

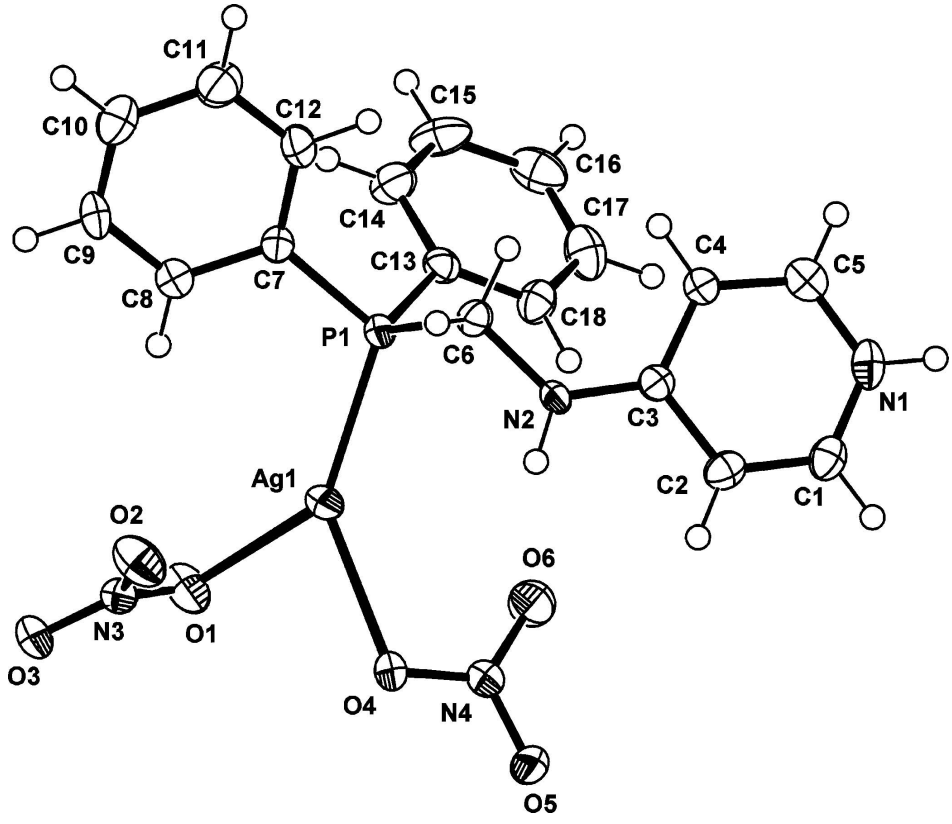

Figure 1

The molecular structure of title complex with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

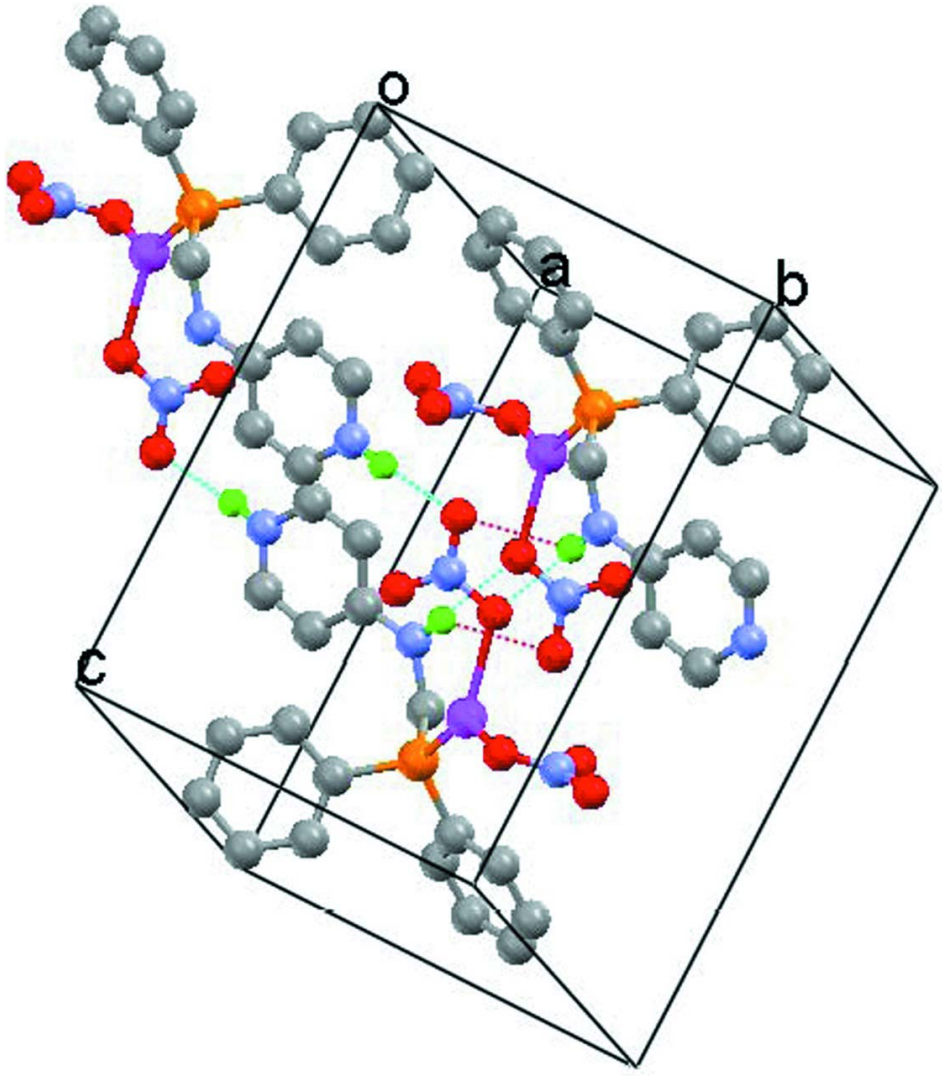

Figure 2

Partial packing diagram of the title compound, showing the intermlecular N—H···O hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding are omitted for clarity.

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Crystal data

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$\beta = 89.170\ (2)°$
$\gamma = 69.439\ (2)°$
$V = 1019.5\ (2)$ Å^3
$Z = 2$
$F(000) = 528$
$D_x = 1.711$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5807 reflections
$\theta = 2.7–27.0°$
$\mu = 1.11$ mm^{-1}
$T = 173$ K
Block, colourless
0.47 × 0.33 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.699, T_{max} = 0.838
8623 measured reflections
4367 independent reflections
3802 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 27.0°, θ_{min} = 2.6°
h = −10→9
k = −12→12
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.109
S = 1.15
4367 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 0.0727P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.46577 (3)	0.46190 (2)	0.297716 (16)	0.03069 (11)
P1	0.20209 (10)	0.64942 (8)	0.24168 (5)	0.02155 (16)
O1	0.6827 (3)	0.2456 (3)	0.24276 (18)	0.0391 (5)
O2	0.4738 (3)	0.1861 (3)	0.31211 (19)	0.0429 (6)
O3	0.6975 (3)	0.0183 (2)	0.25015 (18)	0.0428 (6)
O4	0.6546 (3)	0.4154 (2)	0.43169 (15)	0.0311 (5)
O5	0.7902 (3)	0.5171 (2)	0.52073 (17)	0.0381 (6)
O6	0.6328 (4)	0.6441 (3)	0.39968 (18)	0.0481 (7)
N1	0.1753 (3)	1.2090 (3)	0.45460 (18)	0.0283 (5)
H1A	0.1774	1.2963	0.4667	0.034*
N2	0.1655 (3)	0.7994 (2)	0.40482 (16)	0.0219 (5)
H2A	0.2357	0.7271	0.4428	0.026*
N3	0.6180 (4)	0.1481 (3)	0.26837 (18)	0.0288 (5)
N4	0.6919 (3)	0.5284 (3)	0.44974 (17)	0.0265 (5)
C1	0.2731 (4)	1.0885 (3)	0.5089 (2)	0.0269 (6)
H1B	0.3442	1.0991	0.5594	0.032*

C2	0.2720 (4)	0.9528 (3)	0.4930 (2)	0.0256 (6)
H2B	0.3420	0.8693	0.5321	0.031*
C3	0.1658 (3)	0.9348 (3)	0.41738 (19)	0.0204 (5)
C4	0.0664 (4)	1.0632 (3)	0.3620 (2)	0.0231 (6)
H4A	−0.0059	1.0567	0.3108	0.028*
C5	0.0740 (4)	1.1971 (3)	0.3818 (2)	0.0284 (6)
H5A	0.0070	1.2831	0.3438	0.034*
C6	0.0617 (4)	0.7590 (3)	0.33523 (19)	0.0230 (5)
H6A	−0.0272	0.8500	0.3051	0.028*
H6B	−0.0049	0.7010	0.3680	0.028*
C7	0.0424 (4)	0.5829 (3)	0.18720 (19)	0.0229 (5)
C8	0.0942 (4)	0.4339 (3)	0.1700 (2)	0.0325 (7)
H8A	0.2135	0.3697	0.1835	0.039*
C9	−0.0290 (5)	0.3790 (3)	0.1330 (3)	0.0394 (8)
H9A	0.0068	0.2772	0.1217	0.047*
C10	−0.1997 (5)	0.4697 (4)	0.1129 (2)	0.0375 (8)
H10A	−0.2831	0.4310	0.0884	0.045*
C11	−0.2522 (4)	0.6186 (4)	0.1281 (2)	0.0378 (8)
H11A	−0.3711	0.6822	0.1129	0.045*
C12	−0.1322 (4)	0.6748 (3)	0.1652 (2)	0.0335 (7)
H12A	−0.1692	0.7770	0.1758	0.040*
C13	0.2342 (4)	0.7867 (3)	0.15637 (19)	0.0227 (5)
C14	0.1854 (4)	0.7949 (4)	0.0613 (2)	0.0339 (7)
H14A	0.1303	0.7297	0.0404	0.041*
C15	0.2167 (5)	0.8975 (4)	−0.0029 (2)	0.0424 (8)
H15A	0.1858	0.9011	−0.0680	0.051*
C16	0.2934 (5)	0.9955 (4)	0.0282 (3)	0.0414 (8)
H16A	0.3104	1.0689	−0.0150	0.050*
C17	0.3444 (5)	0.9857 (4)	0.1215 (3)	0.0378 (8)
H17A	0.3977	1.0519	0.1425	0.045*
C18	0.3189 (4)	0.8801 (3)	0.1855 (2)	0.0285 (6)
H18A	0.3593	0.8716	0.2493	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03087 (16)	0.02167 (15)	0.03252 (16)	0.00010 (10)	−0.00920 (10)	−0.00312 (9)
P1	0.0243 (4)	0.0165 (3)	0.0215 (3)	−0.0036 (3)	−0.0032 (3)	−0.0036 (3)
O1	0.0364 (13)	0.0254 (12)	0.0523 (15)	−0.0074 (10)	0.0050 (11)	−0.0014 (10)
O2	0.0350 (13)	0.0333 (13)	0.0535 (15)	−0.0049 (10)	0.0092 (11)	0.0023 (11)
O3	0.0476 (14)	0.0205 (11)	0.0509 (15)	0.0013 (10)	−0.0151 (11)	−0.0095 (10)
O4	0.0377 (12)	0.0186 (10)	0.0362 (12)	−0.0080 (9)	−0.0105 (9)	−0.0035 (8)
O5	0.0479 (14)	0.0260 (12)	0.0433 (13)	−0.0169 (11)	−0.0224 (11)	0.0037 (10)
O6	0.0708 (18)	0.0321 (13)	0.0454 (15)	−0.0250 (13)	−0.0217 (13)	0.0142 (11)
N1	0.0319 (13)	0.0239 (13)	0.0343 (14)	−0.0151 (11)	0.0092 (11)	−0.0096 (10)
N2	0.0283 (12)	0.0136 (11)	0.0207 (11)	−0.0034 (9)	−0.0046 (9)	−0.0004 (8)
N3	0.0320 (14)	0.0225 (13)	0.0275 (13)	−0.0035 (11)	−0.0083 (10)	−0.0036 (10)
N4	0.0292 (13)	0.0214 (12)	0.0271 (12)	−0.0068 (10)	−0.0038 (10)	0.0000 (10)

C1	0.0248 (14)	0.0313 (16)	0.0276 (15)	−0.0123 (12)	0.0047 (11)	−0.0092 (12)
C2	0.0234 (14)	0.0331 (16)	0.0205 (13)	−0.0096 (12)	0.0016 (10)	−0.0042 (11)
C3	0.0171 (12)	0.0223 (14)	0.0205 (13)	−0.0049 (10)	0.0035 (10)	−0.0043 (10)
C4	0.0230 (13)	0.0214 (14)	0.0240 (14)	−0.0064 (11)	−0.0002 (10)	−0.0025 (11)
C5	0.0286 (15)	0.0275 (16)	0.0277 (15)	−0.0085 (12)	0.0053 (11)	−0.0001 (11)
C6	0.0243 (13)	0.0240 (14)	0.0202 (13)	−0.0074 (11)	−0.0008 (10)	−0.0039 (10)
C7	0.0267 (14)	0.0198 (13)	0.0229 (13)	−0.0086 (11)	−0.0025 (11)	−0.0024 (10)
C8	0.0340 (17)	0.0243 (16)	0.0362 (17)	−0.0058 (13)	−0.0082 (13)	−0.0045 (12)
C9	0.053 (2)	0.0170 (15)	0.049 (2)	−0.0121 (15)	−0.0120 (16)	−0.0056 (13)
C10	0.0388 (18)	0.0405 (19)	0.0408 (18)	−0.0222 (16)	−0.0018 (14)	−0.0082 (14)
C11	0.0276 (16)	0.043 (2)	0.0406 (19)	−0.0075 (14)	0.0001 (13)	−0.0133 (15)
C12	0.0316 (16)	0.0225 (16)	0.0429 (18)	−0.0033 (13)	−0.0039 (13)	−0.0111 (13)
C13	0.0206 (13)	0.0209 (13)	0.0233 (13)	−0.0030 (11)	0.0012 (10)	−0.0025 (10)
C14	0.0360 (17)	0.0389 (18)	0.0293 (16)	−0.0166 (15)	−0.0054 (13)	0.0011 (13)
C15	0.0381 (19)	0.063 (2)	0.0269 (16)	−0.0213 (18)	−0.0099 (13)	0.0133 (15)
C16	0.0333 (17)	0.0385 (19)	0.049 (2)	−0.0107 (15)	0.0033 (15)	0.0135 (15)
C17	0.0393 (19)	0.0294 (17)	0.048 (2)	−0.0156 (15)	0.0118 (15)	−0.0065 (14)
C18	0.0282 (15)	0.0315 (16)	0.0276 (15)	−0.0118 (13)	0.0031 (12)	−0.0081 (12)

Geometric parameters (Å, º)

Ag1—P1	2.3500 (8)	C5—H5A	0.9500
Ag1—O4	2.354 (2)	C6—H6A	0.9900
Ag1—O1	2.370 (2)	C6—H6B	0.9900
P1—C7	1.817 (3)	C7—C12	1.391 (4)
P1—C13	1.817 (3)	C7—C8	1.393 (4)
P1—C6	1.854 (3)	C8—C9	1.393 (4)
O1—N3	1.257 (3)	C8—H8A	0.9500
O2—N3	1.246 (3)	C9—C10	1.358 (5)
O3—N3	1.236 (3)	C9—H9A	0.9500
O4—N4	1.273 (3)	C10—C11	1.385 (5)
O5—N4	1.256 (3)	C10—H10A	0.9500
O6—N4	1.229 (3)	C11—C12	1.381 (5)
N1—C1	1.349 (4)	C11—H11A	0.9500
N1—C5	1.352 (4)	C12—H12A	0.9500
N1—H1A	0.8800	C13—C18	1.390 (4)
N2—C3	1.336 (3)	C13—C14	1.393 (4)
N2—C6	1.452 (3)	C14—C15	1.387 (5)
N2—H2A	0.8800	C14—H14A	0.9500
C1—C2	1.351 (4)	C15—C16	1.394 (5)
C1—H1B	0.9500	C15—H15A	0.9500
C2—C3	1.430 (4)	C16—C17	1.371 (5)
C2—H2B	0.9500	C16—H16A	0.9500
C3—C4	1.408 (4)	C17—C18	1.386 (4)
C4—C5	1.368 (4)	C17—H17A	0.9500
C4—H4A	0.9500	C18—H18A	0.9500
P1—Ag1—O4	136.46 (5)	P1—C6—H6A	109.0

P1—Ag1—O1	138.31 (7)	N2—C6—H6B	109.0
O4—Ag1—O1	84.99 (8)	P1—C6—H6B	109.0
C7—P1—C13	105.94 (13)	H6A—C6—H6B	107.8
C7—P1—C6	100.58 (13)	C12—C7—C8	118.8 (3)
C13—P1—C6	104.39 (13)	C12—C7—P1	122.2 (2)
C7—P1—Ag1	114.33 (10)	C8—C7—P1	119.0 (2)
C13—P1—Ag1	115.36 (9)	C7—C8—C9	120.0 (3)
C6—P1—Ag1	114.65 (9)	C7—C8—H8A	120.0
N3—O1—Ag1	102.13 (18)	C9—C8—H8A	120.0
N4—O4—Ag1	111.82 (16)	C10—C9—C8	120.7 (3)
C1—N1—C5	120.7 (3)	C10—C9—H9A	119.7
C1—N1—H1A	119.7	C8—C9—H9A	119.7
C5—N1—H1A	119.7	C9—C10—C11	120.0 (3)
C3—N2—C6	126.9 (2)	C9—C10—H10A	120.0
C3—N2—H2A	116.5	C11—C10—H10A	120.0
C6—N2—H2A	116.5	C12—C11—C10	120.2 (3)
O3—N3—O2	121.7 (3)	C12—C11—H11A	119.9
O3—N3—O1	120.0 (3)	C10—C11—H11A	119.9
O2—N3—O1	118.3 (3)	C11—C12—C7	120.4 (3)
O6—N4—O5	121.6 (2)	C11—C12—H12A	119.8
O6—N4—O4	121.0 (2)	C7—C12—H12A	119.8
O5—N4—O4	117.5 (2)	C18—C13—C14	119.1 (3)
N1—C1—C2	121.3 (3)	C18—C13—P1	119.2 (2)
N1—C1—H1B	119.3	C14—C13—P1	121.5 (2)
C2—C1—H1B	119.3	C15—C14—C13	120.4 (3)
C1—C2—C3	120.1 (3)	C15—C14—H14A	119.8
C1—C2—H2B	120.0	C13—C14—H14A	119.8
C3—C2—H2B	120.0	C14—C15—C16	119.8 (3)
N2—C3—C4	124.7 (2)	C14—C15—H15A	120.1
N2—C3—C2	118.4 (3)	C16—C15—H15A	120.1
C4—C3—C2	116.9 (3)	C17—C16—C15	119.7 (3)
C5—C4—C3	120.0 (3)	C17—C16—H16A	120.1
C5—C4—H4A	120.0	C15—C16—H16A	120.1
C3—C4—H4A	120.0	C16—C17—C18	120.8 (3)
N1—C5—C4	121.0 (3)	C16—C17—H17A	119.6
N1—C5—H5A	119.5	C18—C17—H17A	119.6
C4—C5—H5A	119.5	C17—C18—C13	120.1 (3)
N2—C6—P1	112.86 (19)	C17—C18—H18A	120.0
N2—C6—H6A	109.0	C13—C18—H18A	120.0

O4—Ag1—P1—C7	−139.96 (13)	C13—P1—C7—C12	−63.3 (3)
O1—Ag1—P1—C7	47.87 (14)	C6—P1—C7—C12	45.2 (3)
O4—Ag1—P1—C13	96.81 (13)	Ag1—P1—C7—C12	168.5 (2)
O1—Ag1—P1—C13	−75.36 (13)	C13—P1—C7—C8	119.1 (2)
O4—Ag1—P1—C6	−24.55 (14)	C6—P1—C7—C8	−132.4 (2)
O1—Ag1—P1—C6	163.29 (13)	Ag1—P1—C7—C8	−9.1 (3)
P1—Ag1—O1—N3	−89.92 (19)	C12—C7—C8—C9	−1.1 (5)
O4—Ag1—O1—N3	95.49 (19)	P1—C7—C8—C9	176.6 (3)

P1—Ag1—O4—N4	−46.8 (2)	C7—C8—C9—C10	0.3 (5)
O1—Ag1—O4—N4	128.01 (19)	C8—C9—C10—C11	0.8 (6)
Ag1—O1—N3—O3	179.4 (2)	C9—C10—C11—C12	−1.1 (5)
Ag1—O1—N3—O2	−0.7 (3)	C10—C11—C12—C7	0.3 (5)
Ag1—O4—N4—O6	−0.5 (4)	C8—C7—C12—C11	0.7 (5)
Ag1—O4—N4—O5	179.1 (2)	P1—C7—C12—C11	−176.9 (3)
C5—N1—C1—C2	−0.5 (4)	C7—P1—C13—C18	166.2 (2)
N1—C1—C2—C3	0.0 (4)	C6—P1—C13—C18	60.5 (3)
C6—N2—C3—C4	−1.9 (4)	Ag1—P1—C13—C18	−66.2 (2)
C6—N2—C3—C2	177.3 (2)	C7—P1—C13—C14	−17.5 (3)
C1—C2—C3—N2	−178.8 (3)	C6—P1—C13—C14	−123.2 (3)
C1—C2—C3—C4	0.4 (4)	Ag1—P1—C13—C14	110.0 (2)
N2—C3—C4—C5	178.9 (3)	C18—C13—C14—C15	−1.7 (5)
C2—C3—C4—C5	−0.2 (4)	P1—C13—C14—C15	−177.9 (3)
C1—N1—C5—C4	0.7 (4)	C13—C14—C15—C16	−1.6 (5)
C3—C4—C5—N1	−0.3 (4)	C14—C15—C16—C17	2.7 (6)
C3—N2—C6—P1	111.1 (3)	C15—C16—C17—C18	−0.6 (5)
C7—P1—C6—N2	167.0 (2)	C16—C17—C18—C13	−2.7 (5)
C13—P1—C6—N2	−83.4 (2)	C14—C13—C18—C17	3.8 (4)
Ag1—P1—C6—N2	43.8 (2)	P1—C13—C18—C17	−179.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O5^{i}	0.88	1.93	2.807 (3)	172
N2—H2*A*···O4^{ii}	0.88	2.16	3.013 (3)	162
N2—H2*A*···O5^{ii}	0.88	2.47	3.075 (3)	127

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