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Bis[(4-methylphenyl)diphenylphosphane-κP]-(nitrato-$\kappa^2 O,O'$)silver(I)

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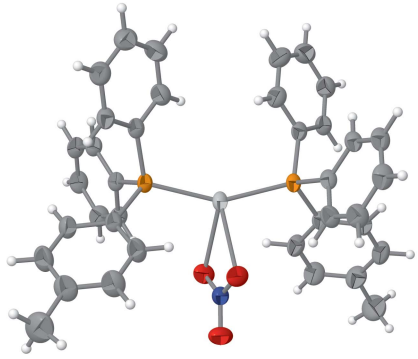
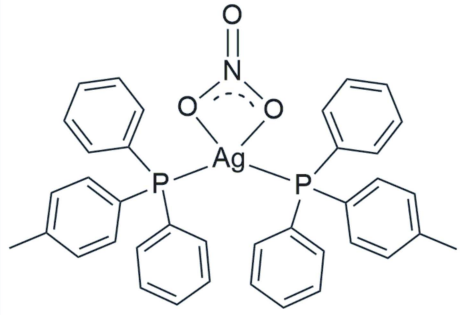
Structural data: full structural data are available from iucrdata.iucr.org

The molecular structure of the title Ag^I complex, $[Ag(NO_3)(C_{19}H_{17}P)_2]$ or $[Ag\{(p\text{-}CH_3C_6H_4)(C_6H_5)_2P\text{-}\kappa P\}_2\text{-}NO_3\text{-}\kappa^2 O{:}O']$, is described, where a distorted trigonal–planar coordination environment is exhibited about the central Ag^I atom; in this description, the two O atoms are assumed to occupy one position in the coordination sphere. The compound crystallized with half a molecule in the asymmetric unit having the Ag^I atom lying on a twofold axis.

3D view



Chemical scheme



Structure description

Silver(I) phosphine complexes have been found to exhibit high antimicrobial, antibacterial and anticancer activity (Potgieter *et al.*, 2016). The continuously expanding library of active compounds leads to a growing interest into their solid- and solution-state characterization, including by single-crystal X-ray diffraction.

The molecular structure of the title compound is shown in Fig. 1. The complex crystallized in the monoclinic space group *C*2/*c*, $Z = 4$ with the asymmetric unit comprising one half of the silver complex molecule, as the central Ag^I atom, along with the nitrato-N and one nitrato-O atom, lying on a twofold axis. Coordinated to the Ag^I atom are two diphenyl-*p*-tolylphosphine ligands, and one nitrato ligand, *via* two O atoms; in this description, the two O atoms are assumed to occupy one position in the coordination environment. The symmetry present in the molecule results in identical Ag—P1 [2.4095 (9) Å] and Ag—O1 [2.522 (3) Å] bond lengths, which fall within the ranges of related compounds (Potgieter *et al.*, 2016). The distorted trigonal–planar coordination displayed by the central Ag^I atom stems from the three coordinating ligands, with corresponding bond angles P1—Ag1—P1^i [152.89 (5)°], P1—Ag1—O1 [109.76 (7)°], and P1—Ag1—O1^i [94.92 (7)°]; symmetry operation: (i) $1-x, y, \frac{3}{2}-z$. The bidentate mode of coordination of the nitrato ligand is confirmed by the O1—Ag1—O1^i bite angle of

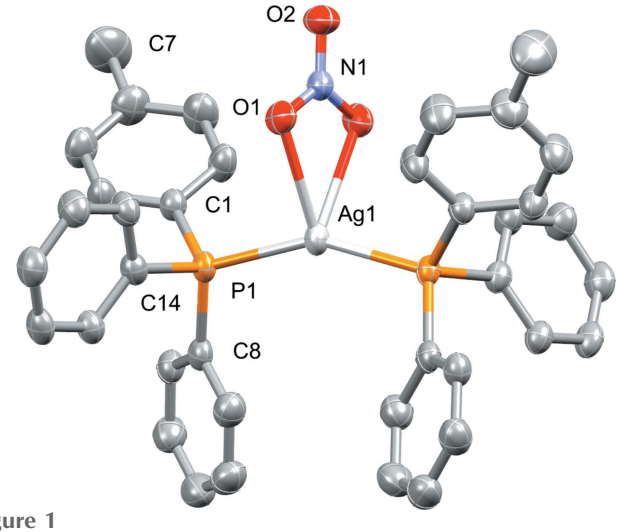


Figure 1
Perspective view of the molecular structure of the title compound showing thermal displacement ellipsoids at the 50% probability level. Hydrogen atoms are omitted for clarity. Unlabelled atoms are related by a twofold axis of symmetry.

50.63 (12)°. The *ipso*-aryl carbon atoms of each of the phosphine ligands overlap in a near-staggered fashion when viewed down the P1–Ag1–P1^{i} axis, presumably due to the steric bulk of the phosphine ligands. The corresponding torsion angles are P1^{i}—Ag1—P1—C1 = −148.40 (15)°, P1^{i}—Ag1—P1—C8 = −24.78 (17)° and P1^{i}—Ag1—P1—C14 = 92.91 (14)°. The plane defined by atoms P1, Ag, P1^{i} and N1 intercepts the plane defined by Ag1, O1, O1^{i} and O2 at an angle of 72.33 (9)°.

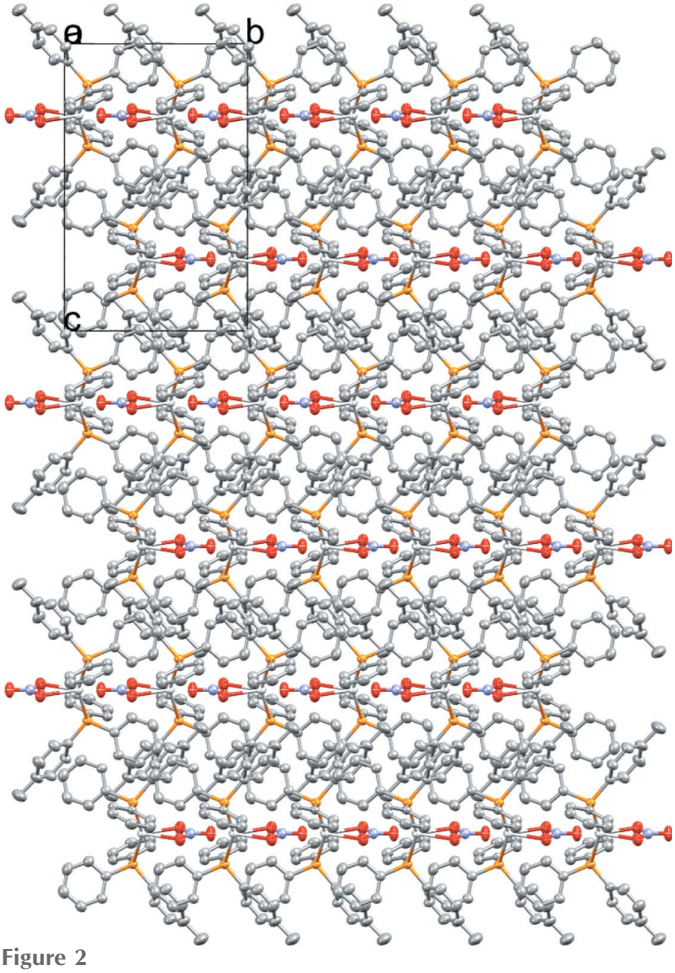


Figure 2
Packing diagram viewed along the *a*-axis.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Ag(NO_3)\{C_{19}H_{17}P)_2]$
M_r	722.47
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	18.1290 (6), 11.0936 (5), 17.9971 (7)
β (°)	104.849 (4)
V (Å^3)	3498.6 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.77
Crystal size (mm)	0.21 × 0.18 × 0.10
Data collection	
Diffractometer	XtaLAB Synergy R, DW system, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.344, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20162, 3668, 3383
R_{int}	0.082
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.637
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.109, 1.06
No. of reflections	3668
No. of parameters	206
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.60, −1.14

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

In the crystal, the complex packs in three-dimensions as layers of isolated complexes. Within these layers a metal-containing NO_3 layer is observed, which alternates with dense arene-ring-filled layers. A view of the unit-cell contents is shown in Fig. 2.

Synthesis and crystallization

Diphenyl-*p*-tolylphosphine (2 mmol) and silver nitrate (1 mmol) were dissolved separately in acetonitrile (10 ml). The solutions were carefully mixed together and heated to 353 K for approximately 2 h. The solution was left to crystallize, and small clear crystals were obtained.

Refinement

For full experimental details including crystal data, data collection and structure refinement details, refer to Table 1. The maximum and minimum residual electron density peaks of 0.60 and 1.14 e Å^{-3} are located 1.29 and 0.83 Å, respectively, from the Ag1 atom, features ascribed to the presence of the strong absorber.

Acknowledgements

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full crystallographic data

IUCrData (2022). **7**, x221045 [https://doi.org/10.1107/S2414314622010458]

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Crystal data

$[Ag(NO_3)\{C_{19}H_{17}P)_2]$
M_r = 722.47
Monoclinic, $C2/c$
a = 18.1290 (6) Å
b = 11.0936 (5) Å
c = 17.9971 (7) Å
β = 104.849 (4)°
V = 3498.6 (2) Å^3
Z = 4
$F(000)$ = 1480
D_x = 1.372 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 14857 reflections
θ = 4.7–78.5°
μ = 5.77 mm^{-1}
T = 150 K
Blade, colourless
0.21 × 0.18 × 0.10 mm

Data collection

XtaLAB Synergy R, DW system, HyPix diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.344, T_{max} = 1.000
20162 measured reflections
3668 independent reflections
3383 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 79.2°, θ_{min} = 4.7°
h = −22→23
k = −13→12
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.109
S = 1.06
3668 reflections
206 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 20.5034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.5000	0.42530 (4)	0.7500	0.03274 (12)
P1	0.39526 (5)	0.37440 (9)	0.64210 (5)	0.0295 (2)
O1	0.55106 (15)	0.6308 (3)	0.72975 (18)	0.0428 (7)
O2	0.5000	0.7999 (4)	0.7500	0.0573 (12)
N1	0.5000	0.6886 (4)	0.7500	0.0361 (10)
C8	0.4038 (2)	0.2263 (4)	0.6014 (2)	0.0332 (8)
C14	0.3048 (2)	0.3676 (3)	0.6690 (2)	0.0317 (8)
C1	0.3777 (2)	0.4809 (4)	0.5629 (2)	0.0329 (8)
C13	0.3896 (2)	0.2044 (4)	0.5231 (2)	0.0378 (9)
H13	0.3746	0.2688	0.4877	0.045*
C18	0.1918 (2)	0.2650 (4)	0.6813 (2)	0.0405 (9)
H18	0.1604	0.1952	0.6736	0.049*
C19	0.2580 (2)	0.2661 (4)	0.6569 (2)	0.0349 (8)
H19	0.2717	0.1975	0.6318	0.042*
C15	0.2837 (2)	0.4685 (4)	0.7050 (2)	0.0407 (9)
H15	0.3152	0.5381	0.7136	0.049*
C17	0.1711 (2)	0.3650 (4)	0.7169 (2)	0.0448 (10)
H17	0.1254	0.3639	0.7336	0.054*
C2	0.3067 (2)	0.4939 (4)	0.5108 (2)	0.0426 (9)
H2	0.2650	0.4456	0.5159	0.051*
C6	0.4374 (2)	0.5548 (4)	0.5552 (3)	0.0449 (10)
H6	0.4863	0.5470	0.5902	0.054*
C3	0.2965 (3)	0.5765 (5)	0.4519 (3)	0.0538 (12)
H3	0.2481	0.5826	0.4159	0.065*
C9	0.4264 (3)	0.1314 (4)	0.6525 (3)	0.0466 (10)
H9	0.4370	0.1457	0.7062	0.056*
C12	0.3973 (3)	0.0894 (4)	0.4965 (3)	0.0496 (11)
H12	0.3874	0.0754	0.4428	0.060*
C16	0.2163 (2)	0.4664 (4)	0.7282 (3)	0.0456 (10)
H16	0.2014	0.5353	0.7521	0.055*
C4	0.3559 (3)	0.6513 (5)	0.4439 (3)	0.0533 (11)
C11	0.4192 (3)	−0.0056 (4)	0.5472 (3)	0.0552 (12)
H11	0.4242	−0.0845	0.5285	0.066*
C5	0.4258 (3)	0.6397 (5)	0.4970 (3)	0.0555 (12)
H5	0.4667	0.6909	0.4934	0.067*
C10	0.4338 (3)	0.0157 (4)	0.6257 (3)	0.0540 (11)
H10	0.4488	−0.0489	0.6610	0.065*
C7	0.3448 (4)	0.7468 (6)	0.3819 (3)	0.0817 (19)
H7A	0.3270	0.7088	0.3313	0.123*
H7B	0.3934	0.7878	0.3852	0.123*
H7C	0.3069	0.8055	0.3891	0.123*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02296 (18)	0.0399 (2)	0.0335 (2)	0.000	0.00388 (14)	0.000
P1	0.0214 (4)	0.0375 (5)	0.0295 (4)	−0.0018 (3)	0.0064 (3)	0.0016 (4)
O1	0.0279 (13)	0.0427 (16)	0.0639 (18)	−0.0022 (12)	0.0233 (13)	−0.0038 (14)
O2	0.045 (3)	0.033 (2)	0.095 (4)	0.000	0.020 (2)	0.000
N1	0.026 (2)	0.035 (2)	0.045 (3)	0.000	0.0062 (19)	0.000
C8	0.0216 (16)	0.041 (2)	0.0380 (19)	−0.0008 (14)	0.0088 (14)	0.0016 (16)
C14	0.0285 (17)	0.040 (2)	0.0271 (16)	−0.0037 (15)	0.0079 (14)	0.0028 (15)
C1	0.0276 (17)	0.0384 (19)	0.0331 (18)	−0.0005 (15)	0.0084 (14)	0.0022 (15)
C13	0.0292 (18)	0.045 (2)	0.038 (2)	0.0015 (16)	0.0074 (16)	−0.0025 (17)
C18	0.0287 (19)	0.052 (2)	0.042 (2)	−0.0087 (17)	0.0118 (16)	0.0056 (18)
C19	0.0301 (18)	0.042 (2)	0.0329 (18)	−0.0043 (16)	0.0082 (15)	0.0011 (16)
C15	0.0294 (19)	0.048 (2)	0.047 (2)	−0.0053 (17)	0.0130 (17)	−0.0059 (19)
C17	0.031 (2)	0.062 (3)	0.046 (2)	−0.0012 (19)	0.0179 (18)	0.004 (2)
C2	0.033 (2)	0.050 (2)	0.041 (2)	−0.0052 (18)	0.0032 (17)	0.0079 (18)
C6	0.0280 (19)	0.056 (3)	0.051 (2)	0.0009 (18)	0.0112 (17)	0.013 (2)
C3	0.046 (3)	0.064 (3)	0.045 (2)	0.002 (2)	0.000 (2)	0.013 (2)
C9	0.042 (2)	0.049 (2)	0.047 (2)	0.0025 (19)	0.0088 (19)	0.0061 (19)
C12	0.043 (2)	0.053 (3)	0.051 (2)	0.004 (2)	0.009 (2)	−0.009 (2)
C16	0.036 (2)	0.054 (3)	0.051 (2)	−0.0006 (19)	0.0193 (19)	−0.005 (2)
C4	0.056 (3)	0.062 (3)	0.043 (2)	0.002 (2)	0.014 (2)	0.015 (2)
C11	0.045 (3)	0.047 (3)	0.072 (3)	0.003 (2)	0.013 (2)	−0.009 (2)
C5	0.046 (3)	0.065 (3)	0.058 (3)	−0.006 (2)	0.018 (2)	0.018 (2)
C10	0.050 (3)	0.046 (3)	0.065 (3)	0.007 (2)	0.013 (2)	0.012 (2)
C7	0.096 (5)	0.083 (4)	0.058 (3)	−0.010 (4)	0.003 (3)	0.025 (3)

Geometric parameters (Å, º)

Ag1—P1^{i}	2.4095 (9)	C1—C6	1.393 (5)
Ag1—P1	2.4095 (9)	C13—C12	1.383 (6)
Ag1—O1^{i}	2.522 (3)	C18—C19	1.380 (5)
Ag1—O1	2.522 (3)	C18—C17	1.380 (6)
P1—C8	1.822 (4)	C15—C16	1.388 (5)
P1—C14	1.827 (4)	C17—C16	1.375 (6)
P1—C1	1.815 (4)	C2—C3	1.377 (6)
O1—N1	1.255 (3)	C6—C5	1.384 (6)
O2—N1	1.235 (6)	C3—C4	1.395 (7)
N1—O1^{i}	1.255 (3)	C9—C10	1.390 (7)
C8—C13	1.386 (5)	C12—C11	1.383 (7)
C8—C9	1.389 (6)	C4—C5	1.385 (7)
C14—C19	1.393 (5)	C4—C7	1.514 (7)
C14—C15	1.395 (6)	C11—C10	1.389 (7)
C1—C2	1.392 (5)		
P1^{i}—Ag1—P1	152.89 (5)	C15—C14—P1	117.5 (3)
P1—Ag1—O1	109.76 (7)	C2—C1—P1	122.9 (3)

P1^{i}—Ag1—O1^{i}	109.76 (7)	C2—C1—C6	118.6 (4)
P1^{i}—Ag1—O1	94.92 (7)	C6—C1—P1	118.5 (3)
P1—Ag1—O1^{i}	94.92 (7)	C12—C13—C8	120.3 (4)
O1—Ag1—O1^{i}	50.63 (12)	C19—C18—C17	120.2 (4)
C8—P1—Ag1	113.90 (12)	C18—C19—C14	120.1 (4)
C8—P1—C14	104.11 (17)	C16—C15—C14	119.6 (4)
C14—P1—Ag1	111.84 (12)	C16—C17—C18	120.2 (4)
C1—P1—Ag1	115.07 (12)	C3—C2—C1	120.4 (4)
C1—P1—C8	106.68 (18)	C5—C6—C1	120.4 (4)
C1—P1—C14	104.22 (17)	C2—C3—C4	121.3 (4)
N1—O1—Ag1	95.4 (2)	C8—C9—C10	120.5 (4)
O1—N1—O1^{i}	118.5 (4)	C13—C12—C11	120.8 (4)
O2—N1—O1	120.8 (2)	C17—C16—C15	120.4 (4)
O2—N1—O1^{i}	120.8 (2)	C3—C4—C7	122.2 (5)
C13—C8—P1	123.6 (3)	C5—C4—C3	117.9 (4)
C13—C8—C9	119.1 (4)	C5—C4—C7	119.9 (5)
C9—C8—P1	117.3 (3)	C12—C11—C10	119.3 (4)
C19—C14—P1	122.9 (3)	C6—C5—C4	121.3 (4)
C19—C14—C15	119.5 (3)	C11—C10—C9	120.0 (4)

Symmetry code: (i) $-x+1, y, -z+3/2$.