Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*N*-Phenylthiourea-κ*S*)bis(triphenylphosphane-κ*P*)silver(I) nitrate

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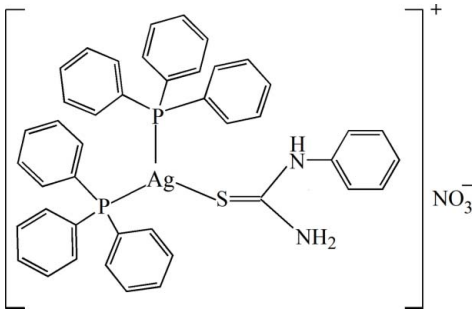
Received 11 June 2014; accepted 17 June 2014

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.064; data-to-parameter ratio = 19.2.

In the title salt, $[Ag(C_7H_8N_2S)(C_{18}H_{15}P)_2]NO_3$, the coordination geometry about the Ag^I atom is shallow trigonal pyramidal, with the metal atom displaced by 0.372 (1) Å from the plane of the P and S atoms. In the crystal, the cations are linked to the anions by N—H···O hydrogen bonds, generating tetramers (two cations and two anions), which feature $R_2^2(8)$ and $R_4^4(8)$ loops. The cations are linked by weak C—H···π interactions, generating a three-dimensional network.

Related literature

For properties of mixed-ligand d^{10} metal(I) complexes, see: Oshio *et al.* (1996); Zheng *et al.* (2001); Sewead *et al.* (2003); Isab *et al.* (2010). For structural studies of mixed-ligand complexes of triphenylphosphane and thione ligands, see: Skoulika *et al.* (1991); Aslanidis *et al.* (1997); Ghassemzadeh *et al.*(2004); Nimthong *et al.* (2008); Isab *et al.* (2010).



Experimental

Crystal data

$[Ag(C_7H_8N_2S)(C_{18}H_{15}P)_2]NO_3$
M_r = 846.63
Monoclinic, $P2_1/c$
a = 13.6113 (5) Å
b = 10.6431 (4) Å
c = 26.4365 (10) Å
β = 96.068 (1)°
V = 3808.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.71 mm^{-1}
T = 173 K
0.27 × 0.14 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.863, T_{max} = 1.000
44417 measured reflections
9196 independent reflections
8261 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.064
S = 1.05
9196 reflections
478 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

*Cg*2 is the centroid of the C11–C16 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3^{i}	0.86	2.02	2.877 (2)	180
N1—H1B···O3^{ii}	0.86	2.17	2.921 (2)	145
N2—H2···O1^{i}	0.86	1.97	2.823 (2)	171
C35—H35···$Cg2^{iii}$	0.93	2.97	3.746 (2)	142
C54—H54···$Cg2^{iv}$	0.93	2.82	3.531 (2)	134

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+1, -z+2$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y+2, -z+2$.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Financial support from the Center of Excellent for Innovation in Chemistry (PERCH–CIC), Office of the Higher Education Commission, Ministry of Education and Graduate School, Prince of Songkla University, are gratefully acknowledged.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7242).

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supporting information

Acta Cryst. (2014). E**70**, m281–m282 [doi:10.1107/S1600536814014147]

(*N*-Phenylthiourea-κS)bis(triphenylphosphane-κP)silver(I) nitrate

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1. Chemical context

Mixed-ligand complexes of group 11 metals dispaly many properties such as magnetism (Oshio *et al.*, 1996); microporousity (Zheng *et al.*, 2001); luminescence (Sewead *et al.*, 2003) and antimicrobial activities (Isab *et al.*,2010). In our earlier work, we synthesized and characterized the neutral monomeric copper(I) complex containing mixed ligands of triphenylphosphane (PPh_3: $C_{18}H_{15}P$) and *N*-phynylthiourea (ptu : $C_7H_8N_2S$), [CuI(ptu)(PPh_3)$_2$] (Nimthong *et al.*, 2008). As part of our continuing studies in this area, we now describe the synthesis and structure of the title compound, [Ag(ptu)(PPh_3)$_2$]NO_3 (Scheme I).

2. Structural commentary

Unlike the previous complex mentioned above (Nimthong *et al.*, 2008), this complex is an ionic complex and it crystallizes in monoclinic system space group $P2_1/c$. The structure consists of the discrete mononuclear [Ag(ptu)(PPh_3)$_2$]$^+$cation and the NO_3^- anion which is similar to those [Ag(PPh_3)$_2$(pymtH)]NO_3 (Aslanidis *et al.*, 1997). A perspective view of the molecular structure of [Ag(ptu)(PPh_3)$_2$]NO_3 with atomic labeling is given in Figure 1. The cation part contains silver(I) atom trigonally coordinated by two phosphorus atoms from two triphenylphosphane molecules and one sulfur atom from *N*–phenylthiourea molecule similar to found in those silver oxyanion complexes containing mixed PPh_3/heterocyclic thione ligands (Aslanidis *et al.*, 1997; Ghassemzadeh *et al.*, 2004). The Ag–P bond lengths of 2.4645 (5) and 2.4693 (4)Å are similar to the values of 2.455 (1) and 2.447 (1) Å observed in [Ag(PPh_3)$_2$(pymtH)]NO_3 (Aslanidis *et al.*, 1997), however, these values are slightly different from the values of 2.458 (2) and 2.507 (2) Å compared to [Ag(TAMTTO)(PPh_3)$_2$]NO_3.1.5THF (Ghassemzadeh *et al.*, 2004) because of the massive and steric effect of TAMTTO heterocyclic ligand. The Ag–S bond length [2.5307 (7) Å] is shorter than in those complexes [Ag(PPh_3)$_2$(pymtH)]NO_3 [2.573 (1)Å] and [Ag(TAMTTO)(PPh_3)$_2$]NO_3.1.5 THF [2.592 (2) Å] (Aslanidis *et al.*, 1997; Ghassemzadeh *et al.*, 2004). The P(1)–Ag–P(2), P(1)–Ag–S(1) and P(2)–Ag–S(1) bond angles are 127.55 (1)° ,113.02 (1)° and 112.69 (1)°, respectively. Due to the steric crowding of six phenyl rings from two bulky triphenyl phosphane ligands and the π(CH)···Ag interaction [3.314 Å] between the centriod of phenyl ring (C2—C7) of the *N*–phenylthiourea and metal atom, the silver centre atom deviates from idealized trigonal planar with this atom lying *ca* 0.372 (1) Å out of the P_2S plane. For the anion, although the oxygen atoms of the nitrate have no influence on coordination, they have great influence on the crystal packing of the complex. It is nearly planar with the bond angles around the nitrogen atom ranging from 119.01 (1)-120.53 (1)° and N(3)–O bond distances are 1.231 (2) – 1.264 (2) Å.

3. Supramolecular features

For the crystal packing, each [Ag(ptu)(PPh_3)$_2$]$^+$ cation is connected to another adjacent cationic part via hydrogen bonding interactions, N–H···O, which are observed between amino and amide groups and nitrate oxygen atoms generate a cyclic hydrogen bond interactions, two $R_2^2(8)$ graph sets for cationic-anionic interactions and one $R_4^4(8)$ graph set for

anionic-anionic interaction, [N(1)–H(1A)···O(3)^{i} : 2.877 (2)Å, N(1)–H(1B)···O(3)^{ii} : 2.921 (2)Å, N(2)–H(2)···O(1) : 2.823 (2) Å and symmetry code : (i) x-1,y,z, (ii) -x+1,-y+1,-z+2] as depicted in Figure 2 and 3. In addition, the cationic parts are linked together by the CH···π interactions between the phenyl rings with the distance of 3.746 (2) Å for C35–H35···Cg2 and 3.531 (2) Å for C54–H54···Cg2 [Cg2 : C11–C16] generating the three dimensional supramolecular network. All interactions are depicted in Figure 4.

4. Synthesis and crystallization

The mixture silver(I) nitrate and triphenylphosphane in ethanol was refluxed at the temperature *ca* 60-70 °C for 2 h. After that, *N*-phenylthiourea ligand was added to the clear mixture solution and then continued to reflux futher for 3 h. The clear filtration was kept and left to evaporate slowly at ambient temperature. After several days, colorless blocks were obtained. The melting point of the complex is 192-194 °C . Elemental analysis,calculated for $[Ag(PPh_3)_2(ptu)]NO_3$: C, 60.99;H, 4.52; N, 4.96; S, 3.78%, found: C, 65.16; H, 4.96; N, 5.16; S, 4.04%.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The structures were solved by direct methods and refined by a full-matrix least-squares procedure based on F^2. All hydrogen atoms were placed in geometrically idealised positions and refined isotropically with a riding model for both of amine N [N—H = 0.86 Å and with U_{iso}(H) =1.2U_{eq}(N)] and phenyl ring C-sp^2[C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C)]. ;

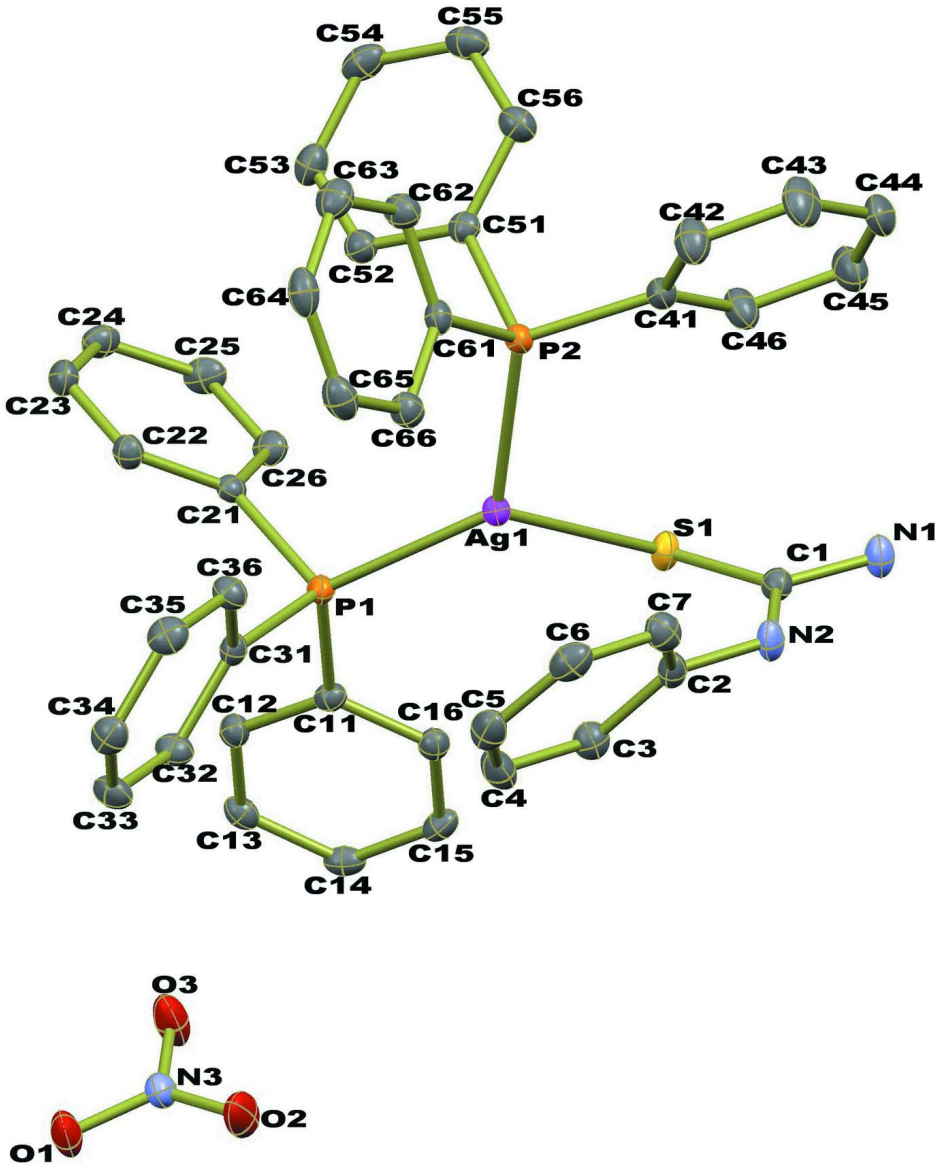

Figure 1

The molecular structure of $[Ag(ptu)(PPh_3)_2]NO_3$ complex. Displacement ellipsoids are shown at 50% probability level.

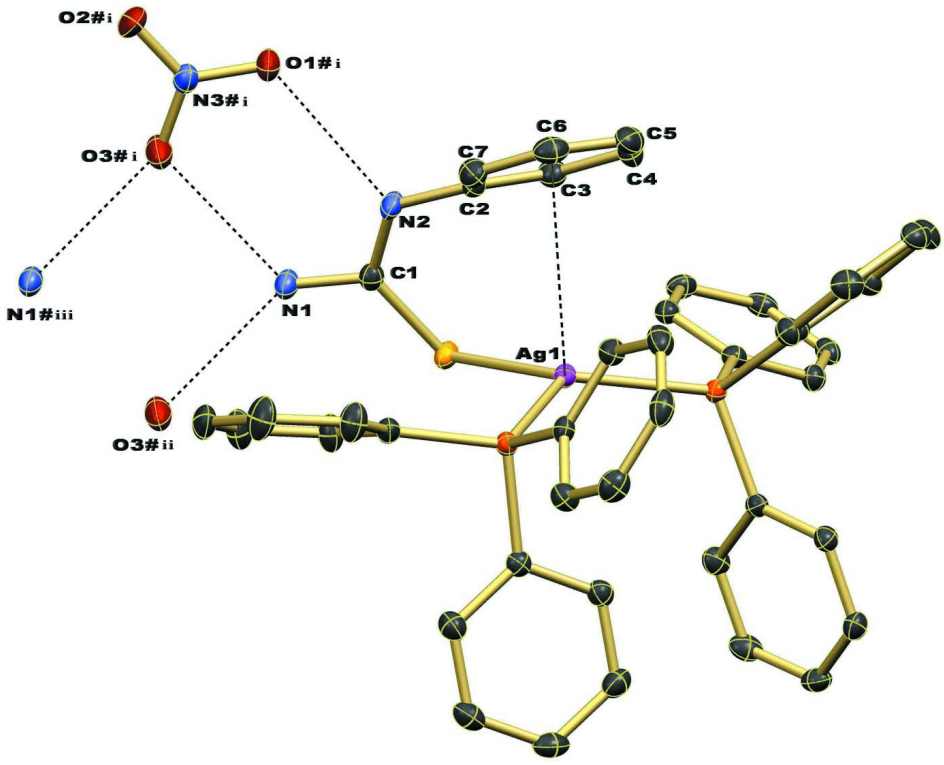

Figure 2

The hydrogen bonding interactions of $[Ag(ptu)(PPh_3)_2]NO_3$ complex (#i: *x* - 1, *y*, *z*, #ii: 1 - *x*, 1 - *y*, 2 - *z*, #iii: -*x*, 1 - *y*,2 - *z*).

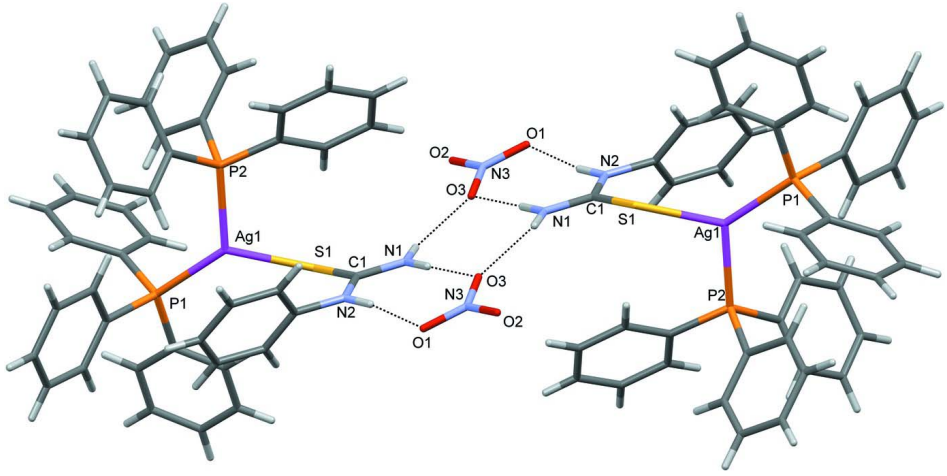

Figure 3

The cyclic of hydrogen bonding interactions containing two $R_2^2(8)$ and one $R_4^4(8)$.

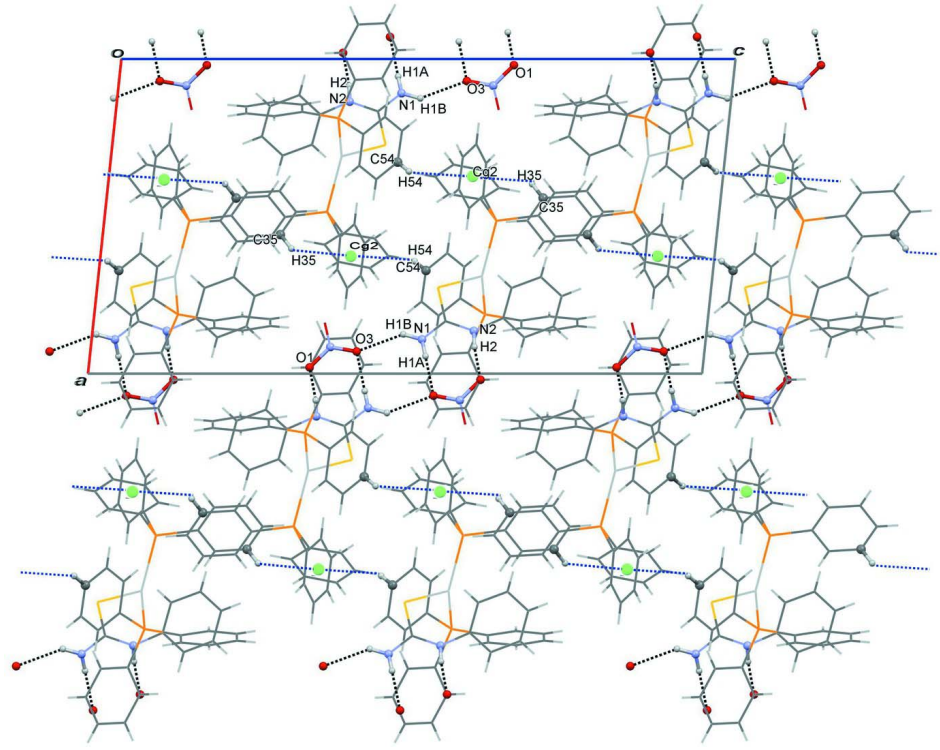

Figure 4

The three-dimensional supramolecular interactions in crystal packing.

(*N*-Phenylthiourea-κ*S*)bis(triphenylphosphane-κ*P*)silver(I) nitrate

Crystal data

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Monoclinic, $P2_1/c$
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b = 10.6431 (4) Å
c = 26.4365 (10) Å
β = 96.068 (1)°
V = 3808.3 (2) Å^3
Z = 4
$F(000)$ = 1736
D_x = 1.477 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 13930 reflections
θ = 2.3–28.0°
μ = 0.71 mm^{-1}
T = 173 K
Block, colourless
0.27 × 0.14 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Frames each covering 0.3 ° in ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.863, T_{max} = 1.000
44417 measured reflections
9196 independent reflections
8261 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 28.0°, θ_{min} = 1.5°
h = −17→17
k = −14→14
l = −34→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.064$
$S = 1.05$
9196 reflections
478 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
$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2 + 2.6456P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.30947 (2)	0.80538 (2)	0.87530 (2)	0.01346 (4)
S1	0.27373 (3)	0.65461 (4)	0.94508 (2)	0.01679 (9)
P1	0.48557 (3)	0.81150 (4)	0.86130 (2)	0.01253 (8)
P2	0.18820 (3)	0.97824 (4)	0.86365 (2)	0.01356 (9)
N1	0.10876 (11)	0.54151 (15)	0.96207 (6)	0.0205 (3)
H1A	0.0553	0.5001	0.9535	0.025*
H1B	0.1249	0.5609	0.9934	0.025*
N2	0.13553 (11)	0.54123 (15)	0.87904 (6)	0.0195 (3)
H2	0.0848	0.4926	0.8754	0.023*
N3	0.91546 (11)	0.35396 (14)	0.88996 (6)	0.0200 (3)
O1	0.98030 (10)	0.36618 (14)	0.85981 (5)	0.0285 (3)
O2	0.83834 (11)	0.29694 (14)	0.87678 (6)	0.0339 (4)
O3	0.92984 (10)	0.40319 (15)	0.93362 (5)	0.0320 (3)
C1	0.16649 (13)	0.57551 (16)	0.92682 (6)	0.0166 (3)
C2	0.17639 (13)	0.57559 (16)	0.83349 (6)	0.0165 (3)
C3	0.27222 (13)	0.54423 (18)	0.82506 (7)	0.0203 (4)
H3	0.3129	0.5015	0.8498	0.024*
C4	0.30689 (14)	0.57740 (19)	0.77919 (7)	0.0246 (4)
H4	0.3714	0.5580	0.7735	0.030*
C5	0.24611 (15)	0.63894 (18)	0.74210 (7)	0.0244 (4)
H5	0.2700	0.6612	0.7117	0.029*
C6	0.14981 (15)	0.66765 (17)	0.75003 (7)	0.0233 (4)
H6	0.1086	0.7080	0.7248	0.028*
C7	0.11484 (14)	0.63599 (18)	0.79586 (7)	0.0212 (4)
H7	0.0502	0.6553	0.8013	0.025*
C11	0.56534 (12)	0.68448 (15)	0.88711 (6)	0.0142 (3)
C12	0.66839 (13)	0.69391 (16)	0.88805 (6)	0.0160 (3)
H12	0.6962	0.7659	0.8756	0.019*

C13	0.72891 (13)	0.59703 (17)	0.90730 (6)	0.0168 (3)
H13	0.7970	0.6032	0.9070	0.020*
C14	0.68800 (13)	0.49043 (16)	0.92701 (6)	0.0178 (3)
H14	0.7285	0.4246	0.9394	0.021*
C15	0.58661 (13)	0.48238 (16)	0.92812 (6)	0.0178 (3)
H15	0.5596	0.4123	0.9425	0.021*
C16	0.52496 (13)	0.57825 (16)	0.90794 (6)	0.0154 (3)
H16	0.4569	0.5716	0.9083	0.018*
C21	0.55372 (12)	0.94570 (15)	0.89023 (6)	0.0136 (3)
C22	0.59006 (12)	1.04369 (16)	0.86294 (6)	0.0161 (3)
H22	0.5778	1.0452	0.8277	0.019*
C23	0.64480 (13)	1.13972 (17)	0.88827 (7)	0.0182 (3)
H23	0.6684	1.2056	0.8698	0.022*
C24	0.66425 (13)	1.13752 (17)	0.94081 (7)	0.0195 (4)
H24	0.7028	1.2001	0.9575	0.023*
C25	0.62590 (14)	1.04144 (17)	0.96837 (7)	0.0211 (4)
H25	0.6374	1.0408	1.0037	0.025*
C26	0.57049 (13)	0.94653 (17)	0.94329 (6)	0.0187 (4)
H26	0.5443	0.8829	0.9619	0.022*
C31	0.50225 (12)	0.81928 (15)	0.79374 (6)	0.0135 (3)
C32	0.57450 (13)	0.75263 (17)	0.77151 (7)	0.0183 (3)
H32	0.6192	0.7031	0.7917	0.022*
C33	0.58030 (14)	0.75957 (18)	0.71953 (7)	0.0213 (4)
H33	0.6288	0.7147	0.7050	0.026*
C34	0.51386 (14)	0.83325 (17)	0.68905 (7)	0.0211 (4)
H34	0.5178	0.8377	0.6542	0.025*
C35	0.44182 (14)	0.90008 (17)	0.71074 (7)	0.0208 (4)
H35	0.3974	0.9498	0.6904	0.025*
C36	0.43562 (13)	0.89312 (17)	0.76278 (7)	0.0181 (3)
H36	0.3868	0.9379	0.7771	0.022*
C41	0.06641 (13)	0.94975 (16)	0.88407 (7)	0.0166 (3)
C42	−0.01987 (14)	0.99999 (19)	0.85980 (8)	0.0263 (4)
H42	−0.0179	1.0465	0.8301	0.032*
C43	−0.10945 (14)	0.9812 (2)	0.87964 (9)	0.0314 (5)
H43	−0.1670	1.0157	0.8633	0.038*
C44	−0.11355 (14)	0.91173 (19)	0.92340 (8)	0.0270 (4)
H44	−0.1735	0.8999	0.9367	0.032*
C45	−0.02773 (15)	0.8597 (2)	0.94747 (8)	0.0288 (4)
H45	−0.0301	0.8124	0.9769	0.035*
C46	0.06196 (14)	0.87786 (19)	0.92784 (7)	0.0242 (4)
H46	0.1192	0.8419	0.9440	0.029*
C51	0.23925 (12)	1.10092 (15)	0.90686 (6)	0.0149 (3)
C52	0.33905 (13)	1.12973 (16)	0.90577 (7)	0.0178 (3)
H52	0.3765	1.0845	0.8846	0.021*
C53	0.38268 (14)	1.22486 (17)	0.93583 (7)	0.0216 (4)
H53	0.4492	1.2435	0.9347	0.026*
C54	0.32787 (15)	1.29242 (17)	0.96757 (7)	0.0237 (4)
H54	0.3572	1.3568	0.9876	0.028*

C55	0.22880 (15)	1.26367 (18)	0.96936 (7)	0.0237 (4)
H55	0.1920	1.3084	0.9910	0.028*
C56	0.18420 (14)	1.16877 (17)	0.93912 (7)	0.0206 (4)
H56	0.1177	1.1504	0.9404	0.025*
C61	0.16834 (12)	1.06410 (16)	0.80372 (6)	0.0153 (3)
C62	0.14519 (14)	1.19195 (17)	0.80202 (7)	0.0200 (4)
H62	0.1353	1.2345	0.8318	0.024*
C63	0.13683 (14)	1.25589 (18)	0.75580 (7)	0.0233 (4)
H63	0.1217	1.3411	0.7548	0.028*
C64	0.15107 (14)	1.19286 (19)	0.71128 (7)	0.0230 (4)
H64	0.1459	1.2358	0.6805	0.028*
C65	0.17304 (14)	1.06573 (19)	0.71274 (7)	0.0237 (4)
H65	0.1819	1.0231	0.6828	0.028*
C66	0.18175 (13)	1.00199 (18)	0.75869 (7)	0.0192 (4)
H66	0.1967	0.9167	0.7594	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.01252 (7)	0.01365 (6)	0.01457 (6)	−0.00079 (4)	0.00304 (4)	0.00008 (5)
S1	0.0166 (2)	0.0204 (2)	0.01331 (19)	−0.00489 (16)	0.00144 (15)	0.00208 (16)
P1	0.01206 (19)	0.01232 (19)	0.01342 (19)	−0.00013 (15)	0.00226 (15)	0.00091 (15)
P2	0.0125 (2)	0.0139 (2)	0.0147 (2)	0.00012 (15)	0.00337 (16)	0.00002 (16)
N1	0.0186 (7)	0.0264 (8)	0.0170 (7)	−0.0071 (6)	0.0043 (6)	0.0003 (6)
N2	0.0160 (7)	0.0250 (8)	0.0178 (7)	−0.0085 (6)	0.0036 (6)	−0.0010 (6)
N3	0.0158 (7)	0.0192 (7)	0.0258 (8)	−0.0008 (6)	0.0057 (6)	−0.0009 (6)
O1	0.0226 (7)	0.0375 (8)	0.0274 (7)	−0.0110 (6)	0.0122 (6)	−0.0076 (6)
O2	0.0222 (7)	0.0362 (8)	0.0449 (9)	−0.0150 (6)	0.0110 (6)	−0.0154 (7)
O3	0.0241 (7)	0.0499 (9)	0.0235 (7)	−0.0120 (7)	0.0093 (6)	−0.0110 (7)
C1	0.0168 (8)	0.0157 (8)	0.0175 (8)	−0.0003 (6)	0.0033 (6)	0.0020 (6)
C2	0.0171 (8)	0.0184 (8)	0.0142 (8)	−0.0059 (7)	0.0033 (6)	−0.0021 (6)
C3	0.0192 (9)	0.0233 (9)	0.0179 (8)	−0.0016 (7)	0.0004 (7)	−0.0015 (7)
C4	0.0212 (9)	0.0318 (10)	0.0221 (9)	−0.0022 (8)	0.0086 (7)	−0.0056 (8)
C5	0.0331 (11)	0.0249 (10)	0.0161 (9)	−0.0078 (8)	0.0076 (8)	−0.0037 (7)
C6	0.0300 (10)	0.0204 (9)	0.0183 (9)	−0.0027 (8)	−0.0032 (7)	−0.0008 (7)
C7	0.0168 (9)	0.0253 (9)	0.0214 (9)	−0.0018 (7)	0.0007 (7)	−0.0029 (7)
C11	0.0164 (8)	0.0131 (7)	0.0129 (7)	0.0005 (6)	0.0013 (6)	−0.0007 (6)
C12	0.0174 (8)	0.0162 (8)	0.0150 (8)	−0.0011 (6)	0.0037 (6)	0.0011 (6)
C13	0.0144 (8)	0.0223 (9)	0.0134 (8)	0.0021 (7)	0.0010 (6)	−0.0021 (7)
C14	0.0231 (9)	0.0159 (8)	0.0136 (8)	0.0049 (7)	−0.0012 (7)	−0.0013 (6)
C15	0.0244 (9)	0.0123 (8)	0.0164 (8)	−0.0021 (7)	0.0010 (7)	0.0011 (6)
C16	0.0159 (8)	0.0159 (8)	0.0144 (8)	−0.0018 (6)	0.0020 (6)	−0.0010 (6)
C21	0.0114 (7)	0.0135 (8)	0.0161 (8)	0.0015 (6)	0.0022 (6)	−0.0014 (6)
C22	0.0169 (8)	0.0187 (8)	0.0128 (8)	−0.0017 (7)	0.0027 (6)	−0.0001 (6)
C23	0.0183 (8)	0.0175 (8)	0.0194 (8)	−0.0029 (7)	0.0051 (7)	0.0014 (7)
C24	0.0186 (9)	0.0173 (8)	0.0220 (9)	−0.0014 (7)	−0.0009 (7)	−0.0050 (7)
C25	0.0288 (10)	0.0213 (9)	0.0127 (8)	0.0016 (7)	−0.0007 (7)	−0.0005 (7)
C26	0.0244 (9)	0.0168 (8)	0.0155 (8)	0.0005 (7)	0.0043 (7)	0.0027 (7)

C31	0.0139 (8)	0.0137 (8)	0.0127 (7)	−0.0033 (6)	0.0012 (6)	−0.0001 (6)
C32	0.0187 (9)	0.0188 (8)	0.0172 (8)	0.0037 (7)	0.0010 (7)	0.0002 (7)
C33	0.0233 (9)	0.0237 (9)	0.0177 (8)	0.0033 (7)	0.0064 (7)	−0.0028 (7)
C34	0.0273 (10)	0.0220 (9)	0.0139 (8)	−0.0034 (7)	0.0022 (7)	−0.0007 (7)
C35	0.0234 (9)	0.0203 (9)	0.0177 (8)	0.0018 (7)	−0.0023 (7)	0.0026 (7)
C36	0.0163 (8)	0.0194 (8)	0.0187 (8)	0.0023 (7)	0.0024 (7)	0.0001 (7)
C41	0.0157 (8)	0.0154 (8)	0.0195 (8)	−0.0010 (6)	0.0052 (7)	−0.0014 (7)
C42	0.0187 (9)	0.0299 (10)	0.0304 (10)	0.0013 (8)	0.0036 (8)	0.0087 (8)
C43	0.0140 (9)	0.0384 (12)	0.0419 (12)	0.0027 (8)	0.0038 (8)	0.0075 (10)
C44	0.0184 (9)	0.0279 (10)	0.0370 (11)	−0.0036 (8)	0.0127 (8)	−0.0025 (9)
C45	0.0280 (10)	0.0315 (11)	0.0292 (10)	0.0013 (8)	0.0134 (8)	0.0067 (9)
C46	0.0187 (9)	0.0277 (10)	0.0273 (10)	0.0044 (7)	0.0074 (7)	0.0059 (8)
C51	0.0166 (8)	0.0140 (8)	0.0140 (8)	0.0008 (6)	0.0014 (6)	0.0021 (6)
C52	0.0204 (9)	0.0167 (8)	0.0169 (8)	0.0002 (7)	0.0042 (7)	0.0001 (7)
C53	0.0221 (9)	0.0205 (9)	0.0219 (9)	−0.0063 (7)	0.0012 (7)	0.0018 (7)
C54	0.0344 (11)	0.0175 (9)	0.0181 (9)	−0.0032 (8)	−0.0020 (8)	−0.0022 (7)
C55	0.0294 (10)	0.0224 (9)	0.0199 (9)	0.0038 (8)	0.0055 (8)	−0.0043 (7)
C56	0.0202 (9)	0.0229 (9)	0.0192 (9)	0.0020 (7)	0.0042 (7)	−0.0015 (7)
C61	0.0117 (8)	0.0179 (8)	0.0165 (8)	−0.0014 (6)	0.0027 (6)	0.0017 (6)
C62	0.0212 (9)	0.0206 (9)	0.0184 (8)	0.0013 (7)	0.0033 (7)	0.0000 (7)
C63	0.0243 (10)	0.0200 (9)	0.0253 (9)	−0.0001 (7)	0.0007 (8)	0.0057 (8)
C64	0.0176 (9)	0.0336 (10)	0.0180 (9)	−0.0039 (8)	0.0021 (7)	0.0077 (8)
C65	0.0208 (9)	0.0346 (11)	0.0162 (8)	−0.0033 (8)	0.0041 (7)	−0.0027 (8)
C66	0.0174 (8)	0.0211 (9)	0.0194 (8)	−0.0014 (7)	0.0028 (7)	−0.0024 (7)

Geometric parameters (Å, º)

Ag1—P1	2.4645 (5)	C24—H24	0.9300
Ag1—P2	2.4693 (4)	C25—C26	1.387 (3)
Ag1—S1	2.5307 (4)	C25—H25	0.9300
S1—C1	1.7098 (18)	C26—H26	0.9300
P1—C11	1.8208 (17)	C31—C32	1.392 (2)
P1—C31	1.8260 (17)	C31—C36	1.398 (2)
P1—C21	1.8262 (17)	C32—C33	1.387 (2)
P2—C41	1.8222 (18)	C32—H32	0.9300
P2—C51	1.8235 (17)	C33—C34	1.389 (3)
P2—C61	1.8241 (17)	C33—H33	0.9300
N1—C1	1.331 (2)	C34—C35	1.384 (3)
N1—H1A	0.8600	C34—H34	0.9300
N1—H1B	0.8600	C35—C36	1.389 (2)
N2—C1	1.339 (2)	C35—H35	0.9300
N2—C2	1.426 (2)	C36—H36	0.9300
N2—H2	0.8600	C41—C42	1.385 (3)
N3—O2	1.231 (2)	C41—C46	1.394 (3)
N3—O1	1.2568 (19)	C42—C43	1.392 (3)
N3—O3	1.264 (2)	C42—H42	0.9300
C2—C3	1.387 (2)	C43—C44	1.379 (3)
C2—C7	1.389 (2)	C43—H43	0.9300

C3—C4	1.392 (3)	C44—C45	1.385 (3)
C3—H3	0.9300	C44—H44	0.9300
C4—C5	1.380 (3)	C45—C46	1.390 (3)
C4—H4	0.9300	C45—H45	0.9300
C5—C6	1.383 (3)	C46—H46	0.9300
C5—H5	0.9300	C51—C56	1.395 (2)
C6—C7	1.389 (3)	C51—C52	1.396 (2)
C6—H6	0.9300	C52—C53	1.382 (2)
C7—H7	0.9300	C52—H52	0.9300
C11—C16	1.396 (2)	C53—C54	1.382 (3)
C11—C12	1.404 (2)	C53—H53	0.9300
C12—C13	1.383 (2)	C54—C55	1.388 (3)
C12—H12	0.9300	C54—H54	0.9300
C13—C14	1.389 (2)	C55—C56	1.387 (3)
C13—H13	0.9300	C55—H55	0.9300
C14—C15	1.386 (3)	C56—H56	0.9300
C14—H14	0.9300	C61—C66	1.391 (2)
C15—C16	1.391 (2)	C61—C62	1.396 (2)
C15—H15	0.9300	C62—C63	1.393 (3)
C16—H16	0.9300	C62—H62	0.9300
C21—C22	1.389 (2)	C63—C64	1.386 (3)
C21—C26	1.397 (2)	C63—H63	0.9300
C22—C23	1.394 (2)	C64—C65	1.385 (3)
C22—H22	0.9300	C64—H64	0.9300
C23—C24	1.387 (2)	C65—C66	1.386 (3)
C23—H23	0.9300	C65—H65	0.9300
C24—C25	1.389 (3)	C66—H66	0.9300

P1—Ag1—P2	127.556 (15)	C26—C25—H25	120.0
P1—Ag1—S1	113.029 (15)	C24—C25—H25	120.0
P2—Ag1—S1	112.694 (15)	C25—C26—C21	120.50 (16)
C1—S1—Ag1	109.30 (6)	C25—C26—H26	119.7
C11—P1—C31	105.62 (8)	C21—C26—H26	119.7
C11—P1—C21	99.64 (8)	C32—C31—C36	118.88 (15)
C31—P1—C21	105.30 (8)	C32—C31—P1	123.80 (13)
C11—P1—Ag1	118.36 (6)	C36—C31—P1	117.27 (13)
C31—P1—Ag1	111.81 (6)	C33—C32—C31	120.52 (16)
C21—P1—Ag1	114.63 (5)	C33—C32—H32	119.7
C41—P2—C51	103.41 (8)	C31—C32—H32	119.7
C41—P2—C61	106.55 (8)	C32—C33—C34	120.23 (17)
C51—P2—C61	101.36 (8)	C32—C33—H33	119.9
C41—P2—Ag1	117.14 (6)	C34—C33—H33	119.9
C51—P2—Ag1	104.48 (6)	C35—C34—C33	119.75 (17)
C61—P2—Ag1	121.15 (6)	C35—C34—H34	120.1
C1—N1—H1A	120.0	C33—C34—H34	120.1
C1—N1—H1B	120.0	C34—C35—C36	120.19 (17)
H1A—N1—H1B	120.0	C34—C35—H35	119.9
C1—N2—C2	127.91 (15)	C36—C35—H35	119.9

C1—N2—H2	116.0	C35—C36—C31	120.42 (16)
C2—N2—H2	116.0	C35—C36—H36	119.8
O2—N3—O1	120.45 (16)	C31—C36—H36	119.8
O2—N3—O3	120.53 (15)	C42—C41—C46	119.18 (17)
O1—N3—O3	119.01 (15)	C42—C41—P2	123.50 (14)
N1—C1—N2	115.86 (16)	C46—C41—P2	117.26 (13)
N1—C1—S1	119.06 (13)	C41—C42—C43	120.24 (18)
N2—C1—S1	125.06 (13)	C41—C42—H42	119.9
C3—C2—C7	120.16 (16)	C43—C42—H42	119.9
C3—C2—N2	122.09 (16)	C44—C43—C42	120.54 (19)
C7—C2—N2	117.64 (16)	C44—C43—H43	119.7
C2—C3—C4	119.35 (17)	C42—C43—H43	119.7
C2—C3—H3	120.3	C43—C44—C45	119.52 (18)
C4—C3—H3	120.3	C43—C44—H44	120.2
C5—C4—C3	120.43 (18)	C45—C44—H44	120.2
C5—C4—H4	119.8	C44—C45—C46	120.28 (19)
C3—C4—H4	119.8	C44—C45—H45	119.9
C4—C5—C6	120.25 (18)	C46—C45—H45	119.9
C4—C5—H5	119.9	C45—C46—C41	120.23 (18)
C6—C5—H5	119.9	C45—C46—H46	119.9
C5—C6—C7	119.74 (18)	C41—C46—H46	119.9
C5—C6—H6	120.1	C56—C51—C52	119.07 (16)
C7—C6—H6	120.1	C56—C51—P2	124.06 (13)
C2—C7—C6	120.05 (17)	C52—C51—P2	116.84 (13)
C2—C7—H7	120.0	C53—C52—C51	120.60 (17)
C6—C7—H7	120.0	C53—C52—H52	119.7
C16—C11—C12	119.03 (15)	C51—C52—H52	119.7
C16—C11—P1	120.35 (13)	C52—C53—C54	120.24 (18)
C12—C11—P1	120.58 (13)	C52—C53—H53	119.9
C13—C12—C11	120.56 (16)	C54—C53—H53	119.9
C13—C12—H12	119.7	C53—C54—C55	119.64 (17)
C11—C12—H12	119.7	C53—C54—H54	120.2
C12—C13—C14	120.01 (16)	C55—C54—H54	120.2
C12—C13—H13	120.0	C56—C55—C54	120.54 (18)
C14—C13—H13	120.0	C56—C55—H55	119.7
C15—C14—C13	119.86 (16)	C54—C55—H55	119.7
C15—C14—H14	120.1	C55—C56—C51	119.91 (17)
C13—C14—H14	120.1	C55—C56—H56	120.0
C14—C15—C16	120.54 (16)	C51—C56—H56	120.0
C14—C15—H15	119.7	C66—C61—C62	119.03 (16)
C16—C15—H15	119.7	C66—C61—P2	118.99 (13)
C15—C16—C11	119.92 (16)	C62—C61—P2	121.89 (13)
C15—C16—H16	120.0	C63—C62—C61	120.10 (17)
C11—C16—H16	120.0	C63—C62—H62	119.9
C22—C21—C26	119.17 (15)	C61—C62—H62	119.9
C22—C21—P1	124.26 (13)	C64—C63—C62	120.18 (18)
C26—C21—P1	116.56 (13)	C64—C63—H63	119.9
C21—C22—C23	120.20 (16)	C62—C63—H63	119.9

C21—C22—H22	119.9	C65—C64—C63	119.90 (17)
C23—C22—H22	119.9	C65—C64—H64	120.1
C24—C23—C22	120.30 (16)	C63—C64—H64	120.1
C24—C23—H23	119.9	C64—C65—C66	120.05 (18)
C22—C23—H23	119.8	C64—C65—H65	120.0
C23—C24—C25	119.70 (16)	C66—C65—H65	120.0
C23—C24—H24	120.2	C65—C66—C61	120.74 (17)
C25—C24—H24	120.2	C65—C66—H66	119.6
C26—C25—C24	120.06 (16)	C61—C66—H66	119.6

C2—N2—C1—N1	172.88 (17)	P1—C31—C32—C33	177.53 (14)
C2—N2—C1—S1	−8.7 (3)	C31—C32—C33—C34	0.0 (3)
Ag1—S1—C1—N1	−147.45 (13)	C32—C33—C34—C35	0.1 (3)
Ag1—S1—C1—N2	34.16 (17)	C33—C34—C35—C36	−0.3 (3)
C1—N2—C2—C3	61.7 (3)	C34—C35—C36—C31	0.4 (3)
C1—N2—C2—C7	−122.0 (2)	C32—C31—C36—C35	−0.3 (3)
C7—C2—C3—C4	2.0 (3)	P1—C31—C36—C35	−177.86 (14)
N2—C2—C3—C4	178.19 (17)	C51—P2—C41—C42	99.52 (17)
C2—C3—C4—C5	−1.1 (3)	C61—P2—C41—C42	−6.87 (18)
C3—C4—C5—C6	−0.4 (3)	Ag1—P2—C41—C42	−146.22 (15)
C4—C5—C6—C7	1.0 (3)	C51—P2—C41—C46	−77.57 (15)
C3—C2—C7—C6	−1.4 (3)	C61—P2—C41—C46	176.04 (14)
N2—C2—C7—C6	−177.76 (16)	Ag1—P2—C41—C46	36.69 (16)
C5—C6—C7—C2	−0.1 (3)	C46—C41—C42—C43	1.5 (3)
C31—P1—C11—C16	−117.34 (14)	P2—C41—C42—C43	−175.56 (16)
C21—P1—C11—C16	133.67 (14)	C41—C42—C43—C44	−0.4 (3)
Ag1—P1—C11—C16	8.77 (16)	C42—C43—C44—C45	−0.5 (3)
C31—P1—C11—C12	65.03 (15)	C43—C44—C45—C46	0.3 (3)
C21—P1—C11—C12	−43.97 (15)	C44—C45—C46—C41	0.7 (3)
Ag1—P1—C11—C12	−168.87 (11)	C42—C41—C46—C45	−1.6 (3)
C16—C11—C12—C13	2.8 (2)	P2—C41—C46—C45	175.61 (16)
P1—C11—C12—C13	−179.50 (13)	C41—P2—C51—C56	−11.67 (17)
C11—C12—C13—C14	−1.5 (3)	C61—P2—C51—C56	98.60 (16)
C12—C13—C14—C15	−1.1 (3)	Ag1—P2—C51—C56	−134.76 (14)
C13—C14—C15—C16	2.4 (3)	C41—P2—C51—C52	170.39 (13)
C14—C15—C16—C11	−1.0 (3)	C61—P2—C51—C52	−79.34 (14)
C12—C11—C16—C15	−1.6 (2)	Ag1—P2—C51—C52	47.30 (14)
P1—C11—C16—C15	−179.23 (13)	C56—C51—C52—C53	−0.6 (3)
C11—P1—C21—C22	121.60 (15)	P2—C51—C52—C53	177.44 (14)
C31—P1—C21—C22	12.36 (16)	C51—C52—C53—C54	0.3 (3)
Ag1—P1—C21—C22	−110.96 (14)	C52—C53—C54—C55	0.4 (3)
C11—P1—C21—C26	−57.49 (14)	C53—C54—C55—C56	−0.8 (3)
C31—P1—C21—C26	−166.73 (13)	C54—C55—C56—C51	0.4 (3)
Ag1—P1—C21—C26	69.95 (14)	C52—C51—C56—C55	0.2 (3)
C26—C21—C22—C23	1.7 (3)	P2—C51—C56—C55	−177.65 (14)
P1—C21—C22—C23	−177.36 (13)	C41—P2—C61—C66	−106.80 (14)
C21—C22—C23—C24	0.7 (3)	C51—P2—C61—C66	145.35 (14)
C22—C23—C24—C25	−2.3 (3)	Ag1—P2—C61—C66	30.55 (16)

C23—C24—C25—C26	1.6 (3)	C41—P2—C61—C62	76.64 (16)
C24—C25—C26—C21	0.8 (3)	C51—P2—C61—C62	−31.20 (16)
C22—C21—C26—C25	−2.4 (3)	Ag1—P2—C61—C62	−146.00 (13)
P1—C21—C26—C25	176.72 (14)	C66—C61—C62—C63	−0.7 (3)
C11—P1—C31—C32	−9.27 (17)	P2—C61—C62—C63	175.88 (14)
C21—P1—C31—C32	95.60 (15)	C61—C62—C63—C64	0.2 (3)
Ag1—P1—C31—C32	−139.30 (13)	C62—C63—C64—C65	0.4 (3)
C11—P1—C31—C36	168.20 (13)	C63—C64—C65—C66	−0.7 (3)
C21—P1—C31—C36	−86.92 (14)	C64—C65—C66—C61	0.2 (3)
Ag1—P1—C31—C36	38.18 (14)	C62—C61—C66—C65	0.4 (3)
C36—C31—C32—C33	0.1 (3)	P2—C61—C66—C65	−176.21 (14)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3^{i}	0.86	2.02	2.877 (2)	180
N1—H1*B*···O3^{ii}	0.86	2.17	2.921 (2)	145
N2—H2···O1^{i}	0.86	1.97	2.823 (2)	171
C35—H35···*Cg*2^{iii}	0.93	2.97	3.746 (2)	142
C54—H54···*Cg*2^{iv}	0.93	2.82	3.531 (2)	134

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) −*x*+1, *y*+1/2, −*z*+3/2; (iv) −*x*+1, −*y*+2, −*z*+2.