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Crystal structure of bis(thiourea-κS)bis(triphenylphosphane-κP)silver(I) nitrate

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In the title salt, $[Ag(CH_4N_2S)_2(PPh_3)_2]NO_3$, the Ag^I atom is coordinated by two thiourea S atoms and two triphenylphosphane P atoms in a distorted tetrahedral geometry, with bond angles in the range 102.90 (4)–123.29 (4)°. The Ag—S═C bond angles are 101.75 (19) and 111.29 (18)°. In the crystal, the component ions are linked by C—H···O, C—H···S, N—H···O and N—H···S hydrogen bonds, generating $(10\bar{1})$ sheets.

Keywords: crystal structure; thiourea; triphenylphosphane; silver(I) complex; hydrogen bonding

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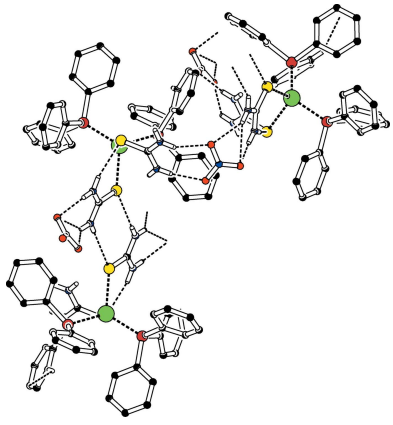
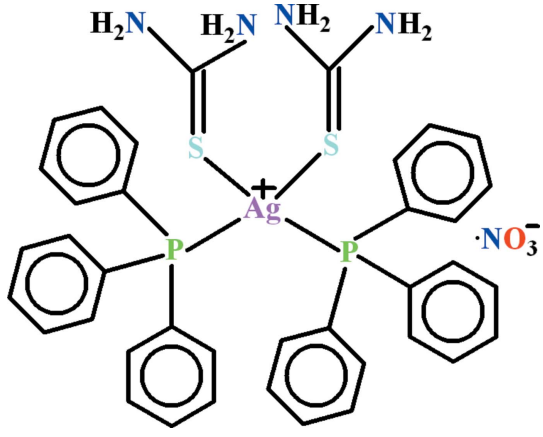
1. Chemical context

Silver(I) forms relatively stable compounds with phosphanes and sulfur donor thione ligands due to favorable soft acid–soft base interactions (Ferrari *et al.*, 2007; Isab *et al.* 2010; Karagiannidis *et al.*, 1990; Nawaz *et al.*, 2011; Rüffer *et al.*, 2011). Interest in these complexes arises from their luminescent (Ferrari *et al.*, 2007), antimicrobial (Ruan *et al.*, 2009) and antitumor properties (Liu *et al.*, 2008). In the light of this, the crystal structures of several silver(I) complexes of phosphanes and thiones have been reported in the literature (Ferrari *et al.*, 2007; Isab *et al.*, 2010; Karagiannidis *et al.*, 1990; Nawaz *et al.*, 2011; Rüffer *et al.*, 2011). Here, we report the crystal structure of a new silver(I) complex of triphenylphosphane (PPh_3) and thiourea (tu), (I) (Fig. 1).





2. Structural commentary

The crystal structure of the title complex consists of $[Ag(PPh_3)_2(tu)_2]^+$ cations and NO_3^- counter-ions. In the cationic complex, $[Ag(PPh_3)_2(tu)_2]^+$, the silver(I) atom is bound to two P atoms of PPh_3 and two sulfur atoms of thiourea, assuming a slightly distorted tetrahedral geometry

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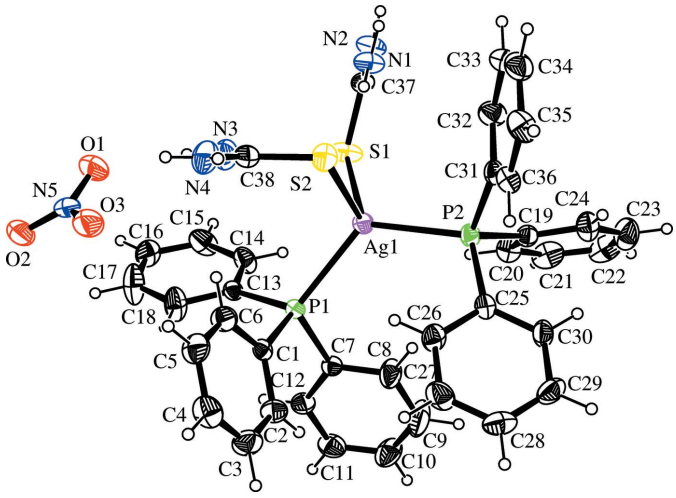

Figure 1
View of the title compound with displacement ellipsoids drawn at the 50% probability level.

(Fig. 1). The spread of bond angles around the Ag atom is 102.90 (4)–123.29 (4)°. The high value of the P1—Ag1—P2 angle [123.29 (4)°] is counterbalanced by the smaller S1—Ag1—S2 bond angle [102.90 (4)°]. The deviation from a tetrahedral geometry is apparently due to steric interaction between the bulky phosphane ligands. The Ag—S, Ag—P and other bond lengths (Table 1) are in agreement with those observed in other reported complexes (Ferrari *et al.*, 2007; Isab *et al.*, 2010; Karagiannidis *et al.*, 1990; Nawaz *et al.*, 2011; Rüffer *et al.*, 2011). The nitrate ion is planar, but exhibits low symmetry due to rather strong hydrogen-bonding interactions with the NH group of the tu ligand.

In (I), the dihedral angle between the phenyl rings *A* (C1–C6), *B* (C7–C12), *C* (C13–C18), *D* (C19–C24), *E* (C25–C30) and *F* (C31–C36) are as follows: *A*/*B*, *A*/*C*, *B*/*C*, *D*/*E*, *D*/*F* and *E*/*F* = 82.67 (15), 62.77 (17), 86.59 (14), 73.72 (14), 85.01 (16) and 84.06 (17)°, respectively. The thiourea units *G* (S1/C37/N1/N2) and *H* (S2/C38/N3/N4) are almost planar with r.m.s. deviations of 0.0031 and 0.0007 Å, respectively, and are oriented at a dihedral angle of 76.82 (11)° to each other.

3. Supramolecular features

In the asymmetric unit, strong N—H···S, N—H···O hydrogen bonds complete distorted $S(6)$ and $R_2^2(8)$ loops. The other hydrogen-bonding interactions are of the C—H···O, C—H···S, N—H···O and N—H···S types (Table 2, Fig. 2) and lead to a two-dimensional polymeric network in the $(10\bar{1})$ plane.

4. Synthesis and crystallization

The title complex was prepared by adding one equivalent of thiourea dissolved in 10 ml methanol to a 1:1 mixture of $AgNO_3$ and PPh_3 in a methanol–acetonitrile medium (10 ml and 15 ml, respectively). Mixing resulted in the formation of a white precipitate. After stirring for half an hour, the mixture was filtered and the filtrate was left for crystallization. Colorless crystals of (I) were isolated from the filtrate. The crystal structure of the product obtained by adding two equivalents of thiourea has already been reported (Isab *et al.*, 2010).

Table 1
Selected bond lengths (Å).

Ag1—P2	2.4888 (13)	Ag1—S1	2.6263 (13)
Ag1—P1	2.5078 (12)	Ag1—S2	2.6683 (13)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.86	2.07	2.899 (5)	161
N1—H1*B*···S2	0.86	2.57	3.417 (4)	169
N2—H2*A*···O2^{i}	0.86	2.54	3.255 (5)	141
N2—H2*A*···O3^{i}	0.86	2.24	2.992 (5)	147
N2—H2*B*···S1^{ii}	0.86	2.66	3.453 (4)	154
N3—H3*A*···O1	0.86	2.09	2.946 (6)	171
N3—H3*B*···S1	0.86	2.91	3.759 (5)	169
N4—H4*A*···O3	0.86	2.26	2.976 (6)	140
C2—H2···O1^{iii}	0.93	2.53	3.174 (6)	126
C14—H14···S1	0.93	2.92	3.520 (5)	124

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

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geome-

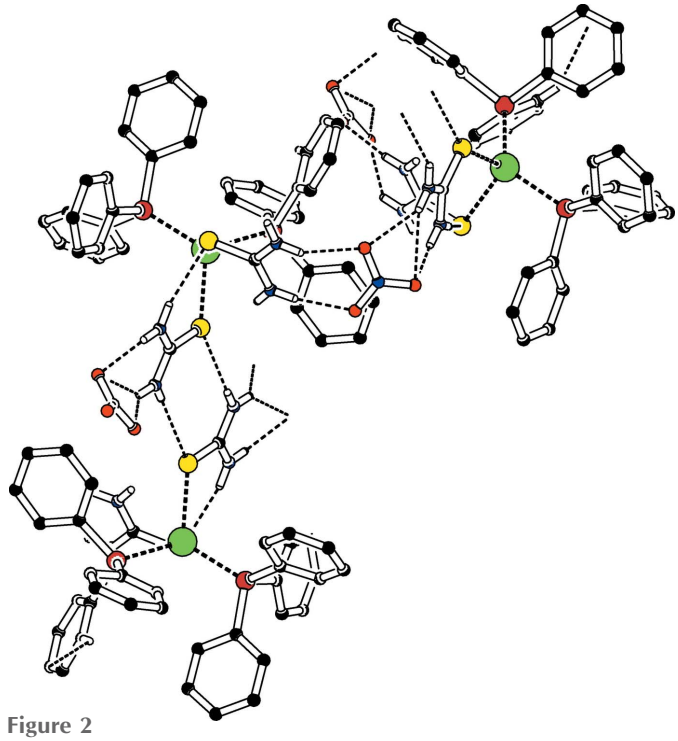

Figure 2
A partial packing diagram (*PLATON*; Spek, 2009) illustrating the formation of sheets of molecules with various loops *via* hydrogen-bonding interactions (shown as dashed lines).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ag(CH_4N_2S)_2(C_{18}H_{15}P)_2]NO_3$
M_r	846.66
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	15.0519 (6), 15.1758 (5), 17.9186 (8)
β (°)	107.886 (2)
V (Å^3)	3895.2 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.75
Crystal size (mm)	0.32 × 0.26 × 0.16
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2005)
T_{min}, T_{max}	0.798, 0.892
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30110, 7659, 3813
R_{int}	0.100
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.088, 0.98
No. of reflections	7659
No. of parameters	460
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

trically (C—H = 0.93, N—H = 0.86 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C, N)$.

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Sidra Nawaz, Muhammad Nawaz Tahir, Muhammad Amir Nadeem, Bushra Mehmood and Saeed Ahmad

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Bis(thiourea-κS)bis(triphenylphosphane-κP)silver(I) nitrate

Crystal data

$[Ag(CH_4N_2S)_2(C_{18}H_{15}P)_2]NO_3$
M_r = 846.66
Monoclinic, $P2_1/n$
a = 15.0519 (6) Å
b = 15.1758 (5) Å
c = 17.9186 (8) Å
β = 107.886 (2)°
V = 3895.2 (3) Å^3
Z = 4
$F(000)$ = 1736
D_x = 1.444 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3813 reflections
θ = 2.4–26.0°
μ = 0.75 mm^{-1}
T = 296 K
Plate, colorless
0.32 × 0.26 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.798, T_{max} = 0.892
30110 measured reflections
7659 independent reflections
3813 reflections with $I > 2\sigma(I)$
R_{int} = 0.100
θ_{max} = 26.0°, θ_{min} = 2.4°
h = −18→18
k = −18→18
l = −22→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.088
S = 0.98
7659 reflections
460 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
$w = 1/[\sigma^2(F_o^2) + (0.0192P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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	0.49184 (3)	0.18428 (2)	0.27125 (2)	0.04076 (12)
P1	0.41457 (8)	0.32439 (7)	0.29245 (7)	0.0352 (3)
P2	0.63642 (9)	0.18065 (8)	0.23159 (7)	0.0387 (3)
S1	0.49005 (11)	0.08173 (7)	0.38885 (7)	0.0603 (5)
S2	0.38377 (10)	0.09742 (8)	0.14694 (8)	0.0520 (4)
N1	0.4763 (3)	−0.0525 (2)	0.2923 (2)	0.0533 (12)
H1A	0.4799	−0.1075	0.2820	0.064*
H1B	0.4609	−0.0147	0.2547	0.064*
N2	0.5177 (3)	−0.0867 (2)	0.4206 (2)	0.0532 (12)
H2A	0.5206	−0.1412	0.4083	0.064*
H2B	0.5300	−0.0719	0.4691	0.064*
N3	0.2637 (3)	0.1110 (3)	0.2272 (3)	0.0677 (14)
H3A	0.2084	0.1177	0.2308	0.081*
H3B	0.3104	0.1049	0.2689	0.081*
N4	0.2023 (3)	0.1198 (3)	0.0959 (3)	0.0744 (15)
H4A	0.1480	0.1263	0.1017	0.089*
H4B	0.2082	0.1195	0.0496	0.089*
C1	0.3488 (3)	0.3837 (3)	0.2050 (3)	0.0334 (12)
C2	0.3714 (4)	0.4676 (3)	0.1868 (3)	0.0495 (14)
H2	0.4220	0.4968	0.2209	0.059*
C3	0.3192 (4)	0.5089 (3)	0.1181 (3)	0.0651 (17)
H3	0.3353	0.5652	0.1065	0.078*
C4	0.2445 (4)	0.4671 (4)	0.0676 (3)	0.0652 (17)
H4	0.2096	0.4953	0.0220	0.078*
C5	0.2209 (4)	0.3842 (4)	0.0839 (3)	0.0628 (17)
H5	0.1700	0.3557	0.0494	0.075*
C6	0.2728 (3)	0.3430 (3)	0.1515 (3)	0.0525 (15)
H6	0.2565	0.2862	0.1619	0.063*
C7	0.4982 (3)	0.4059 (3)	0.3462 (3)	0.0362 (12)
C8	0.5859 (4)	0.4048 (3)	0.3392 (3)	0.0705 (18)
H8	0.6027	0.3600	0.3108	0.085*
C9	0.6508 (4)	0.4701 (4)	0.3740 (4)	0.096 (2)
H9	0.7097	0.4699	0.3675	0.116*
C10	0.6269 (4)	0.5338 (4)	0.4176 (4)	0.0743 (19)
H10	0.6706	0.5761	0.4427	0.089*

C11	0.5400 (4)	0.5362 (3)	0.4245 (3)	0.0619 (17)
H11	0.5239	0.5807	0.4535	0.074*
C12	0.4752 (4)	0.4727 (3)	0.3887 (3)	0.0519 (15)
H12	0.4154	0.4753	0.3934	0.062*
C13	0.3344 (3)	0.3126 (3)	0.3499 (3)	0.0355 (11)
C14	0.3658 (4)	0.2674 (3)	0.4199 (3)	0.0581 (16)
H14	0.4274	0.2482	0.4371	0.070*
C15	0.3088 (5)	0.2502 (3)	0.4649 (3)	0.0699 (18)
H15	0.3321	0.2196	0.5118	0.084*
C16	0.2181 (4)	0.2777 (3)	0.4412 (3)	0.0617 (16)
H16	0.1784	0.2646	0.4705	0.074*
C17	0.1874 (4)	0.3246 (4)	0.3739 (4)	0.090 (2)
H17	0.1261	0.3449	0.3579	0.108*
C18	0.2442 (4)	0.3433 (4)	0.3282 (3)	0.0687 (18)
H18	0.2214	0.3767	0.2828	0.082*
C19	0.7498 (3)	0.1714 (3)	0.3064 (3)	0.0412 (13)
C20	0.7566 (4)	0.1962 (3)	0.3825 (3)	0.0548 (15)
H20	0.7029	0.2116	0.3948	0.066*
C21	0.8416 (5)	0.1982 (4)	0.4402 (4)	0.0734 (19)
H21	0.8455	0.2146	0.4911	0.088*
C22	0.9209 (5)	0.1758 (4)	0.4214 (4)	0.082 (2)
H22	0.9788	0.1788	0.4597	0.098*
C23	0.9158 (4)	0.1494 (4)	0.3484 (4)	0.080 (2)
H23	0.9699	0.1335	0.3369	0.096*
C24	0.8308 (4)	0.1458 (3)	0.2907 (3)	0.0594 (16)
H24	0.8275	0.1261	0.2408	0.071*
C25	0.6492 (4)	0.2776 (3)	0.1747 (3)	0.0388 (13)
C26	0.5705 (4)	0.3294 (3)	0.1437 (3)	0.0503 (14)
H26	0.5141	0.3125	0.1505	0.060*
C27	0.5749 (4)	0.4057 (3)	0.1031 (3)	0.0648 (17)
H27	0.5216	0.4396	0.0824	0.078*
C28	0.6582 (5)	0.4316 (3)	0.0931 (3)	0.0632 (18)
H28	0.6616	0.4837	0.0668	0.076*
C29	0.7358 (4)	0.3803 (4)	0.1219 (3)	0.0628 (17)
H29	0.7917	0.3966	0.1138	0.075*
C30	0.7314 (3)	0.3043 (3)	0.1632 (3)	0.0500 (14)
H30	0.7851	0.2706	0.1836	0.060*
C31	0.6328 (3)	0.0869 (3)	0.1666 (3)	0.0395 (13)
C32	0.6316 (4)	0.0032 (3)	0.1975 (3)	0.0581 (16)
H32	0.6392	−0.0035	0.2507	0.070*
C33	0.6189 (4)	−0.0706 (3)	0.1495 (4)	0.0638 (17)
H33	0.6167	−0.1266	0.1699	0.077*
C34	0.6098 (4)	−0.0596 (4)	0.0717 (4)	0.0653 (18)
H34	0.6014	−0.1087	0.0392	0.078*
C35	0.6127 (4)	0.0224 (4)	0.0410 (3)	0.0636 (17)
H35	0.6077	0.0288	−0.0118	0.076*
C36	0.6233 (3)	0.0960 (3)	0.0886 (3)	0.0486 (14)
H36	0.6240	0.1519	0.0674	0.058*

C37	0.4944 (3)	−0.0262 (3)	0.3655 (3)	0.0411 (13)
C38	0.2767 (4)	0.1101 (3)	0.1581 (4)	0.0501 (15)
N5	0.0359 (4)	0.2164 (3)	0.1905 (3)	0.0634 (15)
O1	0.0756 (3)	0.1552 (2)	0.2336 (2)	0.0767 (13)
O2	−0.0238 (3)	0.2622 (2)	0.2067 (3)	0.0906 (15)
O3	0.0575 (3)	0.2328 (2)	0.1292 (3)	0.0802 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0430 (2)	0.03710 (19)	0.0476 (2)	0.0009 (2)	0.0218 (2)	−0.0015 (2)
P1	0.0355 (8)	0.0314 (7)	0.0395 (8)	0.0020 (6)	0.0128 (7)	0.0002 (6)
P2	0.0383 (8)	0.0434 (7)	0.0382 (8)	0.0034 (7)	0.0173 (7)	0.0006 (7)
S1	0.1117 (14)	0.0337 (7)	0.0409 (8)	0.0012 (8)	0.0313 (9)	0.0007 (6)
S2	0.0517 (10)	0.0620 (9)	0.0426 (9)	−0.0022 (7)	0.0148 (8)	−0.0110 (7)
N1	0.089 (4)	0.037 (2)	0.041 (3)	−0.001 (2)	0.030 (3)	0.000 (2)
N2	0.083 (4)	0.036 (2)	0.038 (3)	0.007 (2)	0.013 (3)	0.000 (2)
N3	0.056 (3)	0.078 (3)	0.077 (4)	−0.002 (2)	0.032 (3)	−0.007 (3)
N4	0.045 (3)	0.087 (3)	0.079 (4)	−0.007 (3)	0.001 (3)	−0.003 (3)
C1	0.037 (3)	0.036 (3)	0.032 (3)	0.005 (2)	0.018 (3)	−0.001 (2)
C2	0.058 (4)	0.045 (3)	0.044 (3)	−0.002 (3)	0.014 (3)	0.005 (3)
C3	0.072 (5)	0.057 (4)	0.067 (4)	−0.004 (3)	0.021 (4)	0.020 (3)
C4	0.069 (5)	0.079 (4)	0.043 (4)	0.016 (4)	0.011 (4)	0.018 (3)
C5	0.048 (4)	0.071 (4)	0.057 (4)	−0.007 (3)	−0.004 (3)	−0.001 (3)
C6	0.050 (4)	0.051 (3)	0.049 (4)	−0.001 (3)	0.004 (3)	0.007 (3)
C7	0.037 (3)	0.035 (3)	0.034 (3)	−0.001 (2)	0.008 (3)	−0.001 (2)
C8	0.050 (4)	0.075 (4)	0.095 (5)	−0.014 (3)	0.034 (4)	−0.042 (4)
C9	0.049 (4)	0.122 (6)	0.128 (6)	−0.028 (4)	0.042 (5)	−0.055 (5)
C10	0.065 (5)	0.078 (4)	0.081 (5)	−0.028 (4)	0.023 (4)	−0.028 (4)
C11	0.073 (5)	0.047 (3)	0.060 (4)	0.001 (3)	0.012 (4)	−0.015 (3)
C12	0.051 (4)	0.040 (3)	0.061 (4)	−0.006 (3)	0.012 (3)	−0.012 (3)
C13	0.038 (3)	0.033 (2)	0.038 (3)	0.003 (2)	0.017 (3)	−0.001 (2)
C14	0.060 (4)	0.063 (3)	0.061 (4)	0.021 (3)	0.032 (4)	0.012 (3)
C15	0.098 (6)	0.063 (4)	0.066 (4)	0.023 (4)	0.050 (5)	0.024 (3)
C16	0.068 (5)	0.071 (4)	0.062 (4)	−0.004 (3)	0.042 (4)	−0.006 (3)
C17	0.048 (4)	0.159 (6)	0.068 (5)	0.022 (5)	0.026 (4)	0.015 (5)
C18	0.051 (4)	0.109 (5)	0.052 (4)	0.020 (4)	0.025 (4)	0.027 (3)
C19	0.040 (3)	0.041 (3)	0.043 (3)	0.001 (3)	0.013 (3)	0.007 (2)
C20	0.056 (4)	0.063 (4)	0.044 (4)	0.001 (3)	0.014 (3)	0.004 (3)
C21	0.086 (5)	0.074 (4)	0.053 (4)	−0.016 (4)	0.011 (4)	−0.001 (3)
C22	0.065 (5)	0.085 (5)	0.071 (5)	−0.020 (4)	−0.016 (5)	0.032 (4)
C23	0.048 (5)	0.095 (5)	0.093 (6)	0.016 (4)	0.015 (5)	0.040 (4)
C24	0.048 (4)	0.075 (4)	0.058 (4)	0.011 (3)	0.019 (4)	0.013 (3)
C25	0.036 (3)	0.049 (3)	0.031 (3)	0.004 (3)	0.010 (3)	−0.001 (2)
C26	0.052 (4)	0.061 (3)	0.045 (3)	0.002 (3)	0.026 (3)	0.004 (3)
C27	0.072 (5)	0.064 (4)	0.062 (4)	0.022 (3)	0.025 (4)	0.025 (3)
C28	0.097 (6)	0.044 (3)	0.055 (4)	−0.013 (4)	0.033 (4)	−0.001 (3)
C29	0.074 (5)	0.058 (4)	0.070 (4)	−0.019 (3)	0.043 (4)	0.000 (3)

C30	0.040 (3)	0.060 (4)	0.057 (4)	0.007 (3)	0.025 (3)	0.008 (3)
C31	0.037 (3)	0.048 (3)	0.040 (3)	0.002 (2)	0.022 (3)	0.000 (3)
C32	0.074 (5)	0.050 (3)	0.058 (4)	0.004 (3)	0.031 (4)	0.007 (3)
C33	0.071 (5)	0.040 (3)	0.085 (5)	0.003 (3)	0.030 (4)	−0.003 (3)
C34	0.059 (4)	0.059 (4)	0.074 (5)	0.002 (3)	0.016 (4)	−0.021 (4)
C35	0.068 (5)	0.074 (4)	0.047 (4)	0.014 (3)	0.015 (3)	−0.008 (3)
C36	0.046 (4)	0.050 (3)	0.050 (4)	0.008 (3)	0.015 (3)	−0.002 (3)
C37	0.050 (4)	0.036 (3)	0.039 (3)	−0.002 (2)	0.016 (3)	0.008 (3)
C38	0.049 (4)	0.039 (3)	0.061 (4)	−0.001 (3)	0.015 (4)	−0.007 (3)
N5	0.059 (4)	0.033 (3)	0.106 (5)	−0.008 (3)	0.036 (4)	−0.002 (3)
O1	0.079 (3)	0.051 (2)	0.103 (3)	0.016 (2)	0.032 (3)	0.020 (2)
O2	0.079 (3)	0.051 (2)	0.164 (4)	0.017 (2)	0.070 (3)	0.019 (3)
O3	0.084 (3)	0.060 (2)	0.109 (4)	0.007 (2)	0.047 (3)	0.020 (2)

Geometric parameters (Å, º)

Ag1—P2	2.4888 (13)	C13—C14	1.379 (6)
Ag1—P1	2.5078 (12)	C14—C15	1.371 (7)
Ag1—S1	2.6263 (13)	C14—H14	0.9300
Ag1—S2	2.6683 (13)	C15—C16	1.365 (7)
P1—C1	1.815 (4)	C15—H15	0.9300
P1—C7	1.816 (4)	C16—C17	1.353 (7)
P1—C13	1.821 (5)	C16—H16	0.9300
P2—C19	1.823 (5)	C17—C18	1.382 (7)
P2—C31	1.828 (5)	C17—H17	0.9300
P2—C25	1.834 (5)	C18—H18	0.9300
S1—C37	1.698 (4)	C19—C20	1.387 (6)
S2—C38	1.695 (6)	C19—C24	1.388 (6)
N1—C37	1.317 (5)	C20—C21	1.376 (6)
N1—H1A	0.8600	C20—H20	0.9300
N1—H1B	0.8600	C21—C22	1.378 (8)
N2—C37	1.315 (5)	C21—H21	0.9300
N2—H2A	0.8600	C22—C23	1.348 (8)
N2—H2B	0.8600	C22—H22	0.9300
N3—C38	1.312 (6)	C23—C24	1.377 (7)
N3—H3A	0.8600	C23—H23	0.9300
N3—H3B	0.8600	C24—H24	0.9300
N4—C38	1.324 (6)	C25—C30	1.376 (6)
N4—H4A	0.8600	C25—C26	1.387 (6)
N4—H4B	0.8600	C26—C27	1.380 (6)
C1—C2	1.382 (5)	C26—H26	0.9300
C1—C6	1.391 (6)	C27—C28	1.377 (7)
C2—C3	1.389 (6)	C27—H27	0.9300
C2—H2	0.9300	C28—C29	1.366 (7)
C3—C4	1.363 (6)	C28—H28	0.9300
C3—H3	0.9300	C29—C30	1.382 (6)
C4—C5	1.363 (6)	C29—H29	0.9300
C4—H4	0.9300	C30—H30	0.9300

C5—C6	1.374 (6)	C31—C36	1.369 (6)
C5—H5	0.9300	C31—C32	1.387 (6)
C6—H6	0.9300	C32—C33	1.390 (6)
C7—C8	1.364 (6)	C32—H32	0.9300
C7—C12	1.375 (6)	C33—C34	1.368 (7)
C8—C9	1.396 (7)	C33—H33	0.9300
C8—H8	0.9300	C34—C35	1.367 (7)
C9—C10	1.359 (7)	C34—H34	0.9300
C9—H9	0.9300	C35—C36	1.384 (6)
C10—C11	1.352 (7)	C35—H35	0.9300
C10—H10	0.9300	C36—H36	0.9300
C11—C12	1.381 (6)	N5—O1	1.237 (5)
C11—H11	0.9300	N5—O2	1.241 (5)
C12—H12	0.9300	N5—O3	1.261 (5)
C13—C18	1.373 (6)		

P2—Ag1—P1	123.29 (4)	C16—C15—H15	119.8
P2—Ag1—S1	116.19 (5)	C14—C15—H15	119.8
P1—Ag1—S1	105.15 (4)	C17—C16—C15	118.2 (6)
P2—Ag1—S2	96.49 (4)	C17—C16—H16	120.9
P1—Ag1—S2	110.67 (4)	C15—C16—H16	120.9
S1—Ag1—S2	102.90 (4)	C16—C17—C18	122.1 (6)
C1—P1—C7	103.0 (2)	C16—C17—H17	118.9
C1—P1—C13	104.9 (2)	C18—C17—H17	118.9
C7—P1—C13	103.8 (2)	C13—C18—C17	120.0 (5)
C1—P1—Ag1	116.41 (14)	C13—C18—H18	120.0
C7—P1—Ag1	112.30 (16)	C17—C18—H18	120.0
C13—P1—Ag1	114.92 (14)	C20—C19—C24	118.0 (5)
C19—P2—C31	104.3 (2)	C20—C19—P2	118.2 (4)
C19—P2—C25	103.7 (2)	C24—C19—P2	123.7 (4)
C31—P2—C25	105.0 (2)	C21—C20—C19	121.0 (5)
C19—P2—Ag1	119.64 (17)	C21—C20—H20	119.5
C31—P2—Ag1	109.93 (16)	C19—C20—H20	119.5
C25—P2—Ag1	113.04 (17)	C20—C21—C22	119.1 (6)
C37—S1—Ag1	111.29 (18)	C20—C21—H21	120.4
C38—S2—Ag1	101.75 (19)	C22—C21—H21	120.4
C37—N1—H1A	120.0	C23—C22—C21	121.0 (6)
C37—N1—H1B	120.0	C23—C22—H22	119.5
H1A—N1—H1B	120.0	C21—C22—H22	119.5
C37—N2—H2A	120.0	C22—C23—C24	120.1 (7)
C37—N2—H2B	120.0	C22—C23—H23	119.9
H2A—N2—H2B	120.0	C24—C23—H23	119.9
C38—N3—H3A	120.0	C23—C24—C19	120.6 (5)
C38—N3—H3B	120.0	C23—C24—H24	119.7
H3A—N3—H3B	120.0	C19—C24—H24	119.7
C38—N4—H4A	120.0	C30—C25—C26	118.1 (4)
C38—N4—H4B	120.0	C30—C25—P2	124.9 (4)
H4A—N4—H4B	120.0	C26—C25—P2	117.0 (4)

C2—C1—C6	117.2 (4)	C27—C26—C25	120.8 (5)
C2—C1—P1	123.5 (4)	C27—C26—H26	119.6
C6—C1—P1	119.3 (3)	C25—C26—H26	119.6
C1—C2—C3	120.7 (5)	C28—C27—C26	120.1 (5)
C1—C2—H2	119.6	C28—C27—H27	120.0
C3—C2—H2	119.6	C26—C27—H27	120.0
C4—C3—C2	120.3 (5)	C29—C28—C27	119.6 (5)
C4—C3—H3	119.8	C29—C28—H28	120.2
C2—C3—H3	119.8	C27—C28—H28	120.2
C3—C4—C5	120.2 (5)	C28—C29—C30	120.2 (5)
C3—C4—H4	119.9	C28—C29—H29	119.9
C5—C4—H4	119.9	C30—C29—H29	119.9
C4—C5—C6	119.5 (5)	C25—C30—C29	121.2 (5)
C4—C5—H5	120.2	C25—C30—H30	119.4
C6—C5—H5	120.2	C29—C30—H30	119.4
C5—C6—C1	122.0 (5)	C36—C31—C32	119.4 (4)
C5—C6—H6	119.0	C36—C31—P2	123.0 (4)
C1—C6—H6	119.0	C32—C31—P2	117.4 (4)
C8—C7—C12	118.4 (4)	C31—C32—C33	120.4 (5)
C8—C7—P1	118.4 (4)	C31—C32—H32	119.8
C12—C7—P1	123.0 (4)	C33—C32—H32	119.8
C7—C8—C9	121.0 (5)	C34—C33—C32	119.0 (5)
C7—C8—H8	119.5	C34—C33—H33	120.5
C9—C8—H8	119.5	C32—C33—H33	120.5
C10—C9—C8	119.3 (6)	C35—C34—C33	121.0 (5)
C10—C9—H9	120.3	C35—C34—H34	119.5
C8—C9—H9	120.3	C33—C34—H34	119.5
C11—C10—C9	120.4 (6)	C34—C35—C36	119.9 (5)
C11—C10—H10	119.8	C34—C35—H35	120.0
C9—C10—H10	119.8	C36—C35—H35	120.0
C10—C11—C12	120.3 (5)	C31—C36—C35	120.3 (5)
C10—C11—H11	119.8	C31—C36—H36	119.9
C12—C11—H11	119.8	C35—C36—H36	119.9
C7—C12—C11	120.6 (5)	N2—C37—N1	117.6 (4)
C7—C12—H12	119.7	N2—C37—S1	120.7 (4)
C11—C12—H12	119.7	N1—C37—S1	121.8 (4)
C18—C13—C14	117.3 (5)	N3—C38—N4	117.5 (6)
C18—C13—P1	125.1 (4)	N3—C38—S2	122.4 (5)
C14—C13—P1	117.5 (4)	N4—C38—S2	120.1 (5)
C15—C14—C13	121.9 (5)	O1—N5—O2	121.3 (6)
C15—C14—H14	119.1	O1—N5—O3	119.3 (5)
C13—C14—H14	119.1	O2—N5—O3	119.4 (5)
C16—C15—C14	120.4 (5)		

C7—P1—C1—C2	6.2 (5)	Ag1—P2—C19—C20	−21.5 (4)
C13—P1—C1—C2	114.6 (4)	C31—P2—C19—C24	39.0 (5)
Ag1—P1—C1—C2	−117.2 (4)	C25—P2—C19—C24	−70.7 (4)
C7—P1—C1—C6	−175.4 (4)	Ag1—P2—C19—C24	162.3 (3)

C13—P1—C1—C6	−67.0 (4)	C24—C19—C20—C21	2.2 (7)
Ag1—P1—C1—C6	61.2 (4)	P2—C19—C20—C21	−174.2 (4)
C6—C1—C2—C3	0.4 (7)	C19—C20—C21—C22	0.4 (8)
P1—C1—C2—C3	178.8 (4)	C20—C21—C22—C23	−2.1 (9)
C1—C2—C3—C4	0.3 (8)	C21—C22—C23—C24	1.0 (9)
C2—C3—C4—C5	−0.6 (9)	C22—C23—C24—C19	1.7 (8)
C3—C4—C5—C6	0.1 (9)	C20—C19—C24—C23	−3.2 (7)
C4—C5—C6—C1	0.6 (8)	P2—C19—C24—C23	172.9 (4)
C2—C1—C6—C5	−0.8 (7)	C19—P2—C25—C30	30.9 (5)
P1—C1—C6—C5	−179.3 (4)	C31—P2—C25—C30	−78.3 (5)
C1—P1—C7—C8	−97.0 (4)	Ag1—P2—C25—C30	161.9 (4)
C13—P1—C7—C8	153.8 (4)	C19—P2—C25—C26	−146.5 (4)
Ag1—P1—C7—C8	29.0 (5)	C31—P2—C25—C26	104.4 (4)
C1—P1—C7—C12	77.7 (4)	Ag1—P2—C25—C26	−15.4 (4)
C13—P1—C7—C12	−31.5 (4)	C30—C25—C26—C27	−0.3 (7)
Ag1—P1—C7—C12	−156.2 (4)	P2—C25—C26—C27	177.2 (4)
C12—C7—C8—C9	−0.2 (9)	C25—C26—C27—C28	−0.3 (8)
P1—C7—C8—C9	174.8 (5)	C26—C27—C28—C29	1.6 (9)
C7—C8—C9—C10	2.1 (10)	C27—C28—C29—C30	−2.1 (9)
C8—C9—C10—C11	−2.7 (10)	C26—C25—C30—C29	−0.2 (7)
C9—C10—C11—C12	1.3 (10)	P2—C25—C30—C29	−177.5 (4)
C8—C7—C12—C11	−1.2 (8)	C28—C29—C30—C25	1.4 (8)
P1—C7—C12—C11	−175.9 (4)	C19—P2—C31—C36	−119.9 (5)
C10—C11—C12—C7	0.6 (8)	C25—P2—C31—C36	−11.2 (5)
C1—P1—C13—C18	0.2 (5)	Ag1—P2—C31—C36	110.7 (4)
C7—P1—C13—C18	108.0 (5)	C19—P2—C31—C32	65.8 (4)
Ag1—P1—C13—C18	−129.0 (4)	C25—P2—C31—C32	174.5 (4)
C1—P1—C13—C14	178.6 (4)	Ag1—P2—C31—C32	−63.7 (4)
C7—P1—C13—C14	−73.6 (4)	C36—C31—C32—C33	−1.3 (8)
Ag1—P1—C13—C14	49.4 (4)	P2—C31—C32—C33	173.2 (4)
C18—C13—C14—C15	2.8 (8)	C31—C32—C33—C34	1.5 (9)
P1—C13—C14—C15	−175.8 (4)	C32—C33—C34—C35	−0.1 (9)
C13—C14—C15—C16	0.0 (8)	C33—C34—C35—C36	−1.3 (9)
C14—C15—C16—C17	−2.2 (9)	C32—C31—C36—C35	−0.1 (8)
C15—C16—C17—C18	1.5 (9)	P2—C31—C36—C35	−174.3 (4)
C14—C13—C18—C17	−3.3 (8)	C34—C35—C36—C31	1.4 (8)
P1—C13—C18—C17	175.1 (4)	Ag1—S1—C37—N2	162.8 (4)
C16—C17—C18—C13	1.3 (10)	Ag1—S1—C37—N1	−16.2 (5)
C31—P2—C19—C20	−144.9 (4)	Ag1—S2—C38—N3	−35.5 (4)
C25—P2—C19—C20	105.5 (4)	Ag1—S2—C38—N4	144.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.86	2.07	2.899 (5)	161
N1—H1*B*···S2	0.86	2.57	3.417 (4)	169
N2—H2*A*···O2^{i}	0.86	2.54	3.255 (5)	141
N2—H2*A*···O3^{i}	0.86	2.24	2.992 (5)	147

N2—H2*B*···S1^{ii}	0.86	2.66	3.453 (4)	154
N3—H3*A*···O1	0.86	2.09	2.946 (6)	171
N3—H3*B*···S1	0.86	2.91	3.759 (5)	169
N4—H4*A*···O3	0.86	2.26	2.976 (6)	140
C2—H2···O1^{iii}	0.93	2.53	3.174 (6)	126
C14—H14···S1	0.93	2.92	3.520 (5)	124

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