

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(*N,N'*-Diethylthiourea- κ S)tris(tri-phenylphosphane- κ P)silver(I) acetate methanol monosolvate

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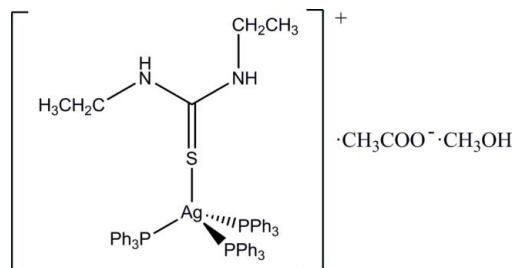
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Received 26 April 2014; accepted 12 May 2014

In the mononuclear title complex, $[\text{Ag}(\text{C}_5\text{H}_{12}\text{N}_2\text{S})(\text{C}_{18}\text{H}_{15}\text{P})_3](\text{CH}_3\text{COO})\cdot\text{CH}_3\text{OH}$, the Ag^{I} ion is in a distorted tetrahedral coordination geometry formed by three P atoms from three triphenylphosphane ligands and one S atom from an *N,N'*-diethylthiourea ligand. In the crystal, the acetate anion is connected to the complex molecule *via* a pair of $\text{N}\cdots\text{H}\cdots\text{O}$ hydrogen bonds [graph-set motif $R_2^2(8)$] and the solvent methanol molecule is connected to the anion *via* an $\text{O}\cdots\text{H}\cdots\text{O}$ hydrogen bond. This aggregate is further connected through a weak $\text{C}\cdots\text{H}\cdots\text{O}$ hydrogen bond, forming a chain along [100]. In addition, sixfold phenyl embraces with intermolecular distances of 6.6463 (13)–6.667 (2) Å are arranged in a chain along [001]. The combination of hydrogen bonding and phenyl \cdots phenyl interactions leads to the formation of a two-dimensional network parallel to (010).

Related literature

For structural reports on silver(I) complexes containing thiourea derivatives as ligands or mixed-ligands with triphenylphosphane, see: Bowmaker *et al.* (2010); Ruffer *et al.* (2011); Pakawatchai *et al.* (2012). For potential applications of silver(I) complexes, see: Ferrari *et al.* (2007); Isab *et al.* (2010). For details of sixfold phenyl embraces, see: Dance & Scudder (2000); Scudder & Dance (2001). For hydrogen-bond graph-set analysis, see: Etter *et al.* (1990).



Experimental

Crystal data

$[\text{Ag}(\text{C}_5\text{H}_{12}\text{N}_2\text{S})(\text{C}_{18}\text{H}_{15}\text{P})_3](\text{C}_2\text{H}_3\text{O}_2)\cdot\text{CH}_4\text{O}$
 $M_r = 1117.99$
 Monoclinic, $P2_1/n$
 $a = 12.950$ (3) Å
 $b = 21.903$ (6) Å
 $c = 19.915$ (5) Å
 $\beta = 103.201$ (4)°
 $V = 5500$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.54$ mm⁻¹
 $T = 100$ K
 $0.18 \times 0.15 \times 0.11$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2012)
 $T_{\text{min}} = 0.608$, $T_{\text{max}} = 0.746$
 59032 measured reflections
 16670 independent reflections
 10564 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.093$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.120$
 $S = 1.00$
 16670 reflections
 653 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.13$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| <i>D</i> — <i>H</i> ⋯ <i>A</i> | <i>D</i> — <i>H</i> | <i>H</i> ⋯ <i>A</i> | <i>D</i> ⋯ <i>A</i> | <i>D</i> — <i>H</i> ⋯ <i>A</i> |
|--------------------------------|---------------------|---------------------|---------------------|--------------------------------|
| N1—H1⋯O1 | 0.88 | 1.93 | 2.811 (3) | 176 |
| N2—H2⋯O2 | 0.88 | 1.89 | 2.754 (3) | 168 |
| O3—H3D⋯O1 | 0.87 | 1.86 | 2.724 (4) | 177 |
| C34—H34⋯O2 [†] | 0.95 | 2.52 | 3.394 (4) | 154 |

Symmetry code: (i) $x - 1, y, z$.

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008) and *SHELXLE* (Hübschle *et al.*, 2011); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

Financial support from the Department of Chemistry, Prince of Songkla University, is gratefully acknowledged. We would like to thank Dr Matthias Zeller for valuable suggestions and assistance with the X-ray structure determination and use of structure refinement programs.

Supporting information for this paper is available from the IUCr electronic archives (Reference: LH5701).

References

- Bowmaker, G. A., Pakawatchai, C., Saithong, S., Skelton, B. W. & White, A. H. (2010). *Dalton Trans.* **39**, 4391–4404.
 Bruker (2012). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Dance, I. & Scudder, M. (2000). *J. Chem. Soc. Dalton Trans.* pp. 1587–1594.
 Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* **B46**, 256–262.
 Ferrari, M. B., Bisceglie, F., Cavalli, E., Pelosi, G., Tarasconi, P. & Verdolino, V. (2007). *Inorg. Chim. Acta*, **360**, 3233–3240.
 Hübschle, C. B., Sheldrick, G. M. & Dittrich, B. (2011). *J. Appl. Cryst.* **44**, 1281–1284.
 Isab, A. A., Nawaz, S., Saleem, M., Altaf, M., Monim-ul-Mehboob, M., Ahmad, S. & Evans, H. S. (2010). *Polyhedron*, **29**, 1251–1256.

- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- Pakawatchai, C., Jantaramas, P., Mokhagul, J. & Nimthong, R. (2012). *Acta Cryst.* **E68**, m1506–m1507.
- Rüffer, T., Lang, H., Nawaz, S., Isab, A. A., Ahmad, S. & Athar, M. M. (2011). *Zh. Strukt. Khim. (Russ. J. Struct. Chem.)*, **52**, 1025–1029.
- Scudder, M. & Dance, I. (2001). *CrystEngCom*, **12**, 1–4.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2014). E70, m216–m217 [doi:10.1107/S1600536814010824]

(*N,N'*-Diethylthiourea- κ S)tris(triphenylphosphane- κ P)silver(I) acetate methanol monosolvate

Yupa Wattanakanjana, Arunpatcha Nimthong and Chanakan Kamrod

1. Experimental

Triphenylphosphane, PPh₃ (0.31 g) was dissolved in 30 mL of methanol at 338 K and then silver acetate, AgOAc (0.10 g) was added. The mixture was stirred for 2 hr and then *N,N'*-diethylthiourea, detu (0.08 g) was added and the new reaction mixture was heated under reflux 5 hr where upon the precipitate gradually disappeared. The resulting clear solution was filtered off and left to evaporate at room temperature. The crystalline complex, which deposited upon standing for several day, was filtered off and dried in vacuo.

1.1. Refinement

Reflections -1 1 1, 0 2 0, 0 -2 1, 1 1 0, -1 0 1, -1 -1 1, 0 0 2, 0 1 1, 0 -1 1, 0 1 2, 0 -1 2, 1 1 1, -1 3 1 and -2 2 3 were affected by the beam stop and were omitted from the refinement. All H atoms were positioned geometrically and refined using a riding-model with C—H = 0.98 Å (CH₃), and U_{iso}(H) = 1.5 U_{eq}(C); 0.99 Å (CH₂), and U_{iso}(H) = 1.2 U_{eq}(C); 0.95 Å (aryl H), and U_{iso}(H) = 1.2 U_{eq}(C); 0.88 Å (NH), and U_{iso}(H) = 1.2 U_{eq}(N); 0.84 Å (OH), and U_{iso}(H) = 1.5 U_{eq}(O).

2. Results and discussion

A large number of structural reports on silver(I) complexes containing thiourea derivatives as ligands or mixed-ligands with triphenylphosphane have been studied in recent years (Bowmaker *et al.*, 2010; Ruffer *et al.*, 2011; Pakawatchai *et al.*, 2012) because these complexes have many applications. Some of these complexes show interesting luminescence properties (Ferrari *et al.*, 2007) and exhibit significant biological activities (Isab *et al.*, 2010). The sixfold phenyl embraces (6PE) is a common motif of a pair of threefold XPh₃ moieties to form a concerted cycle of six edge-to-face (EF) motifs between six phenyl groups, leading to a formation one-, two-, and three-dimensional supramolecular networks (Dance & Scudder, 2000; Scudder & Dance, 2001). Herein, we report the crystal structure a silver(I) complex containing triphenylphosphane and *N,N'*-diethylthiourea.

In the mononuclear title complex, [Ag(C₅H₁₂N₂S)(C₁₈H₁₅P)₃] \cdot CH₃COO \cdot CH₃OH, the Ag^I ion adopts a distorted tetrahedral geometry formed by three P atoms from three triphenylphosphane ligands, one S atom from a *N,N'*-diethylthiourea ligand (Fig. 1). The angles at the Ag^I ion vary from 91.66 (3)° to 115.50 (3)°. In the crystal, the acetate anion is linked to the complex molecule *via* N1—H1 \cdots O1 and N2—H2 \cdots O2 hydrogen bonds [graph-set motif R²₂(8); Etter *et al.*, 1990] and the solvent methanol molecule *via* an O3—H3D \cdots O1 hydrogen bond. Each cation–anion pair is linked through a weak C34(*sp*³)—H34 \cdots O2ⁱ hydrogen bond, forming chains along the *a*-axis direction (see Table 1 and Fig. 2). In addition, sixfold phenyl embraces (6PE) with intermolecular distances P1 \cdots P1ⁱⁱ and P3 \cdots P3ⁱⁱⁱ of 6.6463 (13) Å and 6.667 (2) Å, respectively (symmetry code: (ii) 1-x, 1-y, -z; (iii) 1-x, 1-y, 1-z) are arranged in one-dimensional zigzag chains along the *c*-axis direction (Fig. 3). The combination of hydrogen bonding and phenyl \cdots phenyl interactions lead to the formation of a layer network parallel to (010) (Fig. 4).

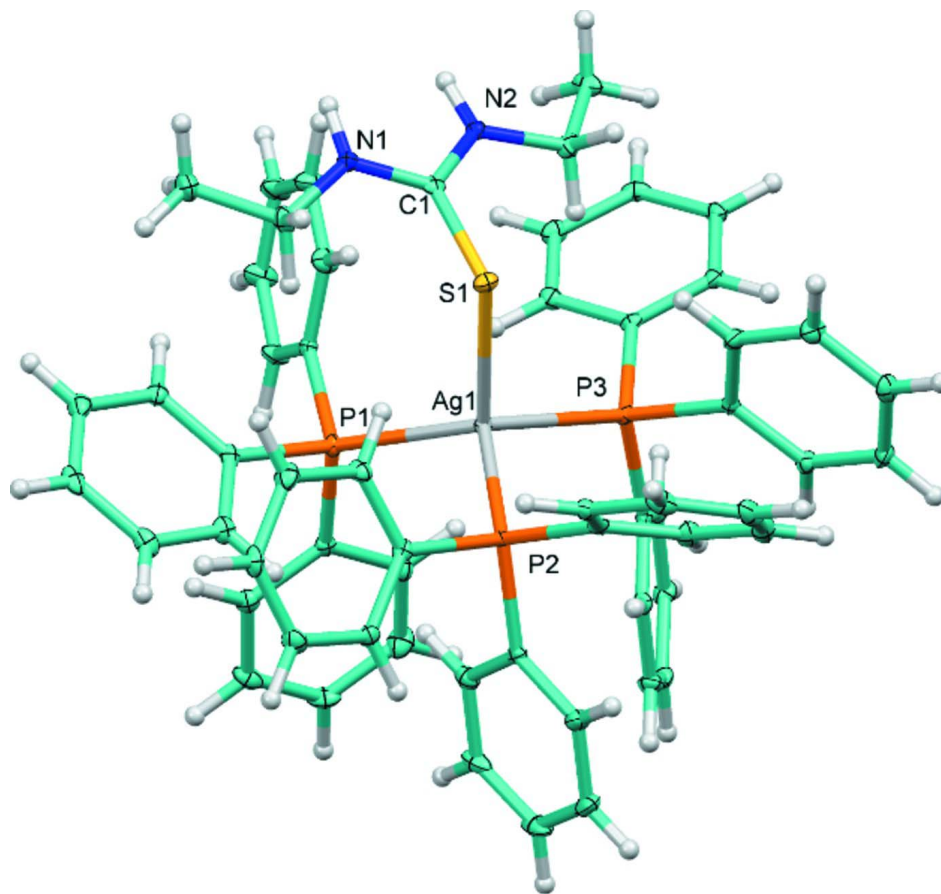


Figure 1

The molecular structure with displacement ellipsoids drawn at the 30% probability level. The acetate anion and methanol molecule are omitted for clarity.

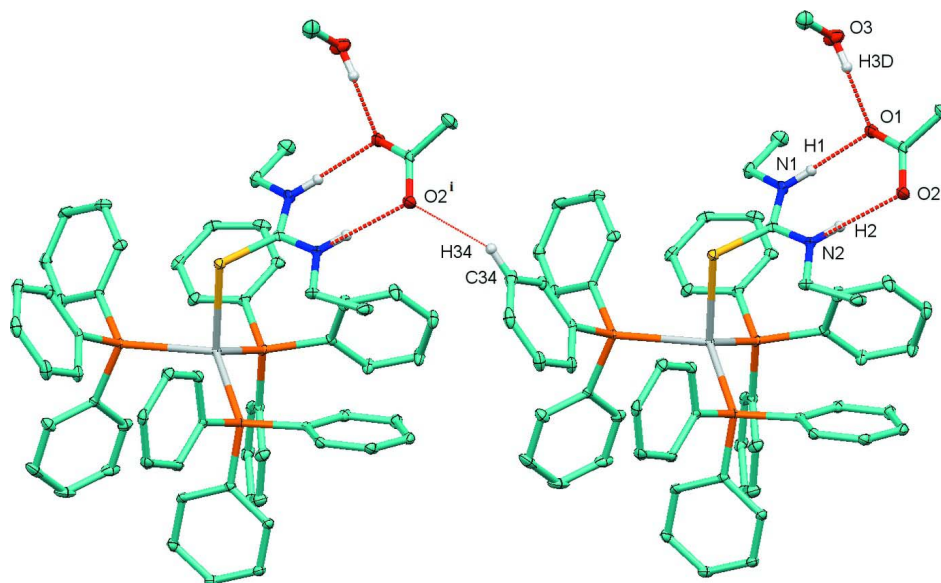


Figure 2

Part of the crystal structure with N—H···O and O—H···O hydrogen bonds shown as red dashed lines (symmetry code (i): $x-1, y, z$).

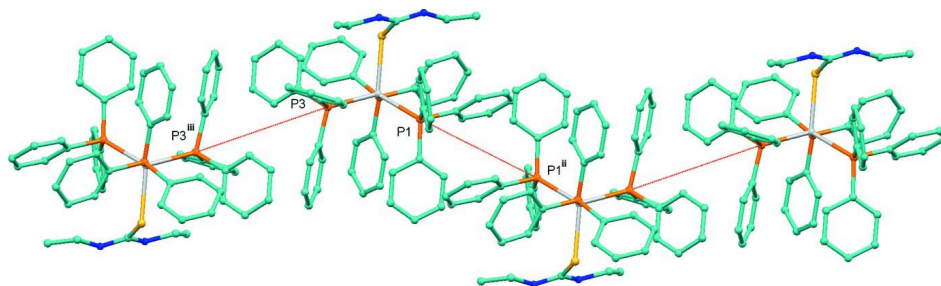
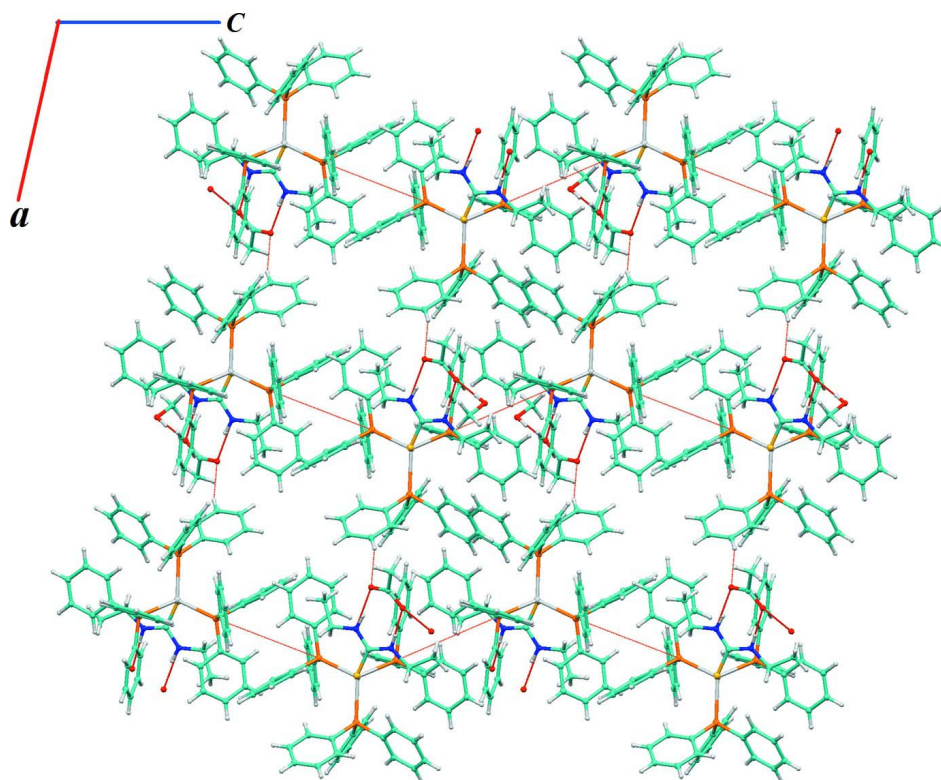


Figure 3

Part of the crystal structure with phenyl···phenyl interactions shown as dashed lines, which link molecules into one-dimensional zigzag chains (symmetry codes: (ii) $1-x, 1-y, -z$; (iii) $1-x, 1-y, 1-z$).


Figure 4

Part of the crystal structure showing formation of a layer network parallel to (010).

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Crystal data

[Ag(C₅H₁₂N₂S)(C₁₈H₁₅P)₃](C₂H₃O₂)·CH₄O

M_r = 1117.99

Monoclinic, $P2_1/n$

a = 12.950 (3) Å

b = 21.903 (6) Å

c = 19.915 (5) Å

β = 103.201 (4)°

V = 5500 (2) Å³

Z = 4

$F(000)$ = 2328

D_x = 1.350 Mg m⁻³

Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 5990 reflections

θ = 2.3–25.9°

μ = 0.54 mm⁻¹

T = 100 K

Block, colourless

0.18 × 0.15 × 0.11 mm

Data collection

Bruker SMART APEX CCD

diffractometer

Radiation source: fine focus sealed tube

ω and π scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2012)

T_{\min} = 0.608, T_{\max} = 0.746

59032 measured reflections

16670 independent reflections

10564 reflections with $I > 2\sigma(I)$

R_{int} = 0.093

θ_{\max} = 30.6°, θ_{\min} = 2.5°

h = -18→18

k = -30→31

l = -28→27

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.120$

$S = 1.00$

16670 reflections

653 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 1.6753P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.23 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -1.13 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|--------------|----------------------------------|
| Ag1 | 0.33154 (2) | 0.60067 (2) | 0.22458 (2) | 0.01296 (6) |
| S1 | 0.33683 (6) | 0.72215 (3) | 0.22711 (4) | 0.01798 (16) |
| P1 | 0.40233 (6) | 0.55336 (4) | 0.12895 (4) | 0.01430 (16) |
| P2 | 0.13005 (6) | 0.60018 (4) | 0.19850 (4) | 0.01245 (14) |
| P3 | 0.41323 (6) | 0.56197 (3) | 0.34445 (4) | 0.01342 (15) |
| N1 | 0.4563 (2) | 0.77443 (12) | 0.14991 (12) | 0.0179 (5) |
| H1 | 0.5131 | 0.7954 | 0.1471 | 0.021* |
| N2 | 0.5416 (2) | 0.75355 (11) | 0.26029 (12) | 0.0151 (5) |
| H2 | 0.5981 | 0.7696 | 0.2495 | 0.018* |
| C1 | 0.4519 (2) | 0.75171 (13) | 0.21146 (15) | 0.0162 (6) |
| C2 | 0.3736 (3) | 0.76719 (16) | 0.08743 (16) | 0.0233 (7) |
| H2A | 0.3153 | 0.7964 | 0.0878 | 0.028* |
| H2B | 0.3442 | 0.7253 | 0.0854 | 0.028* |
| C3 | 0.4183 (3) | 0.77859 (18) | 0.02503 (17) | 0.0306 (8) |
| H3A | 0.4444 | 0.8207 | 0.0261 | 0.046* |
| H3B | 0.3627 | 0.7723 | -0.0169 | 0.046* |
| H3C | 0.4769 | 0.7502 | 0.0253 | 0.046* |
| C4 | 0.5515 (3) | 0.73090 (15) | 0.33009 (16) | 0.0213 (7) |
| H4A | 0.5179 | 0.6902 | 0.3285 | 0.026* |
| H4B | 0.5144 | 0.7589 | 0.3558 | 0.026* |
| C5 | 0.6670 (3) | 0.72634 (16) | 0.36683 (17) | 0.0274 (8) |
| H5A | 0.6990 | 0.7671 | 0.3710 | 0.041* |
| H5B | 0.7042 | 0.6999 | 0.3404 | 0.041* |
| H5C | 0.6727 | 0.7091 | 0.4129 | 0.041* |
| C6 | 0.5431 (2) | 0.57060 (14) | 0.13891 (15) | 0.0153 (6) |
| C7 | 0.5741 (3) | 0.63004 (15) | 0.15736 (18) | 0.0250 (7) |
| H7 | 0.5228 | 0.6590 | 0.1640 | 0.030* |
| C8 | 0.6792 (3) | 0.64759 (16) | 0.16616 (18) | 0.0272 (8) |
| H8 | 0.6998 | 0.6885 | 0.1784 | 0.033* |
| C9 | 0.7535 (3) | 0.60516 (17) | 0.15701 (18) | 0.0275 (8) |

| | | | | |
|-----|-------------|--------------|---------------|------------|
| H9 | 0.8256 | 0.6168 | 0.1625 | 0.033* |
| C10 | 0.7228 (3) | 0.54571 (16) | 0.13985 (19) | 0.0284 (8) |
| H10 | 0.7746 | 0.5163 | 0.1349 | 0.034* |
| C11 | 0.6177 (2) | 0.52847 (15) | 0.12977 (17) | 0.0215 (7) |
| H11 | 0.5970 | 0.4878 | 0.1166 | 0.026* |
| C12 | 0.3419 (2) | 0.57843 (14) | 0.04166 (15) | 0.0171 (6) |
| C13 | 0.3988 (3) | 0.60774 (14) | -0.00032 (16) | 0.0203 (7) |
| H13 | 0.4723 | 0.6157 | 0.0165 | 0.024* |
| C14 | 0.3486 (3) | 0.62551 (15) | -0.06685 (17) | 0.0257 (8) |
| H14 | 0.3879 | 0.6458 | -0.0950 | 0.031* |
| C15 | 0.2425 (3) | 0.61386 (14) | -0.09221 (17) | 0.0253 (8) |
| H15 | 0.2089 | 0.6254 | -0.1380 | 0.030* |
| C16 | 0.1846 (3) | 0.58513 (15) | -0.05066 (16) | 0.0228 (7) |
| H16 | 0.1112 | 0.5772 | -0.0678 | 0.027* |
| C17 | 0.2338 (3) | 0.56809 (15) | 0.01571 (16) | 0.0209 (7) |
| H17 | 0.1935 | 0.5490 | 0.0441 | 0.025* |
| C18 | 0.3954 (2) | 0.47009 (14) | 0.12207 (15) | 0.0162 (6) |
| C19 | 0.4193 (3) | 0.43635 (15) | 0.18297 (17) | 0.0243 (7) |
| H19 | 0.4397 | 0.4567 | 0.2261 | 0.029* |
| C20 | 0.4133 (3) | 0.37296 (17) | 0.18082 (19) | 0.0304 (8) |
| H20 | 0.4305 | 0.3503 | 0.2225 | 0.036* |
| C21 | 0.3829 (3) | 0.34290 (15) | 0.11903 (19) | 0.0262 (8) |
| H21 | 0.3783 | 0.2996 | 0.1179 | 0.031* |
| C22 | 0.3588 (3) | 0.37610 (16) | 0.05847 (18) | 0.0249 (7) |
| H22 | 0.3373 | 0.3554 | 0.0156 | 0.030* |
| C23 | 0.3658 (2) | 0.43917 (15) | 0.05958 (16) | 0.0197 (7) |
| H23 | 0.3503 | 0.4614 | 0.0175 | 0.024* |
| C24 | 0.0644 (2) | 0.62679 (13) | 0.11257 (15) | 0.0147 (6) |
| C25 | 0.1001 (3) | 0.68057 (14) | 0.08859 (16) | 0.0194 (7) |
| H25 | 0.1595 | 0.7013 | 0.1159 | 0.023* |
| C26 | 0.0493 (3) | 0.70410 (16) | 0.02476 (17) | 0.0261 (8) |
| H26 | 0.0732 | 0.7413 | 0.0091 | 0.031* |
| C27 | -0.0358 (3) | 0.67363 (16) | -0.01598 (16) | 0.0250 (7) |
| H27 | -0.0705 | 0.6899 | -0.0595 | 0.030* |
| C28 | -0.0701 (3) | 0.61942 (16) | 0.00689 (17) | 0.0243 (7) |
| H28 | -0.1275 | 0.5979 | -0.0215 | 0.029* |
| C29 | -0.0214 (2) | 0.59630 (15) | 0.07107 (15) | 0.0191 (6) |
| H29 | -0.0465 | 0.5595 | 0.0869 | 0.023* |
| C30 | 0.0609 (2) | 0.64181 (15) | 0.25510 (15) | 0.0167 (6) |
| C31 | 0.0768 (2) | 0.62282 (16) | 0.32355 (16) | 0.0227 (7) |
| H31 | 0.1247 | 0.5905 | 0.3400 | 0.027* |
| C32 | 0.0227 (3) | 0.65100 (18) | 0.36770 (18) | 0.0293 (8) |
| H32 | 0.0322 | 0.6373 | 0.4140 | 0.035* |
| C33 | -0.0451 (3) | 0.69919 (17) | 0.34413 (18) | 0.0289 (8) |
| H33 | -0.0820 | 0.7185 | 0.3744 | 0.035* |
| C34 | -0.0593 (3) | 0.71940 (16) | 0.27687 (19) | 0.0278 (8) |
| H34 | -0.1047 | 0.7531 | 0.2613 | 0.033* |
| C35 | -0.0071 (2) | 0.69032 (15) | 0.23211 (16) | 0.0193 (7) |
| H35 | -0.0179 | 0.7037 | 0.1856 | 0.023* |

| | | | | |
|------|--------------|--------------|--------------|------------|
| C36 | 0.0815 (2) | 0.52212 (14) | 0.20000 (14) | 0.0161 (6) |
| C37 | -0.0046 (3) | 0.50528 (16) | 0.22687 (17) | 0.0243 (7) |
| H37 | -0.0448 | 0.5355 | 0.2437 | 0.029* |
| C38 | -0.0314 (3) | 0.44386 (18) | 0.22893 (18) | 0.0337 (9) |
| H38 | -0.0895 | 0.4323 | 0.2479 | 0.040* |
| C39 | 0.0252 (3) | 0.39995 (17) | 0.20387 (18) | 0.0350 (9) |
| H39 | 0.0061 | 0.3582 | 0.2055 | 0.042* |
| C40 | 0.1096 (3) | 0.41600 (15) | 0.17641 (18) | 0.0282 (8) |
| H40 | 0.1485 | 0.3856 | 0.1587 | 0.034* |
| C41 | 0.1375 (3) | 0.47657 (15) | 0.17474 (16) | 0.0218 (7) |
| H41 | 0.1960 | 0.4875 | 0.1560 | 0.026* |
| C42 | 0.3968 (2) | 0.47973 (14) | 0.35532 (14) | 0.0148 (6) |
| C43 | 0.2959 (2) | 0.45460 (14) | 0.33370 (15) | 0.0186 (7) |
| H43 | 0.2371 | 0.4806 | 0.3164 | 0.022* |
| C44 | 0.2799 (3) | 0.39218 (15) | 0.33711 (16) | 0.0218 (7) |
| H44 | 0.2107 | 0.3755 | 0.3223 | 0.026* |
| C45 | 0.3657 (3) | 0.35437 (15) | 0.36223 (16) | 0.0217 (7) |
| H45 | 0.3553 | 0.3115 | 0.3642 | 0.026* |
| C46 | 0.4659 (3) | 0.37849 (14) | 0.38437 (16) | 0.0199 (7) |
| H46 | 0.5243 | 0.3523 | 0.4018 | 0.024* |
| C47 | 0.4817 (2) | 0.44119 (14) | 0.38122 (15) | 0.0173 (6) |
| H47 | 0.5508 | 0.4577 | 0.3969 | 0.021* |
| C48 | 0.5559 (2) | 0.57202 (13) | 0.37759 (15) | 0.0149 (6) |
| C49 | 0.6217 (2) | 0.56328 (14) | 0.33204 (16) | 0.0199 (7) |
| H49 | 0.5919 | 0.5554 | 0.2847 | 0.024* |
| C50 | 0.7317 (3) | 0.56610 (15) | 0.35607 (17) | 0.0230 (7) |
| H50 | 0.7764 | 0.5605 | 0.3248 | 0.028* |
| C51 | 0.7756 (3) | 0.57685 (14) | 0.42450 (17) | 0.0215 (7) |
| H51 | 0.8506 | 0.5775 | 0.4407 | 0.026* |
| C52 | 0.7108 (2) | 0.58667 (14) | 0.46984 (16) | 0.0201 (7) |
| H52 | 0.7414 | 0.5951 | 0.5170 | 0.024* |
| C53 | 0.6008 (2) | 0.58423 (14) | 0.44665 (16) | 0.0179 (6) |
| H53 | 0.5566 | 0.5909 | 0.4780 | 0.021* |
| C54 | 0.3525 (2) | 0.59660 (14) | 0.40967 (14) | 0.0146 (6) |
| C55 | 0.3145 (2) | 0.56192 (15) | 0.45762 (15) | 0.0183 (6) |
| H55 | 0.3230 | 0.5188 | 0.4586 | 0.022* |
| C56 | 0.2643 (2) | 0.58991 (15) | 0.50379 (16) | 0.0216 (7) |
| H56 | 0.2366 | 0.5659 | 0.5353 | 0.026* |
| C57 | 0.2545 (2) | 0.65292 (16) | 0.50409 (16) | 0.0229 (7) |
| H57 | 0.2214 | 0.6721 | 0.5365 | 0.027* |
| C58 | 0.2928 (3) | 0.68773 (16) | 0.45740 (17) | 0.0232 (7) |
| H58 | 0.2866 | 0.7309 | 0.4580 | 0.028* |
| C59 | 0.3404 (2) | 0.65987 (15) | 0.40960 (16) | 0.0201 (7) |
| H59 | 0.3648 | 0.6840 | 0.3767 | 0.024* |
| O1 | 0.63350 (18) | 0.84663 (11) | 0.14416 (12) | 0.0267 (5) |
| O2 | 0.72376 (18) | 0.81113 (11) | 0.24488 (13) | 0.0306 (6) |
| C60 | 0.7099 (2) | 0.84833 (14) | 0.19575 (17) | 0.0189 (7) |
| C61 | 0.7909 (3) | 0.89894 (18) | 0.2000 (2) | 0.0354 (9) |
| H61A | 0.8114 | 0.9141 | 0.2475 | 0.053* |

| | | | | |
|------|------------|--------------|--------------|-------------|
| H61B | 0.7600 | 0.9324 | 0.1692 | 0.053* |
| H61C | 0.8536 | 0.8831 | 0.1860 | 0.053* |
| O3 | 0.5306 (2) | 0.92864 (13) | 0.04935 (13) | 0.0415 (7) |
| H3D | 0.5652 | 0.9025 | 0.0787 | 0.062* |
| C62 | 0.4790 (3) | 0.9708 (2) | 0.08389 (19) | 0.0386 (10) |
| H62A | 0.4311 | 0.9489 | 0.1071 | 0.058* |
| H62B | 0.4382 | 0.9996 | 0.0505 | 0.058* |
| H62C | 0.5319 | 0.9931 | 0.1181 | 0.058* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Ag1 | 0.01191 (10) | 0.01405 (10) | 0.01316 (10) | 0.00088 (10) | 0.00339 (8) | 0.00021 (9) |
| S1 | 0.0162 (4) | 0.0138 (3) | 0.0248 (4) | -0.0007 (3) | 0.0066 (3) | 0.0009 (3) |
| P1 | 0.0138 (4) | 0.0157 (4) | 0.0141 (4) | 0.0027 (3) | 0.0046 (3) | -0.0009 (3) |
| P2 | 0.0104 (3) | 0.0126 (3) | 0.0146 (3) | -0.0001 (3) | 0.0034 (3) | 0.0007 (3) |
| P3 | 0.0135 (4) | 0.0134 (4) | 0.0134 (4) | 0.0008 (3) | 0.0032 (3) | 0.0024 (3) |
| N1 | 0.0168 (13) | 0.0205 (14) | 0.0166 (13) | -0.0036 (11) | 0.0042 (11) | -0.0018 (10) |
| N2 | 0.0150 (12) | 0.0149 (13) | 0.0154 (12) | 0.0001 (10) | 0.0035 (10) | 0.0011 (10) |
| C1 | 0.0183 (15) | 0.0096 (14) | 0.0212 (15) | 0.0003 (12) | 0.0054 (13) | -0.0032 (11) |
| C2 | 0.0190 (16) | 0.0315 (19) | 0.0190 (16) | 0.0026 (14) | 0.0033 (13) | -0.0025 (14) |
| C3 | 0.036 (2) | 0.036 (2) | 0.0186 (17) | -0.0033 (17) | 0.0035 (16) | -0.0010 (15) |
| C4 | 0.0253 (17) | 0.0188 (16) | 0.0196 (16) | 0.0011 (14) | 0.0046 (14) | 0.0052 (13) |
| C5 | 0.0296 (19) | 0.0205 (17) | 0.0259 (18) | -0.0039 (15) | -0.0066 (15) | 0.0048 (14) |
| C6 | 0.0168 (15) | 0.0174 (15) | 0.0126 (14) | -0.0015 (12) | 0.0050 (12) | -0.0001 (11) |
| C7 | 0.0235 (17) | 0.0202 (17) | 0.0336 (19) | 0.0017 (14) | 0.0117 (15) | -0.0071 (15) |
| C8 | 0.0240 (18) | 0.0214 (18) | 0.038 (2) | -0.0071 (15) | 0.0107 (16) | -0.0100 (15) |
| C9 | 0.0156 (15) | 0.0313 (19) | 0.0356 (19) | -0.0039 (15) | 0.0056 (14) | -0.0097 (16) |
| C10 | 0.0160 (16) | 0.0262 (19) | 0.043 (2) | 0.0010 (14) | 0.0067 (16) | -0.0130 (16) |
| C11 | 0.0165 (15) | 0.0196 (16) | 0.0278 (17) | -0.0002 (13) | 0.0037 (14) | -0.0092 (13) |
| C12 | 0.0205 (16) | 0.0159 (15) | 0.0158 (15) | 0.0043 (13) | 0.0061 (13) | -0.0004 (12) |
| C13 | 0.0244 (16) | 0.0164 (16) | 0.0205 (15) | -0.0002 (14) | 0.0063 (13) | -0.0007 (12) |
| C14 | 0.040 (2) | 0.0176 (16) | 0.0215 (17) | -0.0024 (15) | 0.0101 (16) | 0.0005 (13) |
| C15 | 0.040 (2) | 0.0160 (17) | 0.0172 (16) | 0.0061 (15) | 0.0015 (15) | -0.0012 (12) |
| C16 | 0.0214 (16) | 0.0245 (18) | 0.0200 (16) | 0.0091 (14) | -0.0009 (14) | -0.0033 (13) |
| C17 | 0.0195 (16) | 0.0222 (17) | 0.0217 (16) | 0.0057 (14) | 0.0059 (13) | -0.0010 (13) |
| C18 | 0.0137 (14) | 0.0189 (15) | 0.0165 (15) | 0.0021 (12) | 0.0043 (12) | -0.0002 (12) |
| C19 | 0.0285 (18) | 0.0238 (18) | 0.0209 (17) | 0.0057 (15) | 0.0063 (15) | 0.0003 (14) |
| C20 | 0.036 (2) | 0.0263 (19) | 0.030 (2) | 0.0079 (17) | 0.0105 (17) | 0.0070 (15) |
| C21 | 0.0215 (17) | 0.0135 (16) | 0.043 (2) | 0.0002 (14) | 0.0059 (16) | 0.0007 (15) |
| C22 | 0.0205 (17) | 0.0219 (17) | 0.0300 (19) | 0.0023 (14) | 0.0006 (15) | -0.0062 (14) |
| C23 | 0.0152 (15) | 0.0228 (17) | 0.0208 (16) | 0.0016 (13) | 0.0035 (13) | -0.0001 (13) |
| C24 | 0.0151 (14) | 0.0135 (14) | 0.0162 (14) | 0.0049 (12) | 0.0052 (12) | 0.0020 (11) |
| C25 | 0.0223 (16) | 0.0154 (15) | 0.0197 (16) | 0.0008 (13) | 0.0029 (13) | -0.0012 (12) |
| C26 | 0.035 (2) | 0.0204 (17) | 0.0235 (17) | 0.0030 (15) | 0.0084 (15) | 0.0055 (14) |
| C27 | 0.0286 (18) | 0.0306 (19) | 0.0145 (15) | 0.0071 (15) | 0.0020 (14) | 0.0054 (13) |
| C28 | 0.0174 (16) | 0.0328 (19) | 0.0212 (17) | -0.0005 (14) | 0.0012 (14) | -0.0027 (14) |
| C29 | 0.0146 (14) | 0.0246 (17) | 0.0186 (15) | -0.0014 (14) | 0.0048 (12) | -0.0015 (13) |
| C30 | 0.0093 (13) | 0.0228 (16) | 0.0183 (15) | -0.0050 (12) | 0.0035 (12) | -0.0039 (12) |
| C31 | 0.0135 (15) | 0.0341 (19) | 0.0214 (17) | -0.0004 (14) | 0.0059 (13) | -0.0012 (14) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C32 | 0.0182 (16) | 0.049 (2) | 0.0214 (17) | -0.0053 (16) | 0.0063 (14) | -0.0056 (16) |
| C33 | 0.0197 (17) | 0.041 (2) | 0.0294 (19) | -0.0050 (16) | 0.0118 (15) | -0.0170 (16) |
| C34 | 0.0192 (17) | 0.0244 (18) | 0.039 (2) | 0.0013 (14) | 0.0057 (16) | -0.0106 (16) |
| C35 | 0.0171 (15) | 0.0195 (16) | 0.0209 (16) | -0.0027 (13) | 0.0034 (13) | -0.0034 (13) |
| C36 | 0.0146 (14) | 0.0187 (15) | 0.0124 (14) | -0.0040 (13) | -0.0026 (12) | 0.0031 (12) |
| C37 | 0.0244 (18) | 0.0258 (18) | 0.0227 (17) | -0.0097 (15) | 0.0052 (14) | -0.0001 (14) |
| C38 | 0.039 (2) | 0.037 (2) | 0.0239 (18) | -0.0204 (18) | 0.0051 (17) | 0.0076 (16) |
| C39 | 0.052 (2) | 0.0178 (17) | 0.0268 (18) | -0.0132 (19) | -0.0087 (17) | 0.0071 (15) |
| C40 | 0.037 (2) | 0.0150 (16) | 0.0255 (18) | -0.0025 (15) | -0.0084 (16) | -0.0010 (13) |
| C41 | 0.0238 (17) | 0.0202 (16) | 0.0185 (16) | 0.0009 (14) | -0.0010 (14) | -0.0004 (13) |
| C42 | 0.0177 (15) | 0.0167 (15) | 0.0103 (13) | 0.0005 (12) | 0.0040 (12) | 0.0020 (11) |
| C43 | 0.0172 (15) | 0.0207 (16) | 0.0153 (15) | -0.0004 (13) | -0.0012 (13) | 0.0056 (12) |
| C44 | 0.0186 (15) | 0.0228 (17) | 0.0211 (16) | -0.0072 (14) | -0.0016 (13) | 0.0016 (13) |
| C45 | 0.0279 (18) | 0.0163 (16) | 0.0202 (16) | -0.0005 (14) | 0.0042 (14) | 0.0037 (12) |
| C46 | 0.0216 (16) | 0.0170 (15) | 0.0210 (16) | 0.0038 (13) | 0.0047 (14) | 0.0050 (12) |
| C47 | 0.0163 (15) | 0.0174 (15) | 0.0167 (15) | -0.0008 (13) | 0.0009 (12) | 0.0030 (12) |
| C48 | 0.0151 (14) | 0.0121 (14) | 0.0177 (15) | -0.0001 (12) | 0.0043 (12) | 0.0042 (11) |
| C49 | 0.0188 (16) | 0.0195 (16) | 0.0202 (16) | 0.0008 (13) | 0.0022 (13) | -0.0005 (13) |
| C50 | 0.0189 (16) | 0.0226 (17) | 0.0296 (18) | 0.0019 (14) | 0.0096 (15) | -0.0015 (14) |
| C51 | 0.0150 (15) | 0.0165 (15) | 0.0304 (18) | -0.0006 (13) | -0.0001 (14) | 0.0037 (13) |
| C52 | 0.0209 (16) | 0.0201 (17) | 0.0156 (15) | -0.0052 (13) | -0.0032 (13) | 0.0039 (12) |
| C53 | 0.0185 (15) | 0.0177 (15) | 0.0187 (15) | -0.0023 (12) | 0.0066 (13) | 0.0022 (12) |
| C54 | 0.0106 (13) | 0.0202 (15) | 0.0123 (13) | -0.0008 (13) | 0.0012 (11) | 0.0006 (12) |
| C55 | 0.0188 (15) | 0.0192 (16) | 0.0157 (15) | -0.0013 (13) | 0.0016 (13) | 0.0051 (12) |
| C56 | 0.0206 (16) | 0.0286 (19) | 0.0165 (15) | -0.0017 (14) | 0.0060 (13) | 0.0068 (13) |
| C57 | 0.0153 (15) | 0.034 (2) | 0.0207 (16) | 0.0033 (14) | 0.0070 (13) | -0.0025 (14) |
| C58 | 0.0225 (17) | 0.0212 (17) | 0.0273 (18) | 0.0030 (14) | 0.0087 (14) | -0.0017 (14) |
| C59 | 0.0195 (15) | 0.0208 (16) | 0.0218 (16) | -0.0028 (14) | 0.0082 (13) | 0.0016 (13) |
| O1 | 0.0215 (12) | 0.0335 (14) | 0.0244 (12) | -0.0031 (11) | 0.0035 (10) | 0.0092 (11) |
| O2 | 0.0216 (12) | 0.0336 (14) | 0.0342 (14) | -0.0056 (11) | 0.0010 (11) | 0.0152 (11) |
| C60 | 0.0153 (15) | 0.0198 (16) | 0.0252 (17) | 0.0018 (13) | 0.0119 (13) | -0.0011 (13) |
| C61 | 0.034 (2) | 0.037 (2) | 0.036 (2) | -0.0158 (19) | 0.0097 (17) | 0.0049 (18) |
| O3 | 0.0531 (18) | 0.0419 (17) | 0.0307 (15) | 0.0131 (14) | 0.0122 (13) | 0.0079 (12) |
| C62 | 0.035 (2) | 0.051 (3) | 0.029 (2) | 0.002 (2) | 0.0062 (18) | 0.0029 (18) |

Geometric parameters (Å, °)

| | | | |
|--------|-------------|---------|-----------|
| Ag1—P1 | 2.5178 (9) | C27—C28 | 1.381 (5) |
| Ag1—P3 | 2.5264 (9) | C27—H27 | 0.9500 |
| Ag1—P2 | 2.5415 (10) | C28—C29 | 1.386 (4) |
| Ag1—S1 | 2.6619 (10) | C28—H28 | 0.9500 |
| S1—C1 | 1.717 (3) | C29—H29 | 0.9500 |
| P1—C12 | 1.821 (3) | C30—C35 | 1.389 (4) |
| P1—C6 | 1.827 (3) | C30—C31 | 1.395 (4) |
| P1—C18 | 1.830 (3) | C31—C32 | 1.387 (4) |
| P2—C36 | 1.824 (3) | C31—H31 | 0.9500 |
| P2—C24 | 1.824 (3) | C32—C33 | 1.384 (5) |
| P2—C30 | 1.834 (3) | C32—H32 | 0.9500 |
| P3—C48 | 1.828 (3) | C33—C34 | 1.382 (5) |
| P3—C54 | 1.829 (3) | C33—H33 | 0.9500 |

| | | | |
|---------|-----------|---------|-----------|
| P3—C42 | 1.833 (3) | C34—C35 | 1.391 (4) |
| N1—C1 | 1.336 (4) | C34—H34 | 0.9500 |
| N1—C2 | 1.453 (4) | C35—H35 | 0.9500 |
| N1—H1 | 0.8806 | C36—C37 | 1.392 (4) |
| N2—C1 | 1.334 (4) | C36—C41 | 1.393 (4) |
| N2—C4 | 1.454 (4) | C37—C38 | 1.392 (5) |
| N2—H2 | 0.8807 | C37—H37 | 0.9500 |
| C2—C3 | 1.507 (4) | C38—C39 | 1.371 (6) |
| C2—H2A | 0.9900 | C38—H38 | 0.9500 |
| C2—H2B | 0.9900 | C39—C40 | 1.375 (5) |
| C3—H3A | 0.9800 | C39—H39 | 0.9500 |
| C3—H3B | 0.9800 | C40—C41 | 1.377 (4) |
| C3—H3C | 0.9800 | C40—H40 | 0.9500 |
| C4—C5 | 1.510 (5) | C41—H41 | 0.9500 |
| C4—H4A | 0.9900 | C42—C47 | 1.388 (4) |
| C4—H4B | 0.9900 | C42—C43 | 1.393 (4) |
| C5—H5A | 0.9800 | C43—C44 | 1.387 (4) |
| C5—H5B | 0.9800 | C43—H43 | 0.9500 |
| C5—H5C | 0.9800 | C44—C45 | 1.384 (4) |
| C6—C11 | 1.378 (4) | C44—H44 | 0.9500 |
| C6—C7 | 1.387 (4) | C45—C46 | 1.377 (4) |
| C7—C8 | 1.386 (5) | C45—H45 | 0.9500 |
| C7—H7 | 0.9500 | C46—C47 | 1.392 (4) |
| C8—C9 | 1.380 (5) | C46—H46 | 0.9500 |
| C8—H8 | 0.9500 | C47—H47 | 0.9500 |
| C9—C10 | 1.381 (5) | C48—C53 | 1.391 (4) |
| C9—H9 | 0.9500 | C48—C49 | 1.392 (4) |
| C10—C11 | 1.383 (4) | C49—C50 | 1.396 (4) |
| C10—H10 | 0.9500 | C49—H49 | 0.9500 |
| C11—H11 | 0.9500 | C50—C51 | 1.372 (5) |
| C12—C13 | 1.391 (4) | C50—H50 | 0.9500 |
| C12—C17 | 1.396 (4) | C51—C52 | 1.383 (4) |
| C13—C14 | 1.391 (4) | C51—H51 | 0.9500 |
| C13—H13 | 0.9500 | C52—C53 | 1.395 (4) |
| C14—C15 | 1.375 (5) | C52—H52 | 0.9500 |
| C14—H14 | 0.9500 | C53—H53 | 0.9500 |
| C15—C16 | 1.388 (5) | C54—C59 | 1.395 (4) |
| C15—H15 | 0.9500 | C54—C55 | 1.395 (4) |
| C16—C17 | 1.381 (4) | C55—C56 | 1.384 (4) |
| C16—H16 | 0.9500 | C55—H55 | 0.9500 |
| C17—H17 | 0.9500 | C56—C57 | 1.386 (5) |
| C18—C23 | 1.392 (4) | C56—H56 | 0.9500 |
| C18—C19 | 1.393 (4) | C57—C58 | 1.379 (4) |
| C19—C20 | 1.391 (5) | C57—H57 | 0.9500 |
| C19—H19 | 0.9500 | C58—C59 | 1.388 (4) |
| C20—C21 | 1.372 (5) | C58—H58 | 0.9500 |
| C20—H20 | 0.9500 | C59—H59 | 0.9500 |
| C21—C22 | 1.382 (5) | O1—C60 | 1.254 (4) |
| C21—H21 | 0.9500 | O2—C60 | 1.254 (4) |

| | | | |
|------------|-------------|-------------|-----------|
| C22—C23 | 1.384 (5) | C60—C61 | 1.515 (5) |
| C22—H22 | 0.9500 | C61—H61A | 0.9800 |
| C23—H23 | 0.9500 | C61—H61B | 0.9800 |
| C24—C25 | 1.390 (4) | C61—H61C | 0.9800 |
| C24—C29 | 1.394 (4) | O3—C62 | 1.407 (5) |
| C25—C26 | 1.390 (4) | O3—H3D | 0.8665 |
| C25—H25 | 0.9500 | C62—H62A | 0.9800 |
| C26—C27 | 1.382 (5) | C62—H62B | 0.9800 |
| C26—H26 | 0.9500 | C62—H62C | 0.9800 |
| P1—Ag1—P3 | 115.50 (3) | C27—C26—C25 | 120.3 (3) |
| P1—Ag1—P2 | 112.20 (3) | C27—C26—H26 | 119.8 |
| P3—Ag1—P2 | 112.37 (3) | C25—C26—H26 | 119.8 |
| P1—Ag1—S1 | 114.42 (3) | C28—C27—C26 | 119.7 (3) |
| P3—Ag1—S1 | 108.30 (3) | C28—C27—H27 | 120.2 |
| P2—Ag1—S1 | 91.65 (3) | C26—C27—H27 | 120.2 |
| C1—S1—Ag1 | 113.15 (10) | C27—C28—C29 | 120.3 (3) |
| C12—P1—C6 | 104.00 (14) | C27—C28—H28 | 119.8 |
| C12—P1—C18 | 103.08 (14) | C29—C28—H28 | 119.8 |
| C6—P1—C18 | 104.15 (14) | C28—C29—C24 | 120.4 (3) |
| C12—P1—Ag1 | 116.54 (10) | C28—C29—H29 | 119.8 |
| C6—P1—Ag1 | 111.05 (10) | C24—C29—H29 | 119.8 |
| C18—P1—Ag1 | 116.55 (10) | C35—C30—C31 | 119.4 (3) |
| C36—P2—C24 | 103.07 (13) | C35—C30—P2 | 122.6 (2) |
| C36—P2—C30 | 103.75 (14) | C31—C30—P2 | 118.0 (2) |
| C24—P2—C30 | 103.25 (14) | C32—C31—C30 | 120.3 (3) |
| C36—P2—Ag1 | 110.00 (10) | C32—C31—H31 | 119.9 |
| C24—P2—Ag1 | 115.31 (10) | C30—C31—H31 | 119.9 |
| C30—P2—Ag1 | 119.65 (10) | C33—C32—C31 | 119.8 (3) |
| C48—P3—C54 | 104.88 (13) | C33—C32—H32 | 120.1 |
| C48—P3—C42 | 102.17 (13) | C31—C32—H32 | 120.1 |
| C54—P3—C42 | 104.08 (13) | C34—C33—C32 | 120.4 (3) |
| C48—P3—Ag1 | 118.12 (10) | C34—C33—H33 | 119.8 |
| C54—P3—Ag1 | 112.13 (10) | C32—C33—H33 | 119.8 |
| C42—P3—Ag1 | 113.98 (9) | C33—C34—C35 | 119.8 (3) |
| C1—N1—C2 | 124.6 (3) | C33—C34—H34 | 120.1 |
| C1—N1—H1 | 117.7 | C35—C34—H34 | 120.1 |
| C2—N1—H1 | 117.7 | C30—C35—C34 | 120.2 (3) |
| C1—N2—C4 | 124.0 (3) | C30—C35—H35 | 119.9 |
| C1—N2—H2 | 117.9 | C34—C35—H35 | 119.9 |
| C4—N2—H2 | 118.1 | C37—C36—C41 | 118.5 (3) |
| N2—C1—N1 | 116.4 (3) | C37—C36—P2 | 124.3 (3) |
| N2—C1—S1 | 121.7 (2) | C41—C36—P2 | 117.1 (2) |
| N1—C1—S1 | 121.8 (2) | C36—C37—C38 | 119.6 (3) |
| N1—C2—C3 | 109.9 (3) | C36—C37—H37 | 120.2 |
| N1—C2—H2A | 109.7 | C38—C37—H37 | 120.2 |
| C3—C2—H2A | 109.7 | C39—C38—C37 | 120.6 (3) |
| N1—C2—H2B | 109.7 | C39—C38—H38 | 119.7 |
| C3—C2—H2B | 109.7 | C37—C38—H38 | 119.7 |

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| H2A—C2—H2B | 108.2 | C38—C39—C40 | 120.4 (3) |
| C2—C3—H3A | 109.5 | C38—C39—H39 | 119.8 |
| C2—C3—H3B | 109.5 | C40—C39—H39 | 119.8 |
| H3A—C3—H3B | 109.5 | C39—C40—C41 | 119.5 (4) |
| C2—C3—H3C | 109.5 | C39—C40—H40 | 120.3 |
| H3A—C3—H3C | 109.5 | C41—C40—H40 | 120.3 |
| H3B—C3—H3C | 109.5 | C40—C41—C36 | 121.4 (3) |
| N2—C4—C5 | 110.3 (3) | C40—C41—H41 | 119.3 |
| N2—C4—H4A | 109.6 | C36—C41—H41 | 119.3 |
| C5—C4—H4A | 109.6 | C47—C42—C43 | 118.8 (3) |
| N2—C4—H4B | 109.6 | C47—C42—P3 | 122.5 (2) |
| C5—C4—H4B | 109.6 | C43—C42—P3 | 118.6 (2) |
| H4A—C4—H4B | 108.1 | C44—C43—C42 | 120.9 (3) |
| C4—C5—H5A | 109.5 | C44—C43—H43 | 119.5 |
| C4—C5—H5B | 109.5 | C42—C43—H43 | 119.5 |
| H5A—C5—H5B | 109.5 | C45—C44—C43 | 119.5 (3) |
| C4—C5—H5C | 109.5 | C45—C44—H44 | 120.3 |
| H5A—C5—H5C | 109.5 | C43—C44—H44 | 120.3 |
| H5B—C5—H5C | 109.5 | C46—C45—C44 | 120.4 (3) |
| C11—C6—C7 | 119.6 (3) | C46—C45—H45 | 119.8 |
| C11—C6—P1 | 124.0 (2) | C44—C45—H45 | 119.8 |
| C7—C6—P1 | 116.4 (2) | C45—C46—C47 | 120.1 (3) |
| C8—C7—C6 | 120.7 (3) | C45—C46—H46 | 120.0 |
| C8—C7—H7 | 119.7 | C47—C46—H46 | 120.0 |
| C6—C7—H7 | 119.7 | C42—C47—C46 | 120.3 (3) |
| C9—C8—C7 | 119.4 (3) | C42—C47—H47 | 119.8 |
| C9—C8—H8 | 120.3 | C46—C47—H47 | 119.8 |
| C7—C8—H8 | 120.3 | C53—C48—C49 | 119.4 (3) |
| C8—C9—C10 | 119.8 (3) | C53—C48—P3 | 122.7 (2) |
| C8—C9—H9 | 120.1 | C49—C48—P3 | 117.8 (2) |
| C10—C9—H9 | 120.1 | C48—C49—C50 | 119.9 (3) |
| C9—C10—C11 | 120.7 (3) | C48—C49—H49 | 120.0 |
| C9—C10—H10 | 119.6 | C50—C49—H49 | 120.0 |
| C11—C10—H10 | 119.6 | C51—C50—C49 | 120.5 (3) |
| C6—C11—C10 | 119.7 (3) | C51—C50—H50 | 119.8 |
| C6—C11—H11 | 120.2 | C49—C50—H50 | 119.8 |
| C10—C11—H11 | 120.2 | C50—C51—C52 | 120.0 (3) |
| C13—C12—C17 | 118.5 (3) | C50—C51—H51 | 120.0 |
| C13—C12—P1 | 122.8 (2) | C52—C51—H51 | 120.0 |
| C17—C12—P1 | 118.7 (2) | C51—C52—C53 | 120.3 (3) |
| C12—C13—C14 | 120.3 (3) | C51—C52—H52 | 119.9 |
| C12—C13—H13 | 119.8 | C53—C52—H52 | 119.9 |
| C14—C13—H13 | 119.8 | C48—C53—C52 | 119.9 (3) |
| C15—C14—C13 | 120.5 (3) | C48—C53—H53 | 120.0 |
| C15—C14—H14 | 119.7 | C52—C53—H53 | 120.0 |
| C13—C14—H14 | 119.7 | C59—C54—C55 | 119.0 (3) |
| C14—C15—C16 | 119.7 (3) | C59—C54—P3 | 118.5 (2) |
| C14—C15—H15 | 120.1 | C55—C54—P3 | 122.4 (2) |
| C16—C15—H15 | 120.1 | C56—C55—C54 | 120.4 (3) |

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|---------------|------------|-----------------|------------|
| C17—C16—C15 | 119.9 (3) | C56—C55—H55 | 119.8 |
| C17—C16—H16 | 120.0 | C54—C55—H55 | 119.8 |
| C15—C16—H16 | 120.0 | C55—C56—C57 | 120.1 (3) |
| C16—C17—C12 | 121.0 (3) | C55—C56—H56 | 119.9 |
| C16—C17—H17 | 119.5 | C57—C56—H56 | 119.9 |
| C12—C17—H17 | 119.5 | C58—C57—C56 | 120.0 (3) |
| C23—C18—C19 | 118.8 (3) | C58—C57—H57 | 120.0 |
| C23—C18—P1 | 123.4 (2) | C56—C57—H57 | 120.0 |
| C19—C18—P1 | 117.8 (2) | C57—C58—C59 | 120.2 (3) |
| C20—C19—C18 | 120.2 (3) | C57—C58—H58 | 119.9 |
| C20—C19—H19 | 119.9 | C59—C58—H58 | 119.9 |
| C18—C19—H19 | 119.9 | C58—C59—C54 | 120.2 (3) |
| C21—C20—C19 | 120.6 (3) | C58—C59—H59 | 119.9 |
| C21—C20—H20 | 119.7 | C54—C59—H59 | 119.9 |
| C19—C20—H20 | 119.7 | O1—C60—O2 | 124.4 (3) |
| C20—C21—C22 | 119.5 (3) | O1—C60—C61 | 118.3 (3) |
| C20—C21—H21 | 120.3 | O2—C60—C61 | 117.3 (3) |
| C22—C21—H21 | 120.3 | C60—C61—H61A | 109.5 |
| C21—C22—C23 | 120.7 (3) | C60—C61—H61B | 109.5 |
| C21—C22—H22 | 119.6 | H61A—C61—H61B | 109.5 |
| C23—C22—H22 | 119.6 | C60—C61—H61C | 109.5 |
| C22—C23—C18 | 120.2 (3) | H61A—C61—H61C | 109.5 |
| C22—C23—H23 | 119.9 | H61B—C61—H61C | 109.5 |
| C18—C23—H23 | 119.9 | C62—O3—H3D | 109.4 |
| C25—C24—C29 | 119.0 (3) | O3—C62—H62A | 109.5 |
| C25—C24—P2 | 118.2 (2) | O3—C62—H62B | 109.5 |
| C29—C24—P2 | 122.7 (2) | H62A—C62—H62B | 109.5 |
| C24—C25—C26 | 120.2 (3) | O3—C62—H62C | 109.5 |
| C24—C25—H25 | 119.9 | H62A—C62—H62C | 109.5 |
| C26—C25—H25 | 119.9 | H62B—C62—H62C | 109.5 |
| | | | |
| C4—N2—C1—N1 | -179.9 (3) | C36—P2—C30—C31 | 59.7 (3) |
| C4—N2—C1—S1 | 0.5 (4) | C24—P2—C30—C31 | 167.0 (2) |
| C2—N1—C1—N2 | 168.9 (3) | Ag1—P2—C30—C31 | -63.3 (3) |
| C2—N1—C1—S1 | -11.5 (4) | C35—C30—C31—C32 | 1.8 (5) |
| Ag1—S1—C1—N2 | -79.1 (2) | P2—C30—C31—C32 | -177.1 (3) |
| Ag1—S1—C1—N1 | 101.4 (2) | C30—C31—C32—C33 | -1.7 (5) |
| C1—N1—C2—C3 | -160.5 (3) | C31—C32—C33—C34 | 0.0 (5) |
| C1—N2—C4—C5 | 166.9 (3) | C32—C33—C34—C35 | 1.4 (5) |
| C12—P1—C6—C11 | -97.3 (3) | C31—C30—C35—C34 | -0.4 (5) |
| C18—P1—C6—C11 | 10.4 (3) | P2—C30—C35—C34 | 178.5 (2) |
| Ag1—P1—C6—C11 | 136.6 (2) | C33—C34—C35—C30 | -1.2 (5) |
| C12—P1—C6—C7 | 83.2 (3) | C24—P2—C36—C37 | -95.3 (3) |
| C18—P1—C6—C7 | -169.1 (2) | C30—P2—C36—C37 | 12.1 (3) |
| Ag1—P1—C6—C7 | -42.9 (3) | Ag1—P2—C36—C37 | 141.2 (2) |
| C11—C6—C7—C8 | 0.5 (5) | C24—P2—C36—C41 | 87.1 (2) |
| P1—C6—C7—C8 | 180.0 (3) | C30—P2—C36—C41 | -165.5 (2) |
| C6—C7—C8—C9 | -0.6 (5) | Ag1—P2—C36—C41 | -36.4 (2) |
| C7—C8—C9—C10 | -0.6 (5) | C41—C36—C37—C38 | 1.1 (5) |

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|-----------------|------------|-----------------|------------|
| C8—C9—C10—C11 | 1.8 (6) | P2—C36—C37—C38 | -176.4 (3) |
| C7—C6—C11—C10 | 0.7 (5) | C36—C37—C38—C39 | -0.9 (5) |
| P1—C6—C11—C10 | -178.7 (3) | C37—C38—C39—C40 | 0.1 (5) |
| C9—C10—C11—C6 | -1.9 (5) | C38—C39—C40—C41 | 0.5 (5) |
| C6—P1—C12—C13 | -4.2 (3) | C39—C40—C41—C36 | -0.3 (5) |
| C18—P1—C12—C13 | -112.7 (3) | C37—C36—C41—C40 | -0.5 (5) |
| Ag1—P1—C12—C13 | 118.3 (2) | P2—C36—C41—C40 | 177.2 (2) |
| C6—P1—C12—C17 | 176.0 (2) | C48—P3—C42—C47 | -1.8 (3) |
| C18—P1—C12—C17 | 67.6 (3) | C54—P3—C42—C47 | -110.7 (3) |
| Ag1—P1—C12—C17 | -61.4 (3) | Ag1—P3—C42—C47 | 126.8 (2) |
| C17—C12—C13—C14 | -0.7 (5) | C48—P3—C42—C43 | -178.7 (2) |
| P1—C12—C13—C14 | 179.5 (2) | C54—P3—C42—C43 | 72.4 (3) |
| C12—C13—C14—C15 | -0.6 (5) | Ag1—P3—C42—C43 | -50.1 (3) |
| C13—C14—C15—C16 | 1.2 (5) | C47—C42—C43—C44 | -0.7 (4) |
| C14—C15—C16—C17 | -0.4 (5) | P3—C42—C43—C44 | 176.3 (2) |
| C15—C16—C17—C12 | -1.0 (5) | C42—C43—C44—C45 | -0.1 (5) |
| C13—C12—C17—C16 | 1.6 (5) | C43—C44—C45—C46 | 0.7 (5) |
| P1—C12—C17—C16 | -178.7 (2) | C44—C45—C46—C47 | -0.4 (5) |
| C12—P1—C18—C23 | 9.3 (3) | C43—C42—C47—C46 | 1.0 (4) |
| C6—P1—C18—C23 | -99.1 (3) | P3—C42—C47—C46 | -175.9 (2) |
| Ag1—P1—C18—C23 | 138.2 (2) | C45—C46—C47—C42 | -0.5 (5) |
| C12—P1—C18—C19 | -169.4 (2) | C54—P3—C48—C53 | 18.9 (3) |
| C6—P1—C18—C19 | 82.2 (3) | C42—P3—C48—C53 | -89.5 (3) |
| Ag1—P1—C18—C19 | -40.5 (3) | Ag1—P3—C48—C53 | 144.6 (2) |
| C23—C18—C19—C20 | 0.0 (5) | C54—P3—C48—C49 | -165.1 (2) |
| P1—C18—C19—C20 | 178.7 (3) | C42—P3—C48—C49 | 86.6 (3) |
| C18—C19—C20—C21 | -0.7 (5) | Ag1—P3—C48—C49 | -39.3 (3) |
| C19—C20—C21—C22 | 0.5 (5) | C53—C48—C49—C50 | 0.8 (5) |
| C20—C21—C22—C23 | 0.4 (5) | P3—C48—C49—C50 | -175.4 (2) |
| C21—C22—C23—C18 | -1.1 (5) | C48—C49—C50—C51 | 0.6 (5) |
| C19—C18—C23—C22 | 0.9 (5) | C49—C50—C51—C52 | -1.8 (5) |
| P1—C18—C23—C22 | -177.8 (2) | C50—C51—C52—C53 | 1.6 (5) |
| C36—P2—C24—C25 | -167.0 (2) | C49—C48—C53—C52 | -1.0 (4) |
| C30—P2—C24—C25 | 85.3 (3) | P3—C48—C53—C52 | 175.0 (2) |
| Ag1—P2—C24—C25 | -47.1 (3) | C51—C52—C53—C48 | -0.1 (5) |
| C36—P2—C24—C29 | 14.7 (3) | C48—P3—C54—C59 | 80.7 (3) |
| C30—P2—C24—C29 | -93.1 (3) | C42—P3—C54—C59 | -172.4 (2) |
| Ag1—P2—C24—C29 | 134.6 (2) | Ag1—P3—C54—C59 | -48.7 (3) |
| C29—C24—C25—C26 | 1.4 (5) | C48—P3—C54—C55 | -101.8 (3) |
| P2—C24—C25—C26 | -177.0 (2) | C42—P3—C54—C55 | 5.2 (3) |
| C24—C25—C26—C27 | -1.3 (5) | Ag1—P3—C54—C55 | 128.8 (2) |
| C25—C26—C27—C28 | -0.2 (5) | C59—C54—C55—C56 | 0.8 (4) |
| C26—C27—C28—C29 | 1.6 (5) | P3—C54—C55—C56 | -176.7 (2) |
| C27—C28—C29—C24 | -1.4 (5) | C54—C55—C56—C57 | -2.0 (5) |
| C25—C24—C29—C28 | -0.1 (4) | C55—C56—C57—C58 | 1.3 (5) |
| P2—C24—C29—C28 | 178.3 (2) | C56—C57—C58—C59 | 0.6 (5) |
| C36—P2—C30—C35 | -119.2 (3) | C57—C58—C59—C54 | -1.8 (5) |
| C24—P2—C30—C35 | -12.0 (3) | C55—C54—C59—C58 | 1.1 (4) |
| Ag1—P2—C30—C35 | 117.8 (2) | P3—C54—C59—C58 | 178.7 (2) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|---------------------------|-------------|---------------|-----------------------|-------------------------|
| N1—H1...O1 | 0.88 | 1.93 | 2.811 (3) | 176 |
| N2—H2...O2 | 0.88 | 1.89 | 2.754 (3) | 168 |
| O3—H3D...O1 | 0.87 | 1.86 | 2.724 (4) | 177 |
| C34—H34...O2 ⁱ | 0.95 | 2.52 | 3.394 (4) | 154 |

Symmetry code: (i) $x-1, y, z$.