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# [1*H*-1,2,4-Triazole-5(4*H*)-thione-κ*S*]-bis(triphenylphosphane-κ*P*)(nitrato-κ*O*)-silver(I) methanol monosolvate

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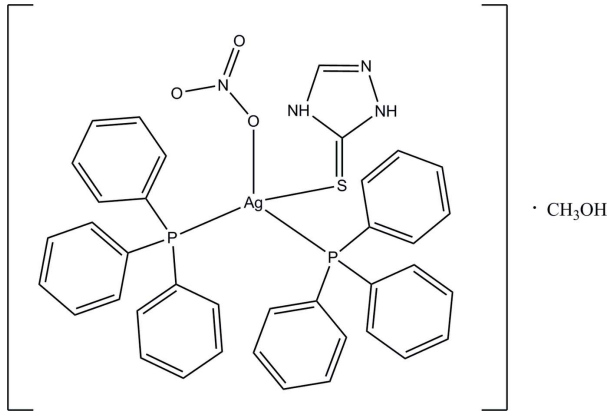
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.041; $wR$ factor = 0.100; data-to-parameter ratio = 23.4.

In the title complex, $[Ag(NO_3)(C_2H_3N_3S)(C_{18}H_{15}P)_2]\cdot CH_3OH$, the $Ag^I$ ion exhibits a distorted tetrahedral coordination geometry formed by two P atoms from two triphenylphosphine ligands, one S atom from a 1*H*-1,2,4-triazole-5(4*H*)-thione ligand and one O atom from a nitrate ion. In the crystal, complex and solvent molecules are linked by O—H···O and N—H···O hydrogen bonds forming a chain along the *b*-axis direction. The chains are linked by weak C—H···O hydrogen bonds forming a two-dimensional supramolecular architecture parallel to (001). In addition, an intramolecular N—H···O hydrogen bond is observed.

## Related literature

For applications of 1,2,4-triazoles and their derivatives, see: Holla *et al.* (1998); Jones *et al.* (1988); Kömürcü *et al.* (1995); Küçükgüzel *et al.* (2001); Wujec & Paneth (2007). For applications of silver(I) complexes with phosphorus and sulfur donor ligands, see: Ferrari *et al.* (2007); Isab *et al.* (2010). For related examples of discrete complexes, see: Nomiya *et al.* (1998); Pakawatchai *et al.* (2012).




## Experimental

### Crystal data

$[Ag(NO_3)(C_2H_3N_3S)(C_{18}H_{15}P)_2]\cdot CH_4O$
$M_r$ = 827.59
Monoclinic, $P2_1/c$
$a$ = 13.2712 (14) Å
$b$ = 14.3999 (15) Å
$c$ = 20.198 (2) Å
$\beta$ = 107.934 (2)°
$V$ = 3672.4 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.74 mm$^{-1}$
$T$ = 100 K
0.37 × 0.19 × 0.18 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
$T_{min}$ = 0.644, $T_{max}$ = 0.746
28287 measured reflections
10825 independent reflections
8714 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
$S$ = 1.02
10825 reflections
462 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.73 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4···O1$^{i}$ | 0.84 | 2.01 | 2.836 (2) | 168 |
| N1—H1···O2 | 0.88 | 1.93 | 2.793 (2) | 167 |
| N3—H3···O4 | 0.88 | 1.91 | 2.769 (3) | 166 |
| C35—H35···O1$^{i}$ | 0.95 | 2.55 | 3.360 (3) | 143 |
| C65—H65···O3$^{ii}$ | 0.95 | 2.48 | 3.340 (3) | 150 |

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

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); 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) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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would like to thank Dr Matthias Zeller for valuable suggestions and assistance with X-ray structure determination and use of structure refinement programs.

Supporting information for this paper is available from the IUCr electronic archives (Reference: LH5682).

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# supporting information

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## [1*H*-1,2,4-Triazole-5(4*H*)-thione-κ*S*]bis(triphenylphosphane-κ*P*)(nitrato-κ*O*)silver(I) methanol monosolvate

**Yupa Wattanakanjana, Sureeporn Palamae, Jenejira Ratthiwan and Ruthairat Nimthong**

### S1. Comment

1,2,4-Triazoles and their derivatives are compounds of considerable interest because of variety of biological properties such as antimicrobial, antiviral, anticonvulsant, activities, anti fungal and antitumor (Holla *et al.*, 1998; Jones *et al.*, 1988; Kömürcü *et al.*, 1995; Küçükgüzel *et al.*, 2001) and also potent inhibitors of enzymes. Therefore, some are approved as drugs, for example, alprazolam, etizolam, or vibrunazole (Wujec & Paneth, 2007).

The coordination chemistry of silver(I) complexes with phosphorus and sulfur donor ligands has attracted great interest in recent years because of their potential applications due to antimicrobial activities and they also often show interesting luminescence properties (Ferrari *et al.*, 2007; Isab *et al.*, 2010). Herein, the crystal structure of a mononuclear silver(I) nitrate complex containing both triphenylphosphine and 1*H*-1,2,4-triazole-5(4*H*)-thione is described.

The molecular structure of the title compound (I) reveals the presence of triphenylphosphine and 2,4-dihydro-3*H*-1,2,4-triazole-3-thione as co-ligands coordinated to the metal ion with two P atoms from two triphenylphosphine ligands, one terminal S atom from the 1*H*-1,2,4-triazole-5(4*H*)-thione ligand and one O atom from nitrate ion as well as one solvent methanol molecule, resulting in a distorted tetrahedral geometry as shown in Fig. 1. The Ag—S bond distance of 2.5591 (6) Å is shorter than in two other structures [Ag(Htsa)($PPh_3$)$_3$] (2.608 (7) Å, Nomiya *et al.*, 1998) and [AgBr($C_3H_6N_2OS$)($C_{18}H_{15}P$)$_2$] (2.8789 (10) Å, Pakawatchai *et al.*, 2012). In the crystal, hydrogen bonds play an important role with the nitrate ion connected to the methanol molecule with intermolecular O4—H4···O1$^{i}$, N1—H1···O2 and N3—H3···O4 interactions (see Table 1) leading to the formation of a 1-D chain along [010], Fig. 2. Furthermore, chains are linked by weak C—H···O hydrogen bonds forming of a 2-D supramolecular architecture parallel to (001). In addition, an intramolecular N—H···O hydrogen bond is observed (Fig. 3).

### S2. Experimental

Triphenylphosphine, $PPh_3$, (0.31g,1.18 mmol) was dissolved in 30 cm$^3$ of methanol at 333 K. $AgNO_3$ (0.10g,0.59 mmol) was added and the mixture was stirred for 3 hours. 1*H*-1,2,4-Triazole-5(4*H*)-thione, (0.06g,0.59 mmol) was added and new reaction mixture was heated under reflux for 3 hours. The resulting clear solution was filtered off and left to evaporate at room temperature. Colorless crystal, which was deposited upon standing for few days, was filtered off and dried under reduced pressure.

### S3. Refinement

H atoms bonded to C, N and O atoms were constrained with a riding model of of 0.95 Å (aryl H), and $U_{iso}$(H) = 1.2$U_{eq}$(C); 0.98 Å($CH_3$) and $U_{iso}$(H) = 1.5$U_{eq}$(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). Reflections 0 1 1, 1 0 0, 16 4 4, -7 8 2, -2 9 25, 7 1 0 were affected by the beam stop and were omitted from the refinement.

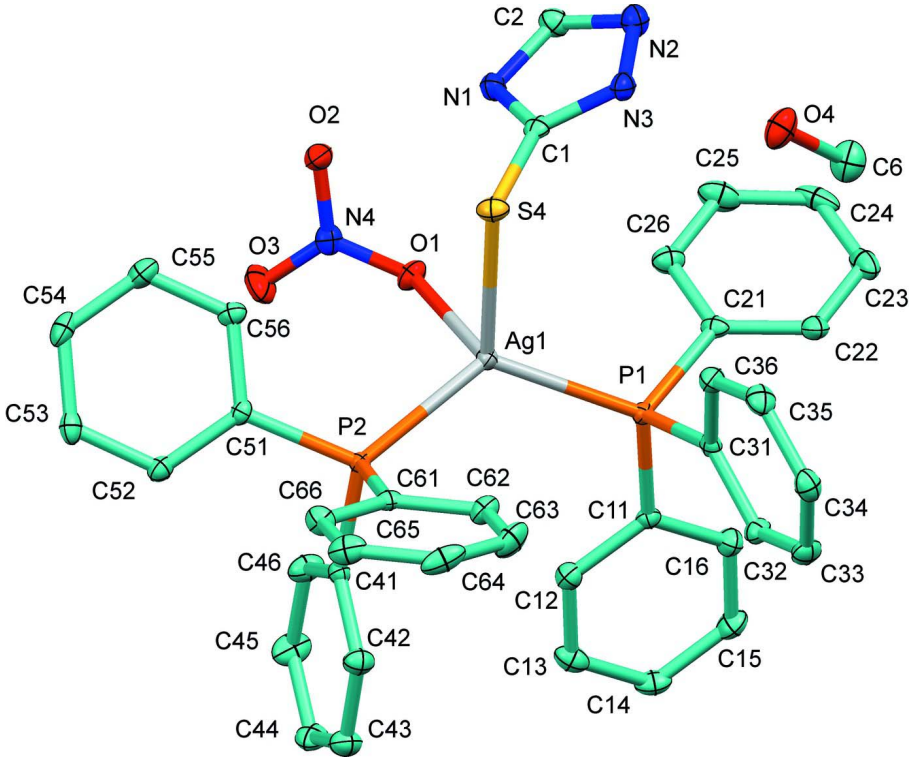


**Figure 1**

The molecular structure with displacement ellipsoids drawn at the 50% probability level. All hydrogen atoms are omitted for clarity.

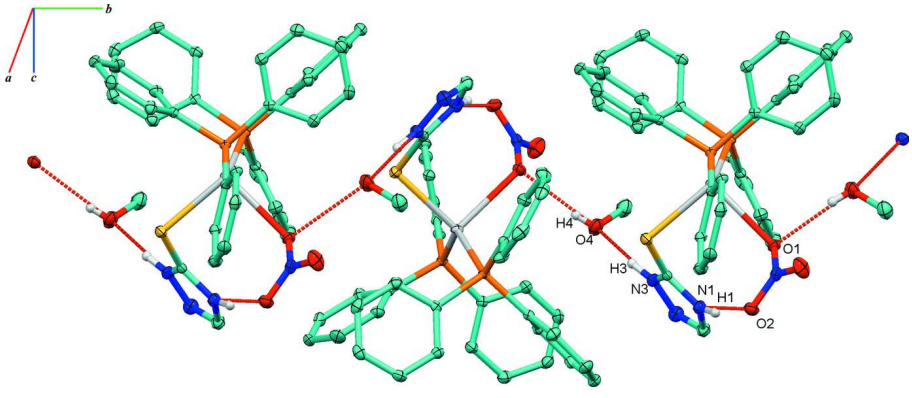


**Figure 2**

Part of the crystal structure showing intermolecular hydrogen bonds (red dashed lines) forming a 1-D chain.

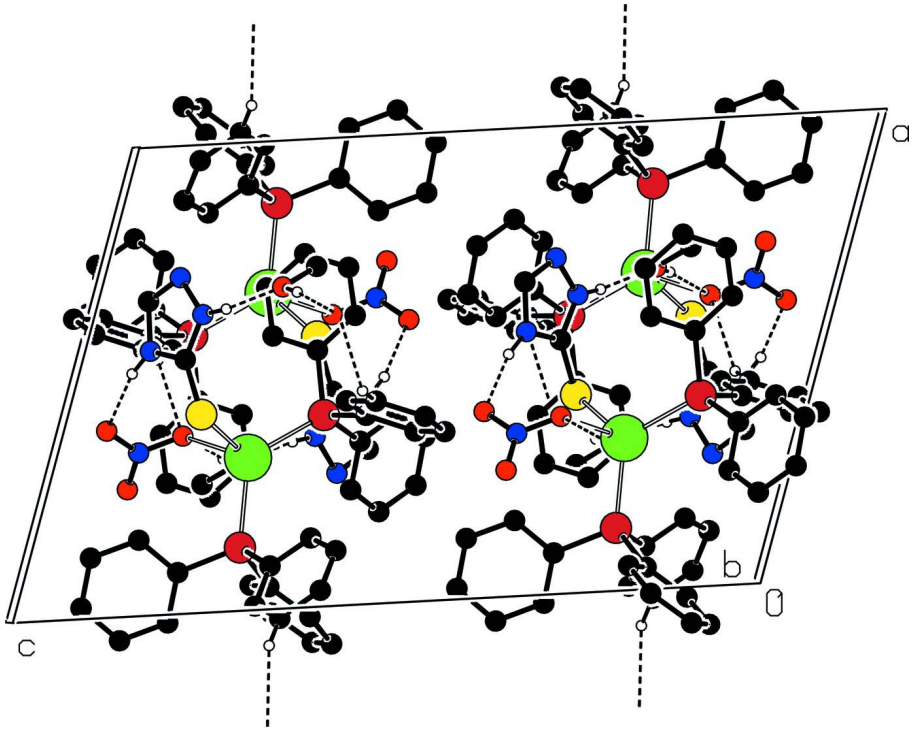


**Figure 3**

Part of the crystal structure with hydrogen bonds shown as dashed lines.

**[1*H*-1,2,4-Triazole-5(4*H*)-thione-κ*S*]bis(triphenylphosphane-κ*P*)(nitrato-κ*O*)silver(I) methanol monosolvate**

*Crystal data*

$[Ag(NO_3)(C_2H_3N_3S)(C_{18}H_{15}P)_2]\cdot CH_4O$
$M_r = 827.59$
Monoclinic, $P2_1/c$
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$b = 14.3999\ (15)$ Å
$c = 20.198\ (2)$ Å
$\beta = 107.934\ (2)°$
$V = 3672.4\ (7)$ Å$^3$
$Z = 4$
$F(000) = 1696$
$D_x = 1.497$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6153 reflections
$\theta = 2.2–30.1°$
$\mu = 0.74$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.37 × 0.19 × 0.18 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine focus sealed tube
$\omega$ and phi scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
$T_{min} = 0.644$, $T_{max} = 0.746$
28287 measured reflections
10825 independent reflections
8714 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 31.4°$, $\theta_{min} = 2.2°$
$h = -19\rightarrow18$
$k = -17\rightarrow20$
$l = -28\rightarrow25$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.100$
$S = 1.02$
10825 reflections
462 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
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.1882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.73$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ag1 | 0.67429 (2) | 0.93151 (2) | 0.76336 (2) | 0.01160 (5) |
| S1 | 0.57664 (4) | 0.80068 (4) | 0.68338 (3) | 0.01644 (12) |
| P1 | 0.59184 (4) | 0.97770 (4) | 0.85134 (3) | 0.01086 (11) |
| P2 | 0.86540 (4) | 0.91525 (4) | 0.78475 (3) | 0.01009 (11) |
| C2 | 0.32936 (18) | 0.93273 (16) | 0.57203 (13) | 0.0181 (5) |
| H2 | 0.2941 | 0.9761 | 0.5371 | 0.022* |
| N2 | 0.28180 (15) | 0.88131 (14) | 0.60609 (11) | 0.0197 (4) |
| O1 | 0.62092 (13) | 1.05965 (11) | 0.66828 (8) | 0.0174 (3) |
| O2 | 0.60167 (13) | 1.01016 (12) | 0.56286 (8) | 0.0194 (4) |
| O3 | 0.72933 (14) | 1.10506 (14) | 0.61295 (10) | 0.0299 (4) |
| O4 | 0.31291 (15) | 0.71893 (13) | 0.74684 (9) | 0.0258 (4) |
| H4 | 0.3255 | 0.6677 | 0.7677 | 0.039* |
| N1 | 0.43582 (15) | 0.91708 (13) | 0.59233 (10) | 0.0155 (4) |
| H1 | 0.4822 | 0.9453 | 0.5761 | 0.019* |
| N3 | 0.36316 (14) | 0.82974 (14) | 0.64945 (10) | 0.0160 (4) |
| H3 | 0.3541 | 0.7879 | 0.6788 | 0.019* |
| N4 | 0.65185 (15) | 1.05927 (13) | 0.61445 (11) | 0.0158 (4) |
| C1 | 0.45739 (17) | 0.85036 (16) | 0.64198 (11) | 0.0138 (4) |
| C6 | 0.2732 (2) | 0.78183 (19) | 0.78606 (14) | 0.0275 (6) |
| H6A | 0.2589 | 0.8417 | 0.7619 | 0.041* |
| H6B | 0.3256 | 0.7904 | 0.8319 | 0.041* |
| H6C | 0.2075 | 0.7572 | 0.7917 | 0.041* |
| C11 | 0.65211 (16) | 1.07206 (15) | 0.91082 (11) | 0.0115 (4) |
| C12 | 0.75475 (17) | 1.09950 (16) | 0.91578 (12) | 0.0149 (4) |
| H12 | 0.7907 | 1.0710 | 0.8871 | 0.018* |
| C13 | 0.80489 (18) | 1.16858 (16) | 0.96255 (13) | 0.0188 (5) |
| H13 | 0.8753 | 1.1865 | 0.9661 | 0.023* |
| C14 | 0.75264 (19) | 1.21114 (16) | 1.00377 (12) | 0.0189 (5) |

| | | | | |
|---|---|---|---|---|
| H14 | 0.7874 | 1.2576 | 1.0361 | 0.023* |
| C15 | 0.64965 (19) | 1.18617 (17) | 0.99799 (12) | 0.0203 (5) |
| H15 | 0.6133 | 1.2164 | 1.0258 | 0.024* |
| C16 | 0.59928 (18) | 1.11716 (17) | 0.95173 (12) | 0.0178 (5) |
| H16 | 0.5284 | 1.1004 | 0.9478 | 0.021* |
| C21 | 0.45256 (16) | 1.00891 (15) | 0.81942 (12) | 0.0132 (4) |
| C22 | 0.38246 (17) | 0.99700 (17) | 0.85794 (12) | 0.0180 (5) |
| H22 | 0.4051 | 0.9664 | 0.9017 | 0.022* |
| C23 | 0.27920 (18) | 1.03002 (19) | 0.83202 (14) | 0.0239 (6) |
| H23 | 0.2317 | 1.0223 | 0.8584 | 0.029* |
| C24 | 0.24512 (19) | 1.07409 (17) | 0.76800 (15) | 0.0256 (6) |
| H24 | 0.1750 | 1.0977 | 0.7510 | 0.031* |
| C25 | 0.3138 (2) | 1.08353 (18) | 0.72893 (15) | 0.0262 (6) |
| H25 | 0.2902 | 1.1123 | 0.6845 | 0.031* |
| C26 | 0.41716 (19) | 1.05108 (16) | 0.75449 (13) | 0.0187 (5) |
| H26 | 0.4639 | 1.0578 | 0.7274 | 0.022* |
| C31 | 0.59714 (15) | 0.87695 (15) | 0.90766 (11) | 0.0112 (4) |
| C32 | 0.63638 (17) | 0.87995 (16) | 0.97996 (12) | 0.0150 (4) |
| H32 | 0.6606 | 0.9373 | 1.0025 | 0.018* |
| C33 | 0.64067 (18) | 0.80025 (17) | 1.01962 (12) | 0.0177 (5) |
| H33 | 0.6672 | 0.8032 | 1.0689 | 0.021* |
| C34 | 0.60578 (17) | 0.71596 (17) | 0.98657 (13) | 0.0176 (5) |
| H34 | 0.6081 | 0.6613 | 1.0134 | 0.021* |
| C35 | 0.56759 (18) | 0.71196 (17) | 0.91447 (13) | 0.0189 (5) |
| H35 | 0.5440 | 0.6545 | 0.8920 | 0.023* |
| C36 | 0.56372 (17) | 0.79166 (16) | 0.87521 (12) | 0.0161 (5) |
| H36 | 0.5382 | 0.7883 | 0.8259 | 0.019* |
| C41 | 0.95262 (15) | 1.00163 (15) | 0.83888 (11) | 0.0115 (4) |
| C42 | 1.02105 (17) | 0.98262 (17) | 0.90534 (12) | 0.0166 (5) |
| H42 | 1.0261 | 0.9213 | 0.9234 | 0.020* |
| C43 | 1.08189 (19) | 1.05348 (17) | 0.94521 (13) | 0.0193 (5) |
| H43 | 1.1275 | 1.0403 | 0.9906 | 0.023* |
| C44 | 1.07645 (18) | 1.14226 (17) | 0.91939 (12) | 0.0191 (5) |
| H44 | 1.1188 | 1.1901 | 0.9467 | 0.023* |
| C45 | 1.0089 (2) | 1.16192 (17) | 0.85322 (13) | 0.0230 (5) |
| H45 | 1.0051 | 1.2231 | 0.8351 | 0.028* |
| C46 | 0.94721 (19) | 1.09224 (17) | 0.81390 (13) | 0.0194 (5) |
| H46 | 0.9003 | 1.1063 | 0.7690 | 0.023* |
| C51 | 0.91175 (16) | 0.90988 (15) | 0.70926 (11) | 0.0115 (4) |
| C52 | 1.01807 (18) | 0.92341 (15) | 0.71397 (12) | 0.0141 (4) |
| H52 | 1.0682 | 0.9377 | 0.7577 | 0.017* |
| C53 | 1.05087 (18) | 0.91613 (16) | 0.65508 (13) | 0.0169 (5) |
| H53 | 1.1234 | 0.9242 | 0.6586 | 0.020* |
| C54 | 0.97678 (19) | 0.89701 (17) | 0.59094 (12) | 0.0188 (5) |
| H54 | 0.9989 | 0.8914 | 0.5506 | 0.023* |
| C55 | 0.87081 (19) | 0.88607 (17) | 0.58562 (12) | 0.0187 (5) |
| H55 | 0.8203 | 0.8751 | 0.5415 | 0.022* |
| C56 | 0.83820 (17) | 0.89111 (16) | 0.64467 (11) | 0.0143 (4) |

| | | | | |
|---|---|---|---|---|
| H56 | 0.7658 | 0.8818 | 0.6410 | 0.017* |
| C61 | 0.90777 (16) | 0.80667 (15) | 0.83114 (11) | 0.0120 (4) |
| C62 | 0.85267 (18) | 0.77704 (16) | 0.87603 (12) | 0.0170 (5) |
| H62 | 0.7950 | 0.8126 | 0.8807 | 0.020* |
| C63 | 0.8822 (2) | 0.69565 (18) | 0.91380 (13) | 0.0247 (5) |
| H63 | 0.8450 | 0.6759 | 0.9447 | 0.030* |
| C64 | 0.9654 (2) | 0.64320 (17) | 0.90676 (12) | 0.0238 (5) |
| H64 | 0.9850 | 0.5875 | 0.9327 | 0.029* |
| C65 | 1.02054 (19) | 0.67137 (17) | 0.86202 (13) | 0.0208 (5) |
| H65 | 1.0775 | 0.6350 | 0.8571 | 0.025* |
| C66 | 0.99194 (17) | 0.75288 (16) | 0.82467 (12) | 0.0171 (5) |
| H66 | 1.0299 | 0.7725 | 0.7943 | 0.020* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ag1 | 0.01102 (8) | 0.01409 (9) | 0.00990 (9) | 0.00083 (6) | 0.00351 (6) | −0.00047 (6) |
| S1 | 0.0177 (2) | 0.0141 (3) | 0.0152 (3) | 0.0004 (2) | 0.0017 (2) | −0.0025 (2) |
| P1 | 0.0107 (2) | 0.0125 (3) | 0.0096 (3) | 0.00039 (19) | 0.0035 (2) | −0.0006 (2) |
| P2 | 0.0097 (2) | 0.0115 (3) | 0.0091 (3) | 0.00054 (19) | 0.0030 (2) | 0.0003 (2) |
| C2 | 0.0169 (10) | 0.0174 (12) | 0.0193 (12) | 0.0005 (8) | 0.0046 (9) | 0.0014 (9) |
| N2 | 0.0178 (9) | 0.0207 (11) | 0.0218 (11) | 0.0012 (8) | 0.0080 (8) | 0.0008 (9) |
| O1 | 0.0242 (8) | 0.0153 (9) | 0.0136 (8) | 0.0014 (6) | 0.0072 (7) | 0.0024 (7) |
| O2 | 0.0215 (8) | 0.0229 (9) | 0.0142 (8) | −0.0053 (7) | 0.0058 (7) | −0.0018 (7) |
| O3 | 0.0267 (9) | 0.0294 (11) | 0.0384 (12) | −0.0152 (8) | 0.0170 (9) | −0.0066 (9) |
| O4 | 0.0398 (11) | 0.0192 (10) | 0.0229 (10) | 0.0015 (8) | 0.0162 (9) | 0.0046 (7) |
| N1 | 0.0151 (8) | 0.0159 (10) | 0.0160 (10) | −0.0016 (7) | 0.0054 (8) | 0.0017 (8) |
| N3 | 0.0175 (9) | 0.0169 (10) | 0.0144 (10) | −0.0032 (7) | 0.0060 (7) | 0.0014 (8) |
| N4 | 0.0177 (9) | 0.0122 (10) | 0.0186 (10) | 0.0008 (7) | 0.0071 (8) | 0.0025 (8) |
| C1 | 0.0175 (10) | 0.0122 (11) | 0.0116 (10) | −0.0033 (8) | 0.0044 (8) | −0.0040 (9) |
| C6 | 0.0324 (14) | 0.0230 (14) | 0.0301 (15) | 0.0051 (11) | 0.0139 (12) | 0.0035 (12) |
| C11 | 0.0120 (9) | 0.0117 (10) | 0.0098 (10) | 0.0008 (7) | 0.0019 (8) | 0.0005 (8) |
| C12 | 0.0157 (10) | 0.0142 (11) | 0.0148 (11) | 0.0018 (8) | 0.0048 (9) | 0.0003 (9) |
| C13 | 0.0156 (10) | 0.0147 (12) | 0.0228 (13) | 0.0001 (8) | 0.0011 (9) | 0.0017 (10) |
| C14 | 0.0231 (11) | 0.0138 (12) | 0.0157 (12) | −0.0009 (9) | 0.0002 (9) | −0.0026 (9) |
| C15 | 0.0260 (12) | 0.0201 (13) | 0.0158 (12) | 0.0023 (9) | 0.0079 (10) | −0.0043 (10) |
| C16 | 0.0163 (10) | 0.0203 (12) | 0.0179 (12) | −0.0005 (9) | 0.0066 (9) | −0.0034 (10) |
| C21 | 0.0125 (9) | 0.0123 (11) | 0.0131 (11) | 0.0015 (8) | 0.0012 (8) | −0.0030 (9) |
| C22 | 0.0141 (10) | 0.0237 (13) | 0.0149 (12) | −0.0017 (9) | 0.0023 (9) | −0.0054 (10) |
| C23 | 0.0143 (10) | 0.0299 (15) | 0.0290 (15) | −0.0020 (10) | 0.0089 (10) | −0.0138 (12) |
| C24 | 0.0125 (10) | 0.0202 (13) | 0.0364 (16) | 0.0028 (9) | −0.0037 (10) | −0.0102 (11) |
| C25 | 0.0205 (12) | 0.0220 (14) | 0.0296 (16) | 0.0034 (10) | −0.0018 (11) | 0.0034 (11) |
| C26 | 0.0199 (11) | 0.0175 (12) | 0.0169 (12) | 0.0000 (9) | 0.0032 (9) | 0.0008 (10) |
| C31 | 0.0091 (8) | 0.0125 (10) | 0.0123 (11) | 0.0018 (7) | 0.0038 (8) | 0.0011 (8) |
| C32 | 0.0161 (10) | 0.0155 (11) | 0.0132 (11) | −0.0002 (8) | 0.0044 (8) | −0.0025 (9) |
| C33 | 0.0193 (10) | 0.0207 (12) | 0.0119 (11) | 0.0018 (9) | 0.0030 (9) | 0.0034 (9) |
| C34 | 0.0158 (10) | 0.0164 (12) | 0.0217 (13) | 0.0012 (8) | 0.0072 (9) | 0.0050 (10) |
| C35 | 0.0197 (11) | 0.0154 (12) | 0.0227 (13) | −0.0043 (9) | 0.0083 (10) | −0.0036 (10) |

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|---|---|---|---|---|---|---|
| C36 | 0.0168 (10) | 0.0176 (12) | 0.0142 (11) | −0.0029 (8) | 0.0053 (9) | −0.0010 (9) |
| C41 | 0.0103 (9) | 0.0131 (11) | 0.0116 (10) | 0.0008 (8) | 0.0039 (8) | −0.0001 (9) |
| C42 | 0.0175 (10) | 0.0152 (12) | 0.0154 (12) | 0.0001 (8) | 0.0024 (9) | 0.0019 (9) |
| C43 | 0.0197 (11) | 0.0196 (13) | 0.0157 (12) | −0.0018 (9) | 0.0014 (9) | 0.0003 (10) |
| C44 | 0.0220 (11) | 0.0168 (12) | 0.0175 (12) | −0.0040 (9) | 0.0047 (10) | −0.0055 (10) |
| C45 | 0.0352 (13) | 0.0113 (12) | 0.0206 (13) | −0.0032 (10) | 0.0058 (11) | 0.0009 (10) |
| C46 | 0.0265 (12) | 0.0140 (12) | 0.0151 (12) | 0.0000 (9) | 0.0024 (10) | 0.0012 (9) |
| C51 | 0.0140 (9) | 0.0104 (10) | 0.0110 (10) | 0.0007 (8) | 0.0052 (8) | 0.0009 (8) |
| C52 | 0.0169 (10) | 0.0140 (11) | 0.0118 (11) | −0.0005 (8) | 0.0051 (9) | 0.0008 (9) |
| C53 | 0.0190 (10) | 0.0140 (11) | 0.0215 (13) | −0.0017 (8) | 0.0117 (9) | 0.0018 (9) |
| C54 | 0.0290 (12) | 0.0163 (12) | 0.0156 (12) | 0.0000 (9) | 0.0136 (10) | −0.0008 (10) |
| C55 | 0.0245 (11) | 0.0188 (12) | 0.0126 (11) | 0.0037 (9) | 0.0057 (9) | 0.0005 (9) |
| C56 | 0.0153 (10) | 0.0140 (11) | 0.0122 (11) | 0.0017 (8) | 0.0021 (8) | −0.0001 (9) |
| C61 | 0.0132 (9) | 0.0109 (10) | 0.0100 (10) | −0.0017 (8) | 0.0010 (8) | −0.0014 (8) |
| C62 | 0.0214 (11) | 0.0172 (12) | 0.0129 (11) | 0.0005 (9) | 0.0059 (9) | 0.0004 (9) |
| C63 | 0.0387 (14) | 0.0223 (14) | 0.0153 (12) | −0.0009 (11) | 0.0117 (11) | 0.0042 (10) |
| C64 | 0.0418 (15) | 0.0114 (12) | 0.0127 (12) | 0.0043 (10) | 0.0005 (11) | 0.0020 (9) |
| C65 | 0.0244 (12) | 0.0153 (12) | 0.0194 (13) | 0.0060 (9) | 0.0019 (10) | −0.0025 (10) |
| C66 | 0.0164 (10) | 0.0150 (12) | 0.0196 (12) | 0.0016 (8) | 0.0052 (9) | 0.0010 (9) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| Ag1—P1 | 2.4485 (6) | C25—H25 | 0.9500 |
| Ag1—P2 | 2.4493 (6) | C26—H26 | 0.9500 |
| Ag1—S1 | 2.5591 (6) | C31—C32 | 1.392 (3) |
| Ag1—O1 | 2.5994 (16) | C31—C36 | 1.398 (3) |
| S1—C1 | 1.703 (2) | C32—C33 | 1.391 (3) |
| P1—C21 | 1.817 (2) | C32—H32 | 0.9500 |
| P1—C11 | 1.827 (2) | C33—C34 | 1.394 (3) |
| P1—C31 | 1.832 (2) | C33—H33 | 0.9500 |
| P2—C51 | 1.813 (2) | C34—C35 | 1.388 (3) |
| P2—C41 | 1.817 (2) | C34—H34 | 0.9500 |
| P2—C61 | 1.821 (2) | C35—C36 | 1.387 (3) |
| C2—N2 | 1.299 (3) | C35—H35 | 0.9500 |
| C2—N1 | 1.363 (3) | C36—H36 | 0.9500 |
| C2—H2 | 0.9500 | C41—C46 | 1.393 (3) |
| N2—N3 | 1.379 (3) | C41—C42 | 1.397 (3) |
| O1—N4 | 1.275 (2) | C42—C43 | 1.393 (3) |
| O2—N4 | 1.266 (3) | C42—H42 | 0.9500 |
| O3—N4 | 1.230 (2) | C43—C44 | 1.374 (3) |
| O4—C6 | 1.408 (3) | C43—H43 | 0.9500 |
| O4—H4 | 0.8400 | C44—C45 | 1.390 (3) |
| N1—C1 | 1.354 (3) | C44—H44 | 0.9500 |
| N1—H1 | 0.8800 | C45—C46 | 1.381 (3) |
| N3—C1 | 1.338 (3) | C45—H45 | 0.9500 |
| N3—H3 | 0.8800 | C46—H46 | 0.9500 |
| C6—H6A | 0.9800 | C51—C56 | 1.394 (3) |
| C6—H6B | 0.9800 | C51—C52 | 1.398 (3) |

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| C6—H6C | 0.9800 | C52—C53 | 1.391 (3) |
| C11—C12 | 1.392 (3) | C52—H52 | 0.9500 |
| C11—C16 | 1.397 (3) | C53—C54 | 1.391 (3) |
| C12—C13 | 1.392 (3) | C53—H53 | 0.9500 |
| C12—H12 | 0.9500 | C54—C55 | 1.386 (3) |
| C13—C14 | 1.380 (3) | C54—H54 | 0.9500 |
| C13—H13 | 0.9500 | C55—C56 | 1.390 (3) |
| C14—C15 | 1.383 (3) | C55—H55 | 0.9500 |
| C14—H14 | 0.9500 | C56—H56 | 0.9500 |
| C15—C16 | 1.387 (3) | C61—C62 | 1.395 (3) |
| C15—H15 | 0.9500 | C61—C66 | 1.398 (3) |
| C16—H16 | 0.9500 | C62—C63 | 1.388 (3) |
| C21—C26 | 1.389 (3) | C62—H62 | 0.9500 |
| C21—C22 | 1.395 (3) | C63—C64 | 1.381 (4) |
| C22—C23 | 1.392 (3) | C63—H63 | 0.9500 |
| C22—H22 | 0.9500 | C64—C65 | 1.387 (4) |
| C23—C24 | 1.385 (4) | C64—H64 | 0.9500 |
| C23—H23 | 0.9500 | C65—C66 | 1.384 (3) |
| C24—C25 | 1.384 (4) | C65—H65 | 0.9500 |
| C24—H24 | 0.9500 | C66—H66 | 0.9500 |
| C25—C26 | 1.390 (3) | | |

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| P1—Ag1—P2 | 124.60 (2) | C21—C26—C25 | 120.4 (2) |
| P1—Ag1—S1 | 113.92 (2) | C21—C26—H26 | 119.8 |
| P2—Ag1—S1 | 109.667 (19) | C25—C26—H26 | 119.8 |
| P1—Ag1—O1 | 105.21 (4) | C32—C31—C36 | 118.8 (2) |
| P2—Ag1—O1 | 103.29 (4) | C32—C31—P1 | 123.88 (17) |
| S1—Ag1—O1 | 94.96 (4) | C36—C31—P1 | 117.30 (17) |
| C1—S1—Ag1 | 102.36 (8) | C33—C32—C31 | 121.0 (2) |
| C21—P1—C11 | 103.94 (10) | C33—C32—H32 | 119.5 |
| C21—P1—C31 | 104.87 (10) | C31—C32—H32 | 119.5 |
| C11—P1—C31 | 104.80 (10) | C32—C33—C34 | 119.6 (2) |
| C21—P1—Ag1 | 116.29 (7) | C32—C33—H33 | 120.2 |
| C11—P1—Ag1 | 118.45 (7) | C34—C33—H33 | 120.2 |
| C31—P1—Ag1 | 107.18 (7) | C35—C34—C33 | 119.9 (2) |
| C51—P2—C41 | 102.53 (10) | C35—C34—H34 | 120.0 |
| C51—P2—C61 | 105.38 (10) | C33—C34—H34 | 120.0 |
| C41—P2—C61 | 103.86 (10) | C36—C35—C34 | 120.2 (2) |
| C51—P2—Ag1 | 117.18 (7) | C36—C35—H35 | 119.9 |
| C41—P2—Ag1 | 118.28 (7) | C34—C35—H35 | 119.9 |
| C61—P2—Ag1 | 108.17 (7) | C35—C36—C31 | 120.5 (2) |
| N2—C2—N1 | 112.0 (2) | C35—C36—H36 | 119.7 |
| N2—C2—H2 | 124.0 | C31—C36—H36 | 119.7 |
| N1—C2—H2 | 124.0 | C46—C41—C42 | 118.5 (2) |
| C2—N2—N3 | 103.30 (18) | C46—C41—P2 | 118.09 (17) |
| N4—O1—Ag1 | 122.75 (13) | C42—C41—P2 | 123.32 (17) |
| C6—O4—H4 | 109.5 | C43—C42—C41 | 120.1 (2) |
| C1—N1—C2 | 107.65 (19) | C43—C42—H42 | 119.9 |

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| C1—N1—H1 | 126.2 | C41—C42—H42 | 119.9 |
| C2—N1—H1 | 126.2 | C44—C43—C42 | 120.6 (2) |
| C1—N3—N2 | 112.65 (19) | C44—C43—H43 | 119.7 |
| C1—N3—H3 | 123.7 | C42—C43—H43 | 119.7 |
| N2—N3—H3 | 123.7 | C43—C44—C45 | 119.8 (2) |
| O3—N4—O2 | 120.7 (2) | C43—C44—H44 | 120.1 |
| O3—N4—O1 | 120.7 (2) | C45—C44—H44 | 120.1 |
| O2—N4—O1 | 118.59 (18) | C46—C45—C44 | 119.8 (2) |
| N3—C1—N1 | 104.42 (19) | C46—C45—H45 | 120.1 |
| N3—C1—S1 | 127.64 (18) | C44—C45—H45 | 120.1 |
| N1—C1—S1 | 127.89 (17) | C45—C46—C41 | 121.1 (2) |
| O4—C6—H6A | 109.5 | C45—C46—H46 | 119.4 |
| O4—C6—H6B | 109.5 | C41—C46—H46 | 119.4 |
| H6A—C6—H6B | 109.5 | C56—C51—C52 | 119.5 (2) |
| O4—C6—H6C | 109.5 | C56—C51—P2 | 118.31 (16) |
| H6A—C6—H6C | 109.5 | C52—C51—P2 | 122.24 (17) |
| H6B—C6—H6C | 109.5 | C53—C52—C51 | 120.4 (2) |
| C12—C11—C16 | 118.9 (2) | C53—C52—H52 | 119.8 |
| C12—C11—P1 | 118.62 (16) | C51—C52—H52 | 119.8 |
| C16—C11—P1 | 122.46 (16) | C52—C53—C54 | 119.6 (2) |
| C11—C12—C13 | 120.3 (2) | C52—C53—H53 | 120.2 |
| C11—C12—H12 | 119.9 | C54—C53—H53 | 120.2 |
| C13—C12—H12 | 119.9 | C55—C54—C53 | 120.3 (2) |
| C14—C13—C12 | 120.2 (2) | C55—C54—H54 | 119.9 |
| C14—C13—H13 | 119.9 | C53—C54—H54 | 119.9 |
| C12—C13—H13 | 119.9 | C54—C55—C56 | 120.3 (2) |
| C13—C14—C15 | 120.0 (2) | C54—C55—H55 | 119.9 |
| C13—C14—H14 | 120.0 | C56—C55—H55 | 119.9 |
| C15—C14—H14 | 120.0 | C55—C56—C51 | 120.0 (2) |
| C14—C15—C16 | 120.1 (2) | C55—C56—H56 | 120.0 |
| C14—C15—H15 | 119.9 | C51—C56—H56 | 120.0 |
| C16—C15—H15 | 119.9 | C62—C61—C66 | 119.0 (2) |
| C15—C16—C11 | 120.4 (2) | C62—C61—P2 | 117.16 (17) |
| C15—C16—H16 | 119.8 | C66—C61—P2 | 123.83 (17) |
| C11—C16—H16 | 119.8 | C63—C62—C61 | 120.0 (2) |
| C26—C21—C22 | 119.4 (2) | C63—C62—H62 | 120.0 |
| C26—C21—P1 | 117.04 (17) | C61—C62—H62 | 120.0 |
| C22—C21—P1 | 123.51 (18) | C64—C63—C62 | 120.3 (2) |
| C23—C22—C21 | 119.8 (2) | C64—C63—H63 | 119.8 |
| C23—C22—H22 | 120.1 | C62—C63—H63 | 119.8 |
| C21—C22—H22 | 120.1 | C63—C64—C65 | 120.4 (2) |
| C24—C23—C22 | 120.5 (2) | C63—C64—H64 | 119.8 |
| C24—C23—H23 | 119.7 | C65—C64—H64 | 119.8 |
| C22—C23—H23 | 119.7 | C66—C65—C64 | 119.5 (2) |
| C25—C24—C23 | 119.6 (2) | C66—C65—H65 | 120.3 |
| C25—C24—H24 | 120.2 | C64—C65—H65 | 120.3 |
| C23—C24—H24 | 120.2 | C65—C66—C61 | 120.8 (2) |
| C24—C25—C26 | 120.2 (3) | C65—C66—H66 | 119.6 |

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|---|---|---|---|
| C24—C25—H25 | 119.9 | C61—C66—H66 | 119.6 |
| C26—C25—H25 | 119.9 | | |
| | | | |
| N1—C2—N2—N3 | −0.8 (3) | C32—C33—C34—C35 | 0.3 (3) |
| N2—C2—N1—C1 | 0.9 (3) | C33—C34—C35—C36 | −0.2 (3) |
| C2—N2—N3—C1 | 0.5 (3) | C34—C35—C36—C31 | −0.6 (3) |
| Ag1—O1—N4—O3 | −96.6 (2) | C32—C31—C36—C35 | 1.3 (3) |
| Ag1—O1—N4—O2 | 82.8 (2) | P1—C31—C36—C35 | 178.64 (17) |
| N2—N3—C1—N1 | 0.0 (3) | C51—P2—C41—C46 | 64.26 (19) |
| N2—N3—C1—S1 | −177.87 (17) | C61—P2—C41—C46 | 173.81 (17) |
| C2—N1—C1—N3 | −0.5 (2) | Ag1—P2—C41—C46 | −66.36 (19) |
| C2—N1—C1—S1 | 177.36 (18) | C51—P2—C41—C42 | −118.73 (19) |
| Ag1—S1—C1—N3 | −110.5 (2) | C61—P2—C41—C42 | −9.2 (2) |
| Ag1—S1—C1—N1 | 72.2 (2) | Ag1—P2—C41—C42 | 110.66 (17) |
| C21—P1—C11—C12 | −145.97 (18) | C46—C41—C42—C43 | 0.1 (3) |
| C31—P1—C11—C12 | 104.21 (18) | P2—C41—C42—C43 | −176.86 (18) |
| Ag1—P1—C11—C12 | −15.2 (2) | C41—C42—C43—C44 | −0.9 (4) |
| C21—P1—C11—C16 | 34.4 (2) | C42—C43—C44—C45 | 0.7 (4) |
| C31—P1—C11—C16 | −75.4 (2) | C43—C44—C45—C46 | 0.3 (4) |
| Ag1—P1—C11—C16 | 165.24 (17) | C44—C45—C46—C41 | −1.1 (4) |
| C16—C11—C12—C13 | 2.2 (3) | C42—C41—C46—C45 | 0.8 (3) |
| P1—C11—C12—C13 | −177.41 (18) | P2—C41—C46—C45 | 178.00 (19) |
| C11—C12—C13—C14 | −0.8 (4) | C41—P2—C51—C56 | −147.58 (18) |
| C12—C13—C14—C15 | −0.9 (4) | C61—P2—C51—C56 | 104.02 (18) |
| C13—C14—C15—C16 | 1.2 (4) | Ag1—P2—C51—C56 | −16.3 (2) |
| C14—C15—C16—C11 | 0.3 (4) | C41—P2—C51—C52 | 32.8 (2) |
| C12—C11—C16—C15 | −1.9 (3) | C61—P2—C51—C52 | −75.6 (2) |
| P1—C11—C16—C15 | 177.65 (18) | Ag1—P2—C51—C52 | 164.03 (15) |
| C11—P1—C21—C26 | 99.22 (19) | C56—C51—C52—C53 | −1.5 (3) |
| C31—P1—C21—C26 | −151.02 (18) | P2—C51—C52—C53 | 178.19 (17) |
| Ag1—P1—C21—C26 | −32.9 (2) | C51—C52—C53—C54 | 1.2 (3) |
| C11—P1—C21—C22 | −77.4 (2) | C52—C53—C54—C55 | 0.6 (4) |
| C31—P1—C21—C22 | 32.3 (2) | C53—C54—C55—C56 | −2.1 (4) |
| Ag1—P1—C21—C22 | 150.51 (17) | C54—C55—C56—C51 | 1.8 (4) |
| C26—C21—C22—C23 | −2.1 (4) | C52—C51—C56—C55 | −0.1 (3) |
| P1—C21—C22—C23 | 174.51 (18) | P2—C51—C56—C55 | −179.74 (18) |
| C21—C22—C23—C24 | 0.5 (4) | C51—P2—C61—C62 | −157.71 (17) |
| C22—C23—C24—C25 | 1.4 (4) | C41—P2—C61—C62 | 94.86 (18) |
| C23—C24—C25—C26 | −1.6 (4) | Ag1—P2—C61—C62 | −31.62 (19) |
| C22—C21—C26—C25 | 1.8 (4) | C51—P2—C61—C66 | 22.9 (2) |
| P1—C21—C26—C25 | −174.95 (19) | C41—P2—C61—C66 | −84.5 (2) |
| C24—C25—C26—C21 | 0.0 (4) | Ag1—P2—C61—C66 | 149.00 (17) |
| C21—P1—C31—C32 | −106.86 (18) | C66—C61—C62—C63 | 0.5 (3) |
| C11—P1—C31—C32 | 2.3 (2) | P2—C61—C62—C63 | −178.93 (19) |
| Ag1—P1—C31—C32 | 128.97 (16) | C61—C62—C63—C64 | −0.6 (4) |
| C21—P1—C31—C36 | 75.99 (18) | C62—C63—C64—C65 | 0.2 (4) |
| C11—P1—C31—C36 | −174.86 (16) | C63—C64—C65—C66 | 0.4 (4) |
| Ag1—P1—C31—C36 | −48.18 (17) | C64—C65—C66—C61 | −0.5 (4) |

| | | | |
|---|---|---|---|
| C36—C31—C32—C33 | −1.2 (3) | C62—C61—C66—C65 | 0.0 (3) |
| P1—C31—C32—C33 | −178.32 (17) | P2—C61—C66—C65 | 179.41 (18) |
| C31—C32—C33—C34 | 0.4 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4···O1$^{i}$ | 0.84 | 2.01 | 2.836 (2) | 168 |
| N1—H1···O2 | 0.88 | 1.93 | 2.793 (2) | 167 |
| N3—H3···O4 | 0.88 | 1.91 | 2.769 (3) | 166 |
| C35—H35···O1$^{i}$ | 0.95 | 2.55 | 3.360 (3) | 143 |
| C65—H65···O3$^{ii}$ | 0.95 | 2.48 | 3.340 (3) | 150 |

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