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# (1,10-Phenanthroline-$\kappa^2N,N'$)(triphenylphosphine-$\kappa P$)silver(I) trifluoromethanesulfonate

**Jie-Qiang Wu,[a] Qiong-Hua Jin,[a]* Ke-Yi Hu[a] and Cun-Lin Zhang[b]**

[a]Department of Chemistry, Capital Normal University, Beijing 100048, People's Republic of China, and [b]Department of Physics, Capital Normal University, Beijing 100048, People's Republic of China
Correspondence e-mail: jinqh204@163.com

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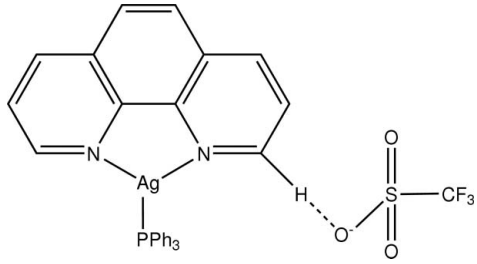
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.042; $wR$ factor = 0.133; data-to-parameter ratio = 25.1.

The structure of the title complex, $[Ag(C_{12}H_8N_2)(C_{18}H_{15}P)]CF_3SO_3$, is based on a distorted trigonal–planar $N_2P$ coordination of the $Ag^I$ ion, provided by two N atoms of the bidentate phenanthroline ligand and one P atom of the triphenylphosphine ligand. The phenanthroline ligand and one phenyl ring of the triphenylphosphine ligand almost lie in one plane (maximum deviation = 0.014 Å from the best planes). The crystal structure may be stabilized by an intermolecular C—H···O hydrogen bond between the phenanthroline ligand and the O atom of the trifluoromethanesulfonate anion.

## Related literature

For related structures, see: Di Nicola *et al.* (2007); Jin *et al.* (1999, 2009); Effendy *et al.* (2007*a*,*b*); Awaleh *et al.* (2005*a*,*b*); Pettinari *et al.* (2007). For general background, see: Howells & Mccown (1977); Bowmaker *et al.* (2005); Lawrance (1986).




## Experimental

### Crystal data

$[Ag(C_{12}H_8N_2)(C_{18}H_{15}P)]CF_3SO_3$ $M_r$ = 699.42
Triclinic, $P\overline{1}$
$a$ = 10.9832 (2) Å
$b$ = 11.7533 (2) Å
$c$ = 12.2642 (3) Å
$\alpha$ = 77.711 (1)°
$\beta$ = 76.183 (1)°
$\gamma$ = 73.440 (1)°
$V$ = 1455.66 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.87 mm$^{-1}$
$T$ = 293 K
0.4 × 0.3 × 0.2 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.735, $T_{max}$ = 0.832
18629 measured reflections
9515 independent reflections
6777 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.133
$S$ = 1.00
9515 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.66 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ag1—N2 | 2.2798 (18) | Ag1—P1 | 2.3469 (5) |
| Ag1—N1 | 2.292 (2) | | |
| N2—Ag1—N1 | 73.53 (8) | N1—Ag1—P1 | 138.03 (6) |
| N2—Ag1—P1 | 147.77 (6) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C20—H16···O2 | 0.93 | 2.36 | 3.285 (6) | 173 |

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2241).

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# supporting information

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# (1,10-Phenanthroline-$\kappa^2N,N'$)(triphenylphosphine-$\kappa P$)silver(I) trifluoromethanesulfonate

**Jie-Qiang Wu, Qiong-Hua Jin, Ke-Yi Hu and Cun-Lin Zhang**

## S1. Comment

A recent report (Di Nicola *et al.*, 2007) describes complexes between silver nitrate, a tertiary phosphine ligand and oligodentate bases, *L* that are derivatives of 2,2′-bipyridyl, which resulted in adducts with general formula $AgNO_3$:P$R_3$:*L*(1:1:1). The silver coordination environment in these complexes is dominated by the quasi-planar $N_2AgP$ or $O_2AgP$ coordination. We have likewise studied mixed-ligand Ag(I) complexes of *N*-heterocyclic and $PPh_3$ ligands, *viz* [AgBr(phen)($PPh_3$)] and [Ag*X*(2-Apy)($PPh_3$)]$_2$ (*X* = Br, Cl, $NO_3$; 2-Apy= 2-aminopyridine) (Jin *et al.*, 1999, Jin *et al.*, 2009) and have synthesized the title complex [Ag(phen)($PPh_3$)](OTf). Furthermore, we have studied the role of several weakly coordinating anions (nitrate, nitrite, acetate, perchlorate trifluoroacetate and trifluoromethanesulfonate) in silver complexes.

The molecular structure of the title complex is depicted in Fig.1. The coordination polyhedron of the silver atom adopts a distorted trigonal-planar geometry, formed by two nitrogen atoms of phen with Ag—N distances of 2.3469 (5) Å and 2.2797 (19) Å, and by one phosphorus atom of the $PPh_3$ ligand with a Ag—P distance of 2.292 (2) Å. The trifluoromethanesulfonate anion is present as a counter anion and, as expected, shows no direct coordination to the metal center, in contrast to the complex [AgBr(phen)($PPh_3$)] where the silver atom is coordinated to two nitrogen atoms of phen (Ag—N 2.376 (8) Å), one phosphorus atom of $PPh_3$ (Ag—P, 2.375 (3) Å) and in addition to one bromide anion (Jin *et al.*, 1999), adopting a distorted tetrahedron as coordination polyhedron.

The molecular structure of the title complex shows little differences in comparison with the structures of compounds AgX:$PPh_3$:*L*, where *X* = nitrate (Di Nicola *et al.*, 2007), nitrite (Pettinari *et al.*, 2007), acetate (Effendy *et al.*, 2007*a*), perchlorate (Effendy *et al.*, 2007*b*) and trifluoroacetate (Awaleh *et al.*, 2005*a*). Considering the large steric hindrance and the weak coordination ability (Awaleh *et al.*, 2005*b*; Howells *et al.*, 1977; Lawrance *et al.*,1986) of the trifluoromethanesulfonate anion, there is only one C—H···O hydrogen-bond between the phenanthroline ligand and the O atom of the anion with the distance O···H of 2.609Å and the angle C—H···O of 173°.

In the title complex, the P—Ag—N1, P—Ag—N2 and N1—Ag—N2 angles are 147.77 (6)°, 138.03 (6)° and 73.54 (8) ° with a sum of 359.54 °, which comfirms the trigonal-planar environment around the silver atom. In the silver nitrate complex, the P—Ag—N (132.66 (9)°, 131.76 (8)°) (Di Nicola *et al.*, 2007) angles are similar. However, contributing to the role of the nitrate anion, the coordination environment of silver changes from distorted trigonal planar to tetrahedral. The P—Ag—N angles in the other complexes are: 136.94 (5)°, 139.60 (5)°, 71.40 (6)° in the perchlorate (Effendy *et al.*, 2007*b*), 129.4 (1)°, 135.7 (1)°, 71.7 (2)° in trifluoroacetate (Awaleh *et al.*, 2005*a*), 116.52 (6)°, 126.12 (7)°, 70.5 (1)° in acetate (Effendy *et al.*, 2007*a*) and 126.72 (8)°, 127.18 (9)°, 70.77 (12)° in the nitrite (Pettinari *et al.*,2007) anion.

Hence, we should consider two types of anions in the complexes AgX:P$R_3$:*L*, *viz* tetrahedral or distorted trigonal-planar anions and planar or quasi-planar anions (Awaleh *et al.*, 2005*a*; Awaleh *et al.*, 2005*b*; Bowmaker *et al.*, 2005). Nitrate,

nitrite and acetate belong to the former type, whereas perchlorate, trifluoroacetate and trifluoromethanesulfonate can play a role in both of them because of large steric hindrance and the weak coordination ability.

## S2. Experimental

A mixture of AgOTf, $Ph_3P$ and phen in the molar ratio of 1:1:1 in MeOH was stirred for 1 h at ambient temperature, then filtered. Subsequent slow evaporation of the filtrate resulted in the formation of colorless crystals of the title complex. Crystals suitable for single-crystal X-ray diffraction were selected directly from the sample as prepared. Analysis found (percentage): C 53.22, H 3.29, N 4.01; calculated: C 53.19, H 3.29, N 4.02.

## S3. Refinement

All hydrogen atoms were located in the calculated sites and included in the final refinement in the riding model approximation with displacement parameters derived from the parent atoms to which they were bonded ($U_{eq}$(H) = 1.2$U_{eq}$(C)).

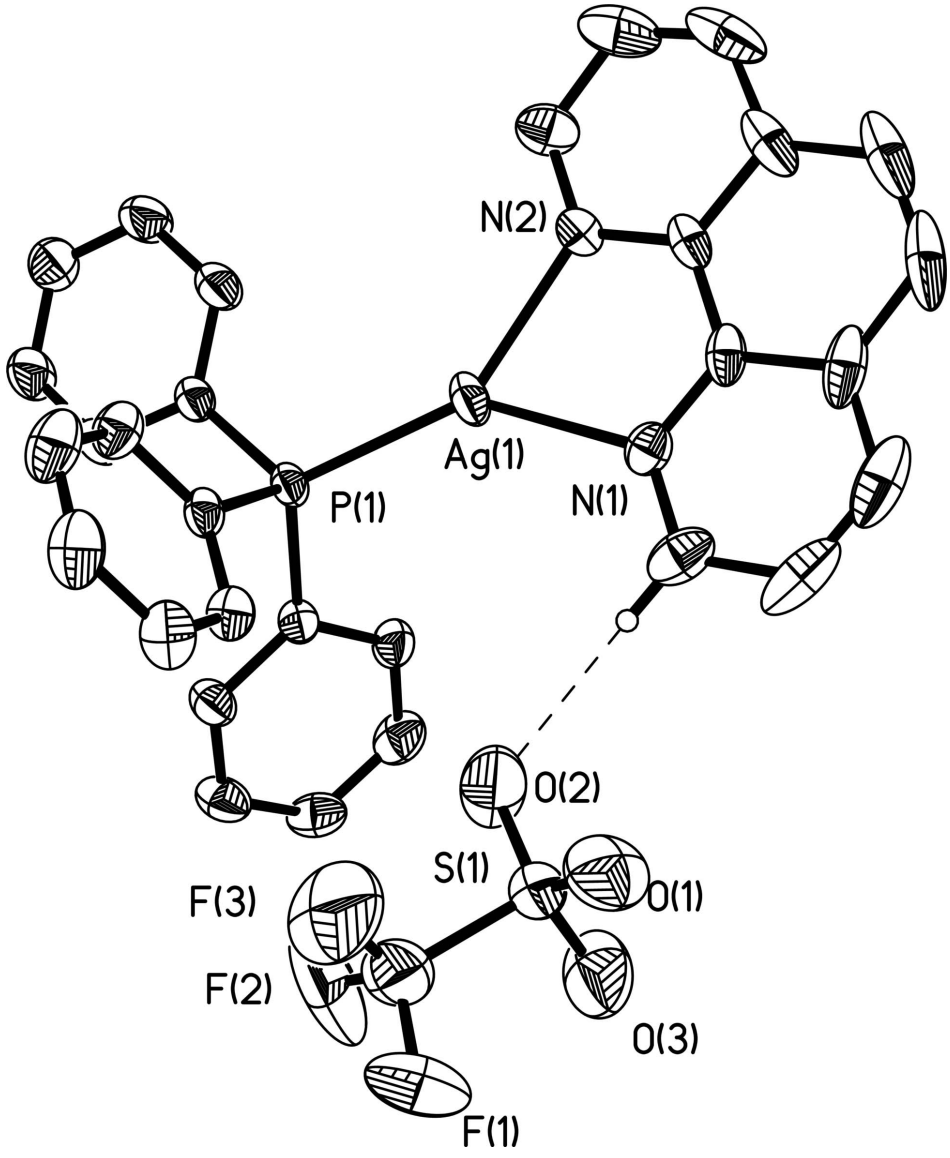


**Figure 1**

Perspective view of the molecule of the title complex; hydrogen atoms are omitted for clarity. Atoms are displayed as ellipsoids at the 35% probability level.

**(1,10-Phenanthroline-$\kappa^2N,N'$)(triphenylphosphine- $\kappa P$)silver(I) trifluoromethanesulfonate**

*Crystal data*

$[Ag(C_{12}H_8N_2)(C_{18}H_{15}P)]CF_3SO_3$
$M_r = 699.42$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.9832$ (2) Å
$b = 11.7533$ (2) Å
$c = 12.2642$ (3) Å
$\alpha = 77.711$ (1)°
$\beta = 76.183$ (1)°
$\gamma = 73.440$ (1)°
$V = 1455.66$ (5) Å$^3$
$Z = 2$
$F(000) = 704$
$D_x = 1.596$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5045 reflections
$\theta = 2.3$–$32.9$°
$\mu = 0.87$ mm$^{-1}$

$T$ = 293 K
Block, colourless

0.4 × 0.3 × 0.2 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.735, $T_{max}$ = 0.832

18629 measured reflections
9515 independent reflections
6777 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021
$\theta_{max}$ = 32.6°, $\theta_{min}$ = 2.0°
$h$ = −15→15
$k$ = −17→16
$l$ = −18→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.133
$S$ = 1.00
9515 reflections
379 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
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.38P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.66 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 | 0.09032 (2) | 0.931304 (15) | 0.211327 (16) | 0.05664 (9) |
| P1 | 0.18488 (6) | 0.77307 (5) | 0.10540 (5) | 0.04241 (13) |
| C24 | −0.0779 (3) | 1.12309 (19) | 0.36019 (18) | 0.0491 (6) |
| C25 | −0.3066 (4) | 1.2209 (4) | 0.3869 (4) | 0.0981 (15) |
| H21 | −0.3787 | 1.2746 | 0.4205 | 0.118* |
| S1 | 0.61400 (9) | 0.77152 (8) | 0.31032 (8) | 0.0748 (2) |
| C1 | 0.0853 (2) | 0.75012 (19) | 0.01682 (19) | 0.0455 (5) |
| C3 | 0.1327 (3) | 0.6742 (3) | −0.0638 (3) | 0.0631 (7) |
| H6 | 0.2207 | 0.6372 | −0.0786 | 0.076* |
| C2 | −0.0452 (3) | 0.8068 (3) | 0.0342 (3) | 0.0644 (7) |
| H10 | −0.0782 | 0.8614 | 0.0852 | 0.077* |
| C4 | 0.3400 (2) | 0.77960 (19) | 0.01460 (18) | 0.0433 (4) |
| C6 | 0.4324 (3) | 0.6788 (2) | −0.0199 (2) | 0.0566 (6) |
| H5 | 0.4166 | 0.6031 | 0.0064 | 0.068* |

| | | | | |
|---|---|---|---|---|
| C7 | 0.4818 (3) | 0.9018 (3) | −0.0982 (3) | 0.0707 (8) |
| H2 | 0.4979 | 0.9772 | −0.1261 | 0.085* |
| C5 | 0.3678 (3) | 0.8918 (2) | −0.0246 (2) | 0.0562 (6) |
| H1 | 0.3088 | 0.9603 | −0.0008 | 0.067* |
| C10 | 0.1297 (3) | 0.5596 (3) | 0.2319 (2) | 0.0602 (7) |
| H15 | 0.0575 | 0.5801 | 0.1981 | 0.072* |
| C8 | 0.2170 (2) | 0.63074 (19) | 0.20106 (18) | 0.0438 (5) |
| C11 | 0.1495 (4) | 0.4583 (3) | 0.3128 (3) | 0.0778 (10) |
| H14 | 0.0894 | 0.4118 | 0.3342 | 0.093* |
| C9 | 0.3237 (3) | 0.5981 (2) | 0.2526 (2) | 0.0544 (6) |
| H11 | 0.3828 | 0.6456 | 0.2335 | 0.065* |
| C12 | 0.5478 (3) | 0.6894 (3) | −0.0929 (3) | 0.0652 (7) |
| H4 | 0.6082 | 0.6213 | −0.1158 | 0.078* |
| C13 | 0.5725 (3) | 0.8001 (3) | −0.1309 (3) | 0.0677 (8) |
| H3 | 0.6504 | 0.8071 | −0.1789 | 0.081* |
| C14 | −0.1276 (3) | 0.7833 (3) | −0.0234 (3) | 0.0766 (9) |
| H9 | −0.2156 | 0.8201 | −0.0094 | 0.092* |
| C16 | 0.0513 (3) | 0.6529 (3) | −0.1223 (3) | 0.0715 (8) |
| H7 | 0.0846 | 0.6022 | −0.1768 | 0.086* |
| C15 | −0.0786 (3) | 0.7058 (3) | −0.1007 (3) | 0.0714 (8) |
| H8 | −0.1336 | 0.6889 | −0.1388 | 0.086* |
| C18 | 0.3430 (4) | 0.4952 (3) | 0.3324 (3) | 0.0685 (8) |
| H12 | 0.4153 | 0.4733 | 0.3662 | 0.082* |
| C17 | 0.2555 (4) | 0.4256 (3) | 0.3616 (3) | 0.0763 (9) |
| H13 | 0.2688 | 0.3561 | 0.4148 | 0.092* |
| O1 | 0.5839 (4) | 0.7776 (4) | 0.4276 (3) | 0.1266 (12) |
| O2 | 0.5105 (4) | 0.7955 (3) | 0.2518 (4) | 0.1519 (17) |
| O3 | 0.7108 (4) | 0.8336 (4) | 0.2534 (4) | 0.1455 (16) |
| C19 | 0.6933 (5) | 0.6175 (4) | 0.2985 (6) | 0.1103 (17) |
| F1 | 0.7991 (3) | 0.5804 (4) | 0.3393 (4) | 0.1752 (17) |
| F2 | 0.7172 (6) | 0.5954 (4) | 0.1989 (4) | 0.218 (3) |
| C23 | 0.0474 (3) | 1.1023 (2) | 0.38492 (18) | 0.0513 (6) |
| C21 | 0.0633 (4) | 1.1640 (3) | 0.4660 (2) | 0.0763 (11) |
| C22 | −0.0480 (7) | 1.2472 (3) | 0.5189 (3) | 0.1041 (18) |
| H19 | −0.0385 | 1.2879 | 0.5723 | 0.125* |
| C20 | 0.2638 (4) | 1.0021 (3) | 0.3561 (3) | 0.0752 (9) |
| H16 | 0.3327 | 0.9473 | 0.3203 | 0.090* |
| N1 | 0.1478 (2) | 1.02361 (18) | 0.33127 (18) | 0.0522 (5) |
| N2 | −0.09368 (19) | 1.06137 (17) | 0.28528 (15) | 0.0489 (5) |
| C26 | −0.1838 (4) | 1.2062 (2) | 0.4146 (2) | 0.0757 (10) |
| C27 | −0.2110 (3) | 1.0794 (3) | 0.2637 (3) | 0.0708 (8) |
| H23 | −0.2217 | 1.0367 | 0.2123 | 0.085* |
| C28 | −0.1636 (6) | 1.2669 (3) | 0.4930 (3) | 0.1029 (17) |
| H20 | −0.2329 | 1.3223 | 0.5277 | 0.124* |
| C29 | −0.3190 (4) | 1.1595 (4) | 0.3146 (4) | 0.0990 (14) |
| H22 | −0.3996 | 1.1693 | 0.2972 | 0.119* |
| C31 | 0.2848 (6) | 1.0623 (5) | 0.4377 (4) | 0.1018 (17) |
| H17 | 0.3670 | 1.0475 | 0.4536 | 0.122* |

| | | | | |
|---|---|---|---|---|
| C30 | 0.1856 (6) | 1.1398 (5) | 0.4908 (3) | 0.1008 (17) |
| H18 | 0.1988 | 1.1777 | 0.5448 | 0.121* |
| F3 | 0.6223 (5) | 0.5475 (3) | 0.3633 (5) | 0.213 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ag1 | 0.06687 (15) | 0.04557 (11) | 0.05563 (12) | −0.00722 (8) | −0.00064 (9) | −0.02543 (8) |
| P1 | 0.0462 (3) | 0.0368 (2) | 0.0428 (3) | −0.0074 (2) | −0.0011 (2) | −0.0152 (2) |
| C24 | 0.0684 (16) | 0.0344 (9) | 0.0358 (9) | −0.0065 (9) | 0.0011 (9) | −0.0071 (7) |
| C25 | 0.072 (2) | 0.074 (2) | 0.094 (3) | 0.0230 (17) | 0.021 (2) | 0.0052 (19) |
| S1 | 0.0677 (5) | 0.0771 (5) | 0.0829 (5) | −0.0120 (4) | −0.0169 (4) | −0.0249 (4) |
| C1 | 0.0490 (13) | 0.0417 (10) | 0.0443 (11) | −0.0082 (8) | −0.0041 (9) | −0.0133 (8) |
| C3 | 0.0536 (15) | 0.0689 (16) | 0.0681 (16) | −0.0009 (12) | −0.0068 (12) | −0.0380 (13) |
| C2 | 0.0545 (16) | 0.0662 (16) | 0.0732 (18) | −0.0011 (12) | −0.0090 (13) | −0.0345 (13) |
| C4 | 0.0472 (12) | 0.0395 (9) | 0.0426 (10) | −0.0110 (8) | −0.0056 (9) | −0.0077 (8) |
| C6 | 0.0523 (15) | 0.0434 (11) | 0.0633 (15) | −0.0094 (10) | 0.0063 (11) | −0.0083 (10) |
| C7 | 0.075 (2) | 0.0628 (16) | 0.077 (2) | −0.0352 (15) | −0.0136 (16) | 0.0069 (14) |
| C5 | 0.0613 (16) | 0.0413 (11) | 0.0690 (16) | −0.0161 (10) | −0.0162 (13) | −0.0062 (10) |
| C10 | 0.0700 (18) | 0.0622 (15) | 0.0540 (14) | −0.0303 (13) | −0.0077 (12) | −0.0061 (11) |
| C8 | 0.0538 (13) | 0.0407 (9) | 0.0377 (9) | −0.0145 (9) | −0.0004 (9) | −0.0133 (8) |
| C11 | 0.107 (3) | 0.0724 (19) | 0.0640 (18) | −0.0527 (19) | −0.0103 (18) | 0.0020 (15) |
| C9 | 0.0615 (16) | 0.0525 (12) | 0.0524 (13) | −0.0168 (11) | −0.0113 (11) | −0.0106 (10) |
| C12 | 0.0510 (15) | 0.0647 (16) | 0.0652 (16) | −0.0060 (12) | 0.0046 (12) | −0.0074 (13) |
| C13 | 0.0497 (16) | 0.082 (2) | 0.0651 (17) | −0.0229 (14) | −0.0056 (13) | 0.0055 (14) |
| C14 | 0.0515 (17) | 0.086 (2) | 0.098 (2) | 0.0036 (14) | −0.0254 (16) | −0.0410 (18) |
| C16 | 0.071 (2) | 0.0799 (19) | 0.0713 (18) | −0.0068 (15) | −0.0163 (15) | −0.0411 (15) |
| C15 | 0.071 (2) | 0.0742 (18) | 0.077 (2) | −0.0096 (15) | −0.0304 (16) | −0.0228 (15) |
| C18 | 0.093 (2) | 0.0581 (15) | 0.0577 (15) | −0.0160 (15) | −0.0278 (15) | −0.0039 (12) |
| C17 | 0.118 (3) | 0.0585 (16) | 0.0554 (16) | −0.0331 (17) | −0.0203 (17) | 0.0037 (12) |
| O1 | 0.105 (2) | 0.169 (4) | 0.097 (2) | −0.019 (2) | 0.0043 (18) | −0.050 (2) |
| O2 | 0.161 (3) | 0.090 (2) | 0.238 (5) | 0.013 (2) | −0.143 (4) | −0.038 (2) |
| O3 | 0.148 (3) | 0.117 (3) | 0.172 (4) | −0.072 (3) | 0.034 (3) | −0.043 (2) |
| C19 | 0.094 (3) | 0.070 (2) | 0.161 (5) | −0.011 (2) | −0.041 (3) | 0.002 (3) |
| F1 | 0.092 (2) | 0.166 (3) | 0.236 (4) | 0.038 (2) | −0.057 (2) | −0.031 (3) |
| F2 | 0.336 (7) | 0.123 (3) | 0.175 (4) | 0.056 (3) | −0.082 (4) | −0.096 (3) |
| C23 | 0.0848 (19) | 0.0382 (10) | 0.0355 (10) | −0.0281 (11) | −0.0072 (10) | −0.0027 (8) |
| C21 | 0.146 (3) | 0.0638 (16) | 0.0408 (12) | −0.068 (2) | −0.0155 (16) | 0.0002 (11) |
| C22 | 0.216 (6) | 0.0626 (19) | 0.0432 (15) | −0.068 (3) | 0.011 (2) | −0.0225 (13) |
| C20 | 0.071 (2) | 0.080 (2) | 0.080 (2) | −0.0389 (17) | −0.0279 (17) | 0.0172 (16) |
| N1 | 0.0608 (13) | 0.0474 (10) | 0.0525 (11) | −0.0202 (9) | −0.0160 (9) | −0.0014 (8) |
| N2 | 0.0510 (12) | 0.0468 (10) | 0.0441 (10) | −0.0026 (8) | −0.0093 (8) | −0.0096 (8) |
| C26 | 0.104 (3) | 0.0428 (12) | 0.0515 (14) | 0.0004 (13) | 0.0185 (15) | −0.0092 (10) |
| C27 | 0.0586 (18) | 0.0790 (19) | 0.0655 (17) | −0.0017 (14) | −0.0208 (14) | −0.0024 (14) |
| C28 | 0.173 (5) | 0.0529 (16) | 0.061 (2) | −0.023 (2) | 0.029 (3) | −0.0266 (14) |
| C29 | 0.060 (2) | 0.108 (3) | 0.093 (3) | 0.011 (2) | −0.0072 (19) | 0.009 (2) |
| C31 | 0.120 (4) | 0.131 (4) | 0.089 (3) | −0.094 (3) | −0.059 (3) | 0.040 (3) |
| C30 | 0.171 (5) | 0.109 (3) | 0.061 (2) | −0.103 (4) | −0.035 (3) | 0.011 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F3 | 0.209 (5) | 0.103 (2) | 0.335 (7) | −0.079 (3) | −0.087 (4) | 0.042 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ag1—N2 | 2.2798 (18) | C11—H14 | 0.9300 |
| Ag1—N1 | 2.292 (2) | C9—C18 | 1.384 (4) |
| Ag1—P1 | 2.3469 (5) | C9—H11 | 0.9300 |
| P1—C4 | 1.812 (2) | C12—C13 | 1.365 (4) |
| P1—C1 | 1.819 (3) | C12—H4 | 0.9300 |
| P1—C8 | 1.823 (2) | C13—H3 | 0.9300 |
| C24—N2 | 1.353 (3) | C14—C15 | 1.364 (5) |
| C24—C26 | 1.418 (3) | C14—H9 | 0.9300 |
| C24—C23 | 1.422 (4) | C16—C15 | 1.370 (5) |
| C25—C29 | 1.308 (7) | C16—H7 | 0.9300 |
| C25—C26 | 1.423 (7) | C15—H8 | 0.9300 |
| C25—H21 | 0.9300 | C18—C17 | 1.371 (5) |
| S1—O1 | 1.409 (3) | C18—H12 | 0.9300 |
| S1—O2 | 1.417 (3) | C17—H13 | 0.9300 |
| S1—O3 | 1.421 (4) | C19—F2 | 1.253 (7) |
| S1—C19 | 1.791 (5) | C19—F1 | 1.298 (6) |
| C1—C3 | 1.381 (3) | C19—F3 | 1.307 (6) |
| C1—C2 | 1.384 (4) | C23—N1 | 1.355 (3) |
| C3—C16 | 1.375 (4) | C23—C21 | 1.416 (3) |
| C3—H6 | 0.9300 | C21—C30 | 1.385 (7) |
| C2—C14 | 1.387 (5) | C21—C22 | 1.442 (7) |
| C2—H10 | 0.9300 | C22—C28 | 1.326 (7) |
| C4—C6 | 1.391 (3) | C22—H19 | 0.9300 |
| C4—C5 | 1.397 (3) | C20—N1 | 1.323 (4) |
| C6—C12 | 1.387 (4) | C20—C31 | 1.435 (6) |
| C6—H5 | 0.9300 | C20—H16 | 0.9300 |
| C7—C5 | 1.376 (4) | N2—C27 | 1.327 (4) |
| C7—C13 | 1.385 (5) | C26—C28 | 1.403 (6) |
| C7—H2 | 0.9300 | C27—C29 | 1.394 (5) |
| C5—H1 | 0.9300 | C27—H23 | 0.9300 |
| C10—C11 | 1.380 (4) | C28—H20 | 0.9300 |
| C10—C8 | 1.382 (4) | C29—H22 | 0.9300 |
| C10—H15 | 0.9300 | C31—C30 | 1.337 (7) |
| C8—C9 | 1.384 (4) | C31—H17 | 0.9300 |
| C11—C17 | 1.356 (5) | C30—H18 | 0.9300 |
| | | | |
| N2—Ag1—N1 | 73.53 (8) | C7—C13—H3 | 119.9 |
| N2—Ag1—P1 | 147.77 (6) | C15—C14—C2 | 119.6 (3) |
| N1—Ag1—P1 | 138.03 (6) | C15—C14—H9 | 120.2 |
| C4—P1—C1 | 106.47 (11) | C2—C14—H9 | 120.2 |
| C4—P1—C8 | 104.71 (10) | C15—C16—C3 | 120.4 (3) |
| C1—P1—C8 | 103.84 (10) | C15—C16—H7 | 119.8 |
| C4—P1—Ag1 | 115.16 (7) | C3—C16—H7 | 119.8 |
| C1—P1—Ag1 | 115.70 (7) | C14—C15—C16 | 120.1 (3) |

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| C8—P1—Ag1 | 109.82 (7) | C14—C15—H8 | 119.9 |
| N2—C24—C26 | 121.2 (3) | C16—C15—H8 | 119.9 |
| N2—C24—C23 | 118.8 (2) | C17—C18—C9 | 120.1 (3) |
| C26—C24—C23 | 120.0 (3) | C17—C18—H12 | 120.0 |
| C29—C25—C26 | 120.5 (3) | C9—C18—H12 | 120.0 |
| C29—C25—H21 | 119.7 | C11—C17—C18 | 119.9 (3) |
| C26—C25—H21 | 119.7 | C11—C17—H13 | 120.0 |
| O1—S1—O2 | 118.2 (3) | C18—C17—H13 | 120.0 |
| O1—S1—O3 | 111.0 (3) | F2—C19—F1 | 109.1 (6) |
| O2—S1—O3 | 113.3 (3) | F2—C19—F3 | 108.5 (6) |
| O1—S1—C19 | 105.7 (3) | F1—C19—F3 | 102.2 (5) |
| O2—S1—C19 | 103.3 (2) | F2—C19—S1 | 113.4 (4) |
| O3—S1—C19 | 103.5 (3) | F1—C19—S1 | 112.9 (4) |
| C3—C1—C2 | 118.2 (3) | F3—C19—S1 | 110.1 (4) |
| C3—C1—P1 | 123.0 (2) | N1—C23—C21 | 121.9 (3) |
| C2—C1—P1 | 118.73 (18) | N1—C23—C24 | 119.3 (2) |
| C16—C3—C1 | 120.6 (3) | C21—C23—C24 | 118.8 (3) |
| C16—C3—H6 | 119.7 | C30—C21—C23 | 117.7 (4) |
| C1—C3—H6 | 119.7 | C30—C21—C22 | 123.6 (4) |
| C1—C2—C14 | 121.0 (3) | C23—C21—C22 | 118.7 (4) |
| C1—C2—H10 | 119.5 | C28—C22—C21 | 121.5 (3) |
| C14—C2—H10 | 119.5 | C28—C22—H19 | 119.2 |
| C6—C4—C5 | 118.1 (2) | C21—C22—H19 | 119.2 |
| C6—C4—P1 | 123.43 (18) | N1—C20—C31 | 120.8 (4) |
| C5—C4—P1 | 118.47 (19) | N1—C20—H16 | 119.6 |
| C12—C6—C4 | 121.0 (2) | C31—C20—H16 | 119.6 |
| C12—C6—H5 | 119.5 | C20—N1—C23 | 119.3 (3) |
| C4—C6—H5 | 119.5 | C20—N1—Ag1 | 126.7 (2) |
| C5—C7—C13 | 120.2 (3) | C23—N1—Ag1 | 113.81 (17) |
| C5—C7—H2 | 119.9 | C27—N2—C24 | 118.7 (2) |
| C13—C7—H2 | 119.9 | C27—N2—Ag1 | 126.7 (2) |
| C7—C5—C4 | 120.5 (3) | C24—N2—Ag1 | 114.57 (16) |
| C7—C5—H1 | 119.7 | C28—C26—C24 | 119.4 (4) |
| C4—C5—H1 | 119.7 | C28—C26—C25 | 123.8 (4) |
| C11—C10—C8 | 120.1 (3) | C24—C26—C25 | 116.9 (3) |
| C11—C10—H15 | 120.0 | N2—C27—C29 | 122.8 (4) |
| C8—C10—H15 | 120.0 | N2—C27—H23 | 118.6 |
| C10—C8—C9 | 118.8 (2) | C29—C27—H23 | 118.6 |
| C10—C8—P1 | 121.0 (2) | C22—C28—C26 | 121.6 (4) |
| C9—C8—P1 | 119.95 (18) | C22—C28—H20 | 119.2 |
| C17—C11—C10 | 120.8 (3) | C26—C28—H20 | 119.2 |
| C17—C11—H14 | 119.6 | C25—C29—C27 | 119.9 (4) |
| C10—C11—H14 | 119.6 | C25—C29—H22 | 120.1 |
| C8—C9—C18 | 120.3 (3) | C27—C29—H22 | 120.1 |
| C8—C9—H11 | 119.9 | C30—C31—C20 | 119.8 (4) |
| C18—C9—H11 | 119.9 | C30—C31—H17 | 120.1 |
| C13—C12—C6 | 119.9 (3) | C20—C31—H17 | 120.1 |
| C13—C12—H4 | 120.1 | C31—C30—C21 | 120.4 (4) |

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| C6—C12—H4 | 120.1 | C31—C30—H18 | 119.8 |
| C12—C13—C7 | 120.2 (3) | C21—C30—H18 | 119.8 |
| C12—C13—H3 | 119.9 | | |

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| N2—Ag1—P1—C4 | 143.08 (12) | O1—S1—C19—F1 | −60.6 (5) |
| N1—Ag1—P1—C4 | −51.26 (12) | O2—S1—C19—F1 | 174.5 (5) |
| N2—Ag1—P1—C1 | 18.06 (13) | O3—S1—C19—F1 | 56.2 (5) |
| N1—Ag1—P1—C1 | −176.27 (11) | O1—S1—C19—F3 | 52.9 (5) |
| N2—Ag1—P1—C8 | −99.05 (13) | O2—S1—C19—F3 | −71.9 (5) |
| N1—Ag1—P1—C8 | 66.61 (12) | O3—S1—C19—F3 | 169.7 (5) |
| C4—P1—C1—C3 | 40.1 (3) | N2—C24—C23—N1 | 1.4 (3) |
| C8—P1—C1—C3 | −70.1 (3) | C26—C24—C23—N1 | −179.3 (2) |
| Ag1—P1—C1—C3 | 169.5 (2) | N2—C24—C23—C21 | −178.0 (2) |
| C4—P1—C1—C2 | −142.9 (2) | C26—C24—C23—C21 | 1.3 (3) |
| C8—P1—C1—C2 | 106.9 (2) | N1—C23—C21—C30 | −1.1 (4) |
| Ag1—P1—C1—C2 | −13.6 (2) | C24—C23—C21—C30 | 178.3 (2) |
| C2—C1—C3—C16 | −2.1 (5) | N1—C23—C21—C22 | 179.5 (2) |
| P1—C1—C3—C16 | 174.9 (3) | C24—C23—C21—C22 | −1.1 (3) |
| C3—C1—C2—C14 | 3.3 (5) | C30—C21—C22—C28 | −179.5 (3) |
| P1—C1—C2—C14 | −173.8 (3) | C23—C21—C22—C28 | −0.1 (5) |
| C1—P1—C4—C6 | −75.7 (2) | C31—C20—N1—C23 | −0.9 (4) |
| C8—P1—C4—C6 | 33.9 (2) | C31—C20—N1—Ag1 | −176.6 (2) |
| Ag1—P1—C4—C6 | 154.6 (2) | C21—C23—N1—C20 | 1.0 (3) |
| C1—P1—C4—C5 | 103.2 (2) | C24—C23—N1—C20 | −178.4 (2) |
| C8—P1—C4—C5 | −147.2 (2) | C21—C23—N1—Ag1 | 177.19 (17) |
| Ag1—P1—C4—C5 | −26.5 (2) | C24—C23—N1—Ag1 | −2.2 (3) |
| C5—C4—C6—C12 | −1.2 (4) | N2—Ag1—N1—C20 | 177.5 (2) |
| P1—C4—C6—C12 | 177.6 (2) | P1—Ag1—N1—C20 | 5.5 (3) |
| C13—C7—C5—C4 | −2.4 (5) | N2—Ag1—N1—C23 | 1.63 (15) |
| C6—C4—C5—C7 | 2.1 (4) | P1—Ag1—N1—C23 | −170.45 (11) |
| P1—C4—C5—C7 | −176.8 (2) | C26—C24—N2—C27 | −0.4 (3) |
| C11—C10—C8—C9 | 0.1 (4) | C23—C24—N2—C27 | 178.9 (2) |
| C11—C10—C8—P1 | −173.6 (3) | C26—C24—N2—Ag1 | −179.12 (18) |
| C4—P1—C8—C10 | −140.7 (2) | C23—C24—N2—Ag1 | 0.2 (3) |
| C1—P1—C8—C10 | −29.2 (2) | N1—Ag1—N2—C27 | −179.6 (2) |
| Ag1—P1—C8—C10 | 95.1 (2) | P1—Ag1—N2—C27 | −9.5 (3) |
| C4—P1—C8—C9 | 45.7 (2) | N1—Ag1—N2—C24 | −0.94 (15) |
| C1—P1—C8—C9 | 157.17 (19) | P1—Ag1—N2—C24 | 169.11 (11) |
| Ag1—P1—C8—C9 | −78.53 (19) | N2—C24—C26—C28 | 179.0 (3) |
| C8—C10—C11—C17 | −1.3 (5) | C23—C24—C26—C28 | −0.3 (4) |
| C10—C8—C9—C18 | 0.8 (4) | N2—C24—C26—C25 | 0.2 (4) |
| P1—C8—C9—C18 | 174.6 (2) | C23—C24—C26—C25 | −179.1 (2) |
| C4—C6—C12—C13 | 0.7 (5) | C29—C25—C26—C28 | −178.6 (4) |
| C6—C12—C13—C7 | −1.0 (5) | C29—C25—C26—C24 | 0.1 (5) |
| C5—C7—C13—C12 | 1.9 (5) | C24—N2—C27—C29 | 0.2 (4) |
| C1—C2—C14—C15 | −1.9 (6) | Ag1—N2—C27—C29 | 178.8 (3) |
| C1—C3—C16—C15 | −0.6 (6) | C21—C22—C28—C26 | 1.2 (6) |
| C2—C14—C15—C16 | −0.9 (6) | C24—C26—C28—C22 | −1.0 (5) |

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|---|---|---|---|
| C3—C16—C15—C14 | 2.1 (6) | C25—C26—C28—C22 | 177.7 (3) |
| C8—C9—C18—C17 | −0.6 (5) | C26—C25—C29—C27 | −0.3 (6) |
| C10—C11—C17—C18 | 1.5 (6) | N2—C27—C29—C25 | 0.1 (6) |
| C9—C18—C17—C11 | −0.5 (5) | N1—C20—C31—C30 | 1.1 (5) |
| O1—S1—C19—F2 | 174.6 (5) | C20—C31—C30—C21 | −1.2 (5) |
| O2—S1—C19—F2 | 49.8 (6) | C23—C21—C30—C31 | 1.2 (5) |
| O3—S1—C19—F2 | −68.6 (6) | C22—C21—C30—C31 | −179.4 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C20—H16···O2 | 0.93 | 2.36 | 3.285 (6) | 173 |