

**(Acetonitrile- $\kappa$ N)(3-amino-4-methylbenzenesulfonato- $\kappa$ N)aqua(triphenylphosphine- $\kappa$ P)silver(I) hemihydrate**

Jia-Jun Han and Ning Li\*

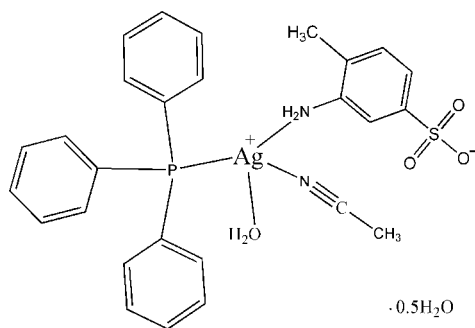
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å; disorder in solvent or counterion;  $R$  factor = 0.035;  $wR$  factor = 0.110; data-to-parameter ratio = 17.8.

The title compound,  $[\text{Ag}(\text{C}_7\text{H}_8\text{NO}_3\text{S})(\text{C}_2\text{H}_3\text{N})(\text{C}_{18}\text{H}_{15}\text{P})(\text{H}_2\text{O})] \cdot 0.5\text{H}_2\text{O}$ , has a mononuclear structure in which the  $\text{Ag}^{\text{I}}$  ion is four-coordinated by the N atoms from a 3-amino-4-methylbenzenesulfonate anion and an acetonitrile molecule, one P atom from a triphenylphosphine ligand and one O atom from a water molecule, forming a distorted tetrahedral configuration. Molecules are linked into a ribbon-like structure along the  $a$  axis by  $\text{O}(\text{water})-\text{H}\cdots\text{O}$  hydrogen bonds involving the coordinated water molecule, and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds. The uncoordinated water molecule is disordered across an inversion centre.

**Related literature**For studies on silver sulfonates, see: Han & Li (2007*a,b*).**Experimental***Crystal data*

$[\text{Ag}(\text{C}_7\text{H}_8\text{NO}_3\text{S})(\text{C}_2\text{H}_3\text{N})(\text{C}_{18}\text{H}_{15}\text{P})(\text{H}_2\text{O})] \cdot 0.5\text{H}_2\text{O}$   
 $M_r = 624.42$   
 Triclinic,  $P\bar{1}$   
 $a = 9.058$  (5) Å

$b = 12.300$  (5) Å  
 $c = 13.500$  (5) Å  
 $\alpha = 90.526$  (5)°  
 $\beta = 105.382$  (5)°  
 $\gamma = 98.637$  (5)°

$V = 1431.9$  (11) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation

$\mu = 0.87$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.27 \times 0.24 \times 0.19$  mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\text{min}} = 0.786$ ,  $T_{\text{max}} = 0.849$

16198 measured reflections  
 6265 independent reflections  
 4674 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.110$   
 $S = 1.00$   
 6265 reflections  
 351 parameters  
 15 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.65$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.60$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Ag1—N1	2.304 (2)	Ag1—N2	2.491 (4)
Ag1—P1	2.3712 (9)	Ag1—O1W	2.524 (3)
N1—Ag1—P1	150.06 (7)	N1—Ag1—O1W	94.06 (8)
N1—Ag1—N2	85.71 (11)	P1—Ag1—O1W	106.81 (6)
P1—Ag1—N2	117.20 (9)	N2—Ag1—O1W	83.54 (11)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1W—H1W1 $\cdots$ O2 <sup>i</sup>	0.854 (10)	1.952 (13)	2.797 (3)	170 (4)
O1W—H1W2 $\cdots$ O3 <sup>ii</sup>	0.853 (10)	2.091 (12)	2.940 (4)	174 (5)
N1—H1N2 $\cdots$ O1 <sup>ii</sup>	0.896 (10)	2.19 (2)	2.965 (3)	144 (3)
N1—H1N1 $\cdots$ O3 <sup>i</sup>	0.885 (10)	2.171 (14)	3.032 (4)	164 (3)

Symmetry codes: (i)  $-x + 1, -y + 1, -z + 2$ ; (ii)  $x + 1, y, z$ .

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2475).

**References**

- Han, J.-J. & Li, N. (2007*a*). *Acta Cryst.* **E63**, m1622–m1623.  
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**supplementary materials**

*Acta Cryst.* (2007). E63, m2807 [ doi:10.1107/S1600536807051549 ]

**(Acetonitrile- $\kappa$ N)(3-amino-4-methylbenzenesulfonato- $\kappa$ N)aqua(triphenylphosphine- $\kappa$ P)silver(I) hemihydrate**

**J.-J. Han and N. Li**

**Comment**

Recently, intense interest has been focused on silver(I) sulfonates because of their interesting structures and properties (Han & Li, 2007*a*). So far, some silver(I) sulfonate compounds modified by secondary ligands that display different structures have been reported (Han & Li, 2007*b*). We selected 3-amino-4-methylbenzenesulfonic acid (HL) as a sulfonate ligand and triphenylphosphine (TPP) as a secondary ligand, generating a new coordination complex,  $[\text{Ag}(L)(\text{TPP})(\text{CNCH}_3)(\text{H}_2\text{O})]\cdot 0.5\text{H}_2\text{O}$ , which is reported here.

In compound (I), each  $\text{Ag}^{\text{I}}$  cation is four-coordinated by two N atoms one each from a 3-amino-4-methylbenzenesulfonate anion and a acetonitrile molecule, one P atom from a triphenylphosphine ligand, and one O atom from the water molecule, forming a distorted tetrahedral configuration (Fig. 1). The Ag—N (sulfonate) distance of the title complex is comparable to that found in a related structure (Han & Li, 2007*b*). The molecules are linked through  $\text{O}_w\text{—H}\cdots\text{O}$  and  $\text{N—H}\cdots\text{O}$  hydrogen bonds (Table 2) to form a ribbon like structure along the *a* axis.

**Experimental**

An aqueous solution (12 ml) of 3-amino-4-methylbenzenesulfonic acid (0.5 mmol) was added to solid  $\text{Ag}_2\text{CO}_3$  (0.25 mmol) and stirred for several minutes until no further  $\text{CO}_2$  was given off. Triphenylphosphine (0.5 mmol) in acetonitrile (5 ml) was then added and a solution formed. Crystals of the title compound were obtained by slow evaporation of the solvent for several days at room temperature.

**Refinement**

The amino H atoms were located in a difference map, and were refined with distance restraints of  $\text{N—H} = 0.90$  (1) Å and  $\text{H}\cdots\text{H} = 1.37$  (2) Å, and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$ . H-atoms of the water molecules were located in a difference map, and were refined with distance restraints of  $\text{O—H} = 0.85$  (1) Å and  $\text{H}\cdots\text{H} = 1.39$  (2) Å, and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$ . C-bound H atoms were positioned geometrically ( $\text{C—H} = 0.93$  Å) and refined as riding, with  $U(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$ . Atom O2W is disordered across an inversion centre and it was refined with an occupancy of 0.50. The  $U^{\text{ij}}$  components of O2W were approximated to isotropic behaviour.

## Figures

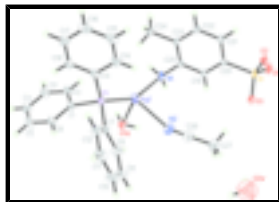


Fig. 1. The structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

## (Acetonitrile- $\kappa N$ )(3-amino-4-methylbenzenesulfonato- $\kappa N$ )aqua(triphenylphosphine- $\kappa P$ )silver(I) hemihydrate

### Crystal data

$[\text{Ag}(\text{C}_7\text{H}_8\text{NO}_3\text{S})(\text{C}_2\text{H}_3\text{N})(\text{C}_{18}\text{H}_{15}\text{P})(\text{H}_2\text{O})] \cdot 0.5\text{H}_2\text{O}$	$Z = 2$
$M_r = 624.42$	$F_{000} = 638$
Triclinic, $P\bar{1}$	$D_x = 1.448 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 9.058 (5) \text{ \AA}$	$\lambda = 0.71069 \text{ \AA}$
$b = 12.300 (5) \text{ \AA}$	Cell parameters from 6198 reflections
$c = 13.500 (5) \text{ \AA}$	$\theta = 3.0\text{--}27.5^\circ$
$\alpha = 90.526 (5)^\circ$	$\mu = 0.87 \text{ mm}^{-1}$
$\beta = 105.382 (5)^\circ$	$T = 293 (2) \text{ K}$
$\gamma = 98.637 (5)^\circ$	Block, colourless
$V = 1431.9 (11) \text{ \AA}^3$	$0.27 \times 0.24 \times 0.19 \text{ mm}$

### Data collection

Rigaku R-AXIS RAPID diffractometer	6265 independent reflections
Radiation source: rotating anode	4674 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.032$
Detector resolution: $10.0 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 27.5^\circ$
$T = 293(2) \text{ K}$	$\theta_{\text{min}} = 1.6^\circ$
$\omega$ scans	$h = 0 \rightarrow 11$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -15 \rightarrow 15$
$T_{\text{min}} = 0.786$ , $T_{\text{max}} = 0.849$	$l = -17 \rightarrow 16$
16198 measured reflections	

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2]$

$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
6265 reflections	$(\Delta/\sigma)_{\max} = 0.001$
351 parameters	$\Delta\rho_{\max} = 0.65 \text{ e } \text{\AA}^{-3}$
15 restraints	$\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ag1	0.82067 (3)	0.71412 (2)	0.812387 (19)	0.05643 (11)	
S1	0.24990 (7)	0.64963 (6)	1.03695 (5)	0.03917 (16)	
P1	0.89270 (8)	0.83242 (6)	0.68962 (5)	0.03976 (17)	
O1	0.1360 (2)	0.72108 (19)	1.00246 (19)	0.0587 (6)	
O2	0.2681 (3)	0.6244 (2)	1.14346 (18)	0.0603 (6)	
O3	0.2255 (2)	0.55291 (18)	0.96984 (19)	0.0582 (6)	
O1W	0.9384 (3)	0.5422 (2)	0.8028 (2)	0.0617 (6)	
H1W1	0.868 (3)	0.497 (3)	0.819 (3)	0.092*	
H1W2	1.021 (3)	0.550 (4)	0.853 (2)	0.092*	
O2W	-0.0549 (18)	0.4784 (15)	0.5433 (11)	0.237 (7)	0.50
H2W1	0.0000	0.5000	0.5000	0.355*	
H2W2	0.000 (12)	0.50 (2)	0.6040 (16)	0.355*	0.50
N1	0.7966 (2)	0.6867 (2)	0.97637 (19)	0.0424 (5)	
H1N1	0.782 (3)	0.6141 (9)	0.979 (3)	0.064*	
H1N2	0.8959 (17)	0.709 (2)	1.011 (2)	0.064*	
C1	1.0808 (3)	0.8162 (2)	0.6725 (2)	0.0414 (6)	
C2	1.1987 (4)	0.8086 (3)	0.7591 (2)	0.0547 (8)	
H2	1.1784	0.8062	0.8231	0.066*	
C3	1.3482 (4)	0.8046 (4)	0.7521 (3)	0.0700 (10)	
H3	1.4282	0.8008	0.8110	0.084*	
C4	1.3763 (4)	0.8063 (3)	0.6554 (3)	0.0740 (11)	
H4	1.4757	0.8038	0.6496	0.089*	
C5	1.2592 (4)	0.8117 (3)	0.5700 (3)	0.0697 (10)	
H5	1.2786	0.8117	0.5057	0.084*	
C6	1.1114 (4)	0.8171 (3)	0.5775 (2)	0.0577 (8)	

## supplementary materials

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H6	1.0321	0.8214	0.5183	0.069*
C7	0.7559 (3)	0.8004 (2)	0.5636 (2)	0.0455 (6)
C8	0.6856 (5)	0.6923 (3)	0.5389 (3)	0.0700 (10)
H8	0.7095	0.6390	0.5865	0.084*
C9	0.5807 (6)	0.6623 (4)	0.4452 (3)	0.0878 (13)
H9	0.5352	0.5891	0.4293	0.105*
C10	0.5433 (5)	0.7408 (4)	0.3747 (3)	0.0885 (14)
H10	0.4722	0.7206	0.3114	0.106*
C11	0.6097 (5)	0.8475 (4)	0.3974 (3)	0.0802 (12)
H11	0.5847	0.9005	0.3497	0.096*
C12	0.7160 (4)	0.8775 (3)	0.4929 (3)	0.0619 (9)
H12	0.7604	0.9509	0.5087	0.074*
C13	0.9072 (3)	0.9809 (2)	0.7080 (2)	0.0430 (6)
C14	0.7906 (4)	1.0222 (3)	0.7386 (2)	0.0559 (8)
H14	0.7072	0.9745	0.7497	0.067*
C15	0.7994 (5)	1.1354 (3)	0.7526 (3)	0.0688 (10)
H15	0.7205	1.1631	0.7719	0.083*
C16	0.9230 (5)	1.2066 (3)	0.7384 (3)	0.0706 (10)
H16	0.9284	1.2821	0.7489	0.085*
C17	1.0364 (5)	1.1670 (3)	0.7093 (3)	0.0662 (9)
H17	1.1197	1.2157	0.6994	0.079*
C18	1.0311 (4)	1.0546 (3)	0.6936 (2)	0.0542 (8)
H18	1.1105	1.0286	0.6734	0.065*
C19	0.5426 (3)	0.6758 (2)	1.0080 (2)	0.0354 (5)
H19	0.5231	0.6006	0.9914	0.043*
C20	0.4308 (3)	0.7267 (2)	1.0332 (2)	0.0367 (6)
C21	0.4580 (3)	0.8378 (2)	1.0601 (2)	0.0469 (7)
H21	0.3828	0.8716	1.0780	0.056*
C22	0.6002 (4)	0.8980 (2)	1.0597 (3)	0.0509 (7)
H22	0.6201	0.9727	1.0787	0.061*
C23	0.7131 (3)	0.8505 (2)	1.0321 (2)	0.0406 (6)
C24	0.8614 (3)	0.9190 (3)	1.0249 (3)	0.0539 (8)
H24A	0.9473	0.8967	1.0747	0.081*
H24B	0.8581	0.9953	1.0384	0.081*
H24C	0.8738	0.9089	0.9572	0.081*
C25	0.6851 (3)	0.7374 (2)	1.00730 (19)	0.0346 (5)
N2	0.5710 (4)	0.5851 (3)	0.7540 (3)	0.0848 (10)
C26	0.4561 (6)	0.5415 (4)	0.7544 (4)	0.0868 (12)
C27	0.3062 (7)	0.4811 (5)	0.7599 (5)	0.129 (2)
H27A	0.3103	0.4036	0.7603	0.194*
H27B	0.2263	0.4959	0.7012	0.194*
H27C	0.2838	0.5044	0.8217	0.194*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.06167 (17)	0.06053 (17)	0.05768 (17)	0.01306 (12)	0.03202 (12)	0.01829 (11)
S1	0.0240 (3)	0.0411 (4)	0.0537 (4)	-0.0004 (3)	0.0156 (3)	0.0031 (3)

P1	0.0409 (4)	0.0445 (4)	0.0372 (4)	0.0092 (3)	0.0149 (3)	0.0054 (3)
O1	0.0282 (10)	0.0637 (14)	0.0861 (16)	0.0109 (10)	0.0164 (10)	0.0087 (11)
O2	0.0504 (12)	0.0696 (14)	0.0584 (13)	-0.0098 (11)	0.0211 (10)	0.0121 (11)
O3	0.0404 (11)	0.0536 (13)	0.0801 (16)	-0.0093 (10)	0.0252 (11)	-0.0142 (11)
O1W	0.0545 (13)	0.0586 (14)	0.0737 (16)	0.0033 (12)	0.0234 (12)	0.0091 (12)
O2W	0.238 (10)	0.224 (9)	0.246 (10)	0.058 (8)	0.051 (8)	-0.025 (8)
N1	0.0279 (10)	0.0525 (14)	0.0506 (14)	0.0078 (10)	0.0160 (10)	0.0148 (11)
C1	0.0425 (14)	0.0416 (14)	0.0440 (15)	0.0119 (12)	0.0157 (12)	0.0043 (11)
C2	0.0546 (18)	0.068 (2)	0.0478 (17)	0.0212 (16)	0.0174 (14)	0.0113 (14)
C3	0.0513 (19)	0.094 (3)	0.067 (2)	0.0285 (19)	0.0103 (17)	0.012 (2)
C4	0.053 (2)	0.083 (3)	0.099 (3)	0.0261 (19)	0.036 (2)	0.009 (2)
C5	0.068 (2)	0.096 (3)	0.063 (2)	0.032 (2)	0.0375 (19)	0.0152 (19)
C6	0.0546 (18)	0.080 (2)	0.0454 (17)	0.0218 (17)	0.0198 (14)	0.0096 (15)
C7	0.0393 (14)	0.0556 (17)	0.0414 (15)	0.0054 (13)	0.0117 (12)	-0.0015 (13)
C8	0.083 (3)	0.058 (2)	0.062 (2)	0.0081 (19)	0.0110 (19)	-0.0077 (17)
C9	0.093 (3)	0.072 (3)	0.081 (3)	-0.003 (2)	0.002 (2)	-0.026 (2)
C10	0.072 (3)	0.115 (4)	0.064 (3)	0.021 (3)	-0.009 (2)	-0.023 (3)
C11	0.070 (3)	0.098 (3)	0.061 (2)	0.020 (2)	-0.0063 (19)	0.005 (2)
C12	0.0559 (19)	0.067 (2)	0.0537 (19)	0.0054 (17)	0.0019 (15)	0.0075 (16)
C13	0.0464 (15)	0.0482 (15)	0.0367 (14)	0.0138 (13)	0.0117 (12)	0.0029 (11)
C14	0.0483 (17)	0.067 (2)	0.0537 (18)	0.0158 (16)	0.0123 (14)	-0.0024 (15)
C15	0.077 (3)	0.074 (2)	0.061 (2)	0.039 (2)	0.0134 (18)	-0.0072 (18)
C16	0.104 (3)	0.0498 (19)	0.060 (2)	0.029 (2)	0.016 (2)	0.0022 (16)
C17	0.090 (3)	0.0454 (18)	0.065 (2)	0.0023 (18)	0.0281 (19)	0.0037 (15)
C18	0.066 (2)	0.0505 (17)	0.0548 (18)	0.0129 (16)	0.0290 (16)	0.0056 (14)
C19	0.0276 (12)	0.0347 (13)	0.0458 (14)	0.0038 (10)	0.0133 (10)	0.0070 (11)
C20	0.0246 (11)	0.0392 (14)	0.0466 (15)	0.0015 (11)	0.0120 (10)	0.0068 (11)
C21	0.0391 (14)	0.0376 (14)	0.070 (2)	0.0051 (12)	0.0261 (14)	0.0026 (13)
C22	0.0526 (17)	0.0343 (14)	0.067 (2)	-0.0023 (13)	0.0239 (15)	-0.0010 (13)
C23	0.0310 (12)	0.0440 (15)	0.0438 (14)	-0.0059 (12)	0.0114 (11)	0.0053 (11)
C24	0.0406 (15)	0.0572 (18)	0.0580 (18)	-0.0154 (14)	0.0160 (13)	0.0039 (14)
C25	0.0246 (11)	0.0429 (14)	0.0366 (13)	0.0038 (11)	0.0093 (10)	0.0099 (10)
N2	0.0546 (19)	0.095 (3)	0.094 (3)	-0.0099 (19)	0.0144 (18)	-0.002 (2)
C26	0.081 (3)	0.092 (3)	0.083 (3)	0.006 (3)	0.020 (2)	-0.009 (2)
C27	0.104 (4)	0.161 (6)	0.116 (4)	-0.044 (4)	0.055 (4)	-0.026 (4)

*Geometric parameters (Å, °)*

Ag1—N1	2.304 (2)	C9—H9	0.93
Ag1—P1	2.3712 (9)	C10—C11	1.355 (6)
Ag1—N2	2.491 (4)	C10—H10	0.93
Ag1—O1W	2.524 (3)	C11—C12	1.396 (5)
S1—O1	1.441 (2)	C11—H11	0.93
S1—O3	1.442 (2)	C12—H12	0.93
S1—O2	1.445 (2)	C13—C18	1.390 (4)
S1—C20	1.779 (3)	C13—C14	1.391 (4)
P1—C1	1.818 (3)	C14—C15	1.391 (5)
P1—C7	1.818 (3)	C14—H14	0.93
P1—C13	1.821 (3)	C15—C16	1.371 (6)

## supplementary materials

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O1W—H1W1	0.854 (10)	C15—H15	0.93
O1W—H1W2	0.853 (10)	C16—C17	1.345 (6)
O2W—O2W <sup>i</sup>	1.762 (17)	C16—H16	0.93
O2W—H2W1	0.881 (9)	C17—C18	1.388 (5)
O2W—H2W2	0.845 (10)	C17—H17	0.93
N1—C25	1.411 (4)	C18—H18	0.93
N1—H1N1	0.885 (10)	C19—C20	1.379 (4)
N1—H1N2	0.896 (10)	C19—C25	1.397 (3)
C1—C2	1.373 (4)	C19—H19	0.93
C1—C6	1.383 (4)	C20—C21	1.379 (4)
C2—C3	1.390 (5)	C21—C22	1.387 (4)
C2—H2	0.93	C21—H21	0.93
C3—C4	1.393 (6)	C22—C23	1.379 (4)
C3—H3	0.9300	C22—H22	0.93
C4—C5	1.353 (6)	C23—C25	1.397 (4)
C4—H4	0.93	C23—C24	1.502 (4)
C5—C6	1.380 (5)	C24—H24A	0.96
C5—H5	0.93	C24—H24B	0.96
C6—H6	0.93	C24—H24C	0.96
C7—C12	1.371 (5)	N2—C26	1.099 (6)
C7—C8	1.382 (5)	C26—C27	1.467 (7)
C8—C9	1.374 (5)	C27—H27A	0.96
C8—H8	0.93	C27—H27B	0.96
C9—C10	1.377 (7)	C27—H27C	0.96
N1—Ag1—P1	150.06 (7)	C9—C10—H10	119.9
N1—Ag1—N2	85.71 (11)	C10—C11—C12	119.6 (4)
P1—Ag1—N2	117.20 (9)	C10—C11—H11	120.2
N1—Ag1—O1W	94.06 (8)	C12—C11—H11	120.2
P1—Ag1—O1W	106.81 (6)	C7—C12—C11	121.0 (4)
N2—Ag1—O1W	83.54 (11)	C7—C12—H12	119.5
O1—S1—O3	113.35 (15)	C11—C12—H12	119.5
O1—S1—O2	112.03 (15)	C18—C13—C14	118.7 (3)
O3—S1—O2	112.98 (15)	C18—C13—P1	122.6 (2)
O1—S1—C20	106.06 (13)	C14—C13—P1	118.7 (2)
O3—S1—C20	106.33 (13)	C13—C14—C15	119.5 (3)
O2—S1—C20	105.33 (13)	C13—C14—H14	120.2
C1—P1—C7	105.53 (13)	C15—C14—H14	120.2
C1—P1—C13	103.30 (13)	C16—C15—C14	120.9 (4)
C7—P1—C13	103.75 (14)	C16—C15—H15	119.6
C1—P1—Ag1	112.36 (9)	C14—C15—H15	119.6
C7—P1—Ag1	110.54 (10)	C17—C16—C15	119.8 (3)
C13—P1—Ag1	120.07 (10)	C17—C16—H16	120.1
Ag1—O1W—H1W1	97 (3)	C15—C16—H16	120.1
Ag1—O1W—H1W2	105 (3)	C16—C17—C18	121.1 (4)
H1W1—O1W—H1W2	109 (2)	C16—C17—H17	119.5
H2W1—O2W—H2W2	109 (3)	C18—C17—H17	119.5
C25—N1—Ag1	117.66 (16)	C17—C18—C13	120.1 (3)
C25—N1—H1N1	114 (2)	C17—C18—H18	120.0



Ag1—N1—H1N1	103 (2)	C13—C18—H18	120.0
C25—N1—H1N2	116 (2)	C20—C19—C25	120.0 (2)
Ag1—N1—H1N2	98 (2)	C20—C19—H19	120.0
H1N1—N1—H1N2	105 (2)	C25—C19—H19	120.0
C2—C1—C6	119.2 (3)	C19—C20—C21	121.1 (2)
C2—C1—P1	117.8 (2)	C19—C20—S1	120.8 (2)
C6—C1—P1	123.0 (2)	C21—C20—S1	118.0 (2)
C1—C2—C3	120.7 (3)	C20—C21—C22	118.3 (3)
C1—C2—H2	119.6	C20—C21—H21	120.8
C3—C2—H2	119.6	C22—C21—H21	120.8
C2—C3—C4	119.0 (3)	C23—C22—C21	122.1 (3)
C2—C3—H3	120.5	C23—C22—H22	118.9
C4—C3—H3	120.5	C21—C22—H22	118.9
C5—C4—C3	120.2 (3)	C22—C23—C25	118.8 (2)
C5—C4—H4	119.9	C22—C23—C24	121.0 (3)
C3—C4—H4	119.9	C25—C23—C24	120.1 (3)
C4—C5—C6	120.6 (3)	C23—C24—H24A	109.5
C4—C5—H5	119.7	C23—C24—H24B	109.5
C6—C5—H5	119.7	H24A—C24—H24B	109.5
C5—C6—C1	120.3 (3)	C23—C24—H24C	109.5
C5—C6—H6	119.9	H24A—C24—H24C	109.5
C1—C6—H6	119.9	H24B—C24—H24C	109.5
C12—C7—C8	118.2 (3)	C19—C25—C23	119.5 (2)
C12—C7—P1	123.8 (2)	C19—C25—N1	120.1 (2)
C8—C7—P1	117.9 (3)	C23—C25—N1	120.2 (2)
C9—C8—C7	121.0 (4)	C26—N2—Ag1	158.9 (4)
C9—C8—H8	119.5	N2—C26—C27	177.2 (6)
C7—C8—H8	119.5	C26—C27—H27A	109.5
C8—C9—C10	119.9 (4)	C26—C27—H27B	109.5
C8—C9—H9	120.1	H27A—C27—H27B	109.5
C10—C9—H9	120.1	C26—C27—H27C	109.5
C11—C10—C9	120.3 (4)	H27A—C27—H27C	109.5
C11—C10—H10	119.9	H27B—C27—H27C	109.5

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

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W1 $\cdots$ O2 <sup>ii</sup>	0.854 (10)	1.952 (13)	2.797 (3)	170 (4)
O1W—H1W2 $\cdots$ O3 <sup>iii</sup>	0.853 (10)	2.091 (12)	2.940 (4)	174 (5)
N1—H1N2 $\cdots$ O1 <sup>iii</sup>	0.896 (10)	2.19 (2)	2.965 (3)	144 (3)
N1—H1N1 $\cdots$ O3 <sup>ii</sup>	0.885 (10)	2.171 (14)	3.032 (4)	164 (3)

Symmetry codes: (ii)  $-x+1, -y+1, -z+2$ ; (iii)  $x+1, y, z$ .

