Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[bis(triphenylphosphine)-silver(I)]-μ-6-aminonaphthalene-1-sulfonato-κ^2O:N] monohydrate]

Hua Wu,[a,b] Ying-Ying Liu[a]* and Hong-Ye Bai[a]

[a]Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China, and [b]School of Heilongjiang Agricultural College of Vocational Technology, Jiamusi 154007, People's Republic of China
Correspondence e-mail: liuyy21@yahoo.com.cn

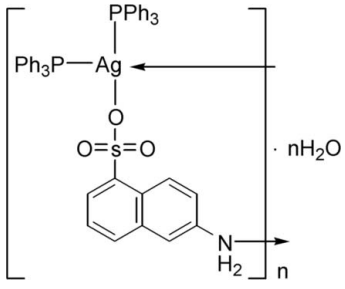
Received 25 October 2007; accepted 8 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.040; wR factor = 0.108; data-to-parameter ratio = 16.5.

In the title compound, $\{[Ag(C_{10}H_8NO_3S)(C_{18}H_{15}P)_2]\cdot H_2O\}_n$, each Ag^I cation is four coordinated by two P atoms from two different triphenylphosphine ligands, and by one N atom and one sulfonate O atom from different 6-aminonaphthalene-1-sulfonate anions in a distorted tetrahedral geometry. Each 6-aminonaphthalene-1-sulfonate ligand bridges two Ag^I centers, resulting in the formation of polymeric chains parallel to the a axis. Intermolecular O—H···O and N—H···O hydrogen bonds contribute to the crystal packing stability. One phenyl ring is disordered over two positions; the site occupancies are 0.68 and 0.32.

Related literature

For related literature, see: Wang *et al.* (2007).



Experimental

Crystal data

$[Ag(C_{10}H_8NO_3S)(C_{18}H_{15}P)_2]\cdot H_2O$
M_r = 872.66
Triclinic, $P\overline{1}$
a = 10.017 (2) Å
b = 13.696 (3) Å
c = 16.792 (3) Å
α = 69.84 (3)°
β = 81.37 (3)°
γ = 69.09 (3)°
V = 2019.1 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 293 (2) K
0.29 × 0.24 × 0.19 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.823, T_{max} = 0.886
9249 measured reflections
8991 independent reflections
5525 reflections with $I > 2\sigma(I)$
R_{int} = 0.006

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.108
S = 0.91
8991 reflections
545 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—P1	2.4598 (13)	Ag1—O1	2.478 (3)
Ag1—N1^{i}	2.460 (3)	Ag1—P2	2.4837 (14)
P1—Ag1—N1^{i}	117.56 (9)	P1—Ag1—P2	123.55 (5)
P1—Ag1—O1	105.72 (7)	N1^{i}—Ag1—P2	103.02 (9)
N1^{i}—Ag1—O1	90.32 (10)	O1—Ag1—P2	111.83 (8)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1C···O2	0.92 (6)	1.88 (3)	2.789 (5)	166 (8)
N1—H1B···O2^{ii}	0.87 (4)	2.31 (2)	3.140 (4)	162 (4)
N1—H1A···O3^{iii}	0.85 (4)	2.17 (2)	2.975 (4)	159 (4)

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

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 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*.

We thank the Science Foundation for Young Teachers of Northeast Normal University (grant No. 20070314) for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2332).

References

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku Corporation (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-Ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, X.-Y., Ma, C.-H., Gao, Q.-Q., Lu, S.-Q. & Dong, X.-W. (2007). *Acta Cryst.* E**63**, m2361.

supplementary materials

Acta Cryst. (2007). E**63**, m3027 [**doi:10.1107/S1600536807057121**]

catena-Poly[[[bis(triphenylphosphine)silver(I)]-μ-6-aminonaphthalene-1-sulfonato-κ^2O:N] monohydrate]

H. Wu, Y.-Y. Liu and H.-Y. Bai

Comment

In the title compound, (I), each Ag^I cation is four-coordinated by two P atoms from two triphenylphosphine ligands, one N atom and one O atom from the different 6-aminonaphthalene-1-sulfonate anions (Fig. 1). The Ag—O (sulfonate) distance in (I) is similar to the equivalent value in a related compound (Wang *et al.*, 2007).

There are two intermolecular N—H···O hydrogen bonds involving the amino N atom and two sulfonate O atoms among the adjacent 6-aminonaphthalene-1-sulfonate anions (Table 1), and the whole structure displays a double chain supramolecular framework, The lattice water molecule connects the units *via* hydrogen bond (Fig. 2).

Experimental

An aqueous solution (10 ml) of 6-aminonaphthalene-1-sulfonic acid (0.1115 g, 0.5 mmol) was added to solid Ag_2CO_3 (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO_2 was given off; triphenylphosphine (0.113 g, 0.5 mmol) in acetonitrile (10 ml) was then added and a white precipitate formed. The precipitate was dissolved by dropwise addition of an aqueous solution of NH_3 (14 *M*). Colourless blocks of (I) were obtained by evaporation of the solution for several days at room temperature.

Refinement

C-bound H-atoms were geometrically positioned (C—H 0.93 Å) and refined using a riding model, with $U_{iso} = 1.2U_{eq}$ (C). The H atoms of the amino group and water molecule were located in a difference map and refined freely, with U_{iso}(H) = $1.2U_{eq}$ (N, O). One phenyl ring in triphenylphosphine ligand was treated as disordered between two orientations with the refined occupancies of 0.677 (15) and 0.323 (15), respectively.

Figures

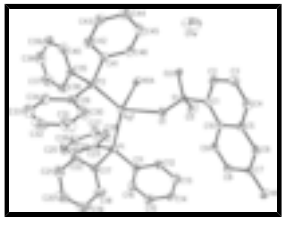


Fig. 1. A portion of the polymeric chain in (I), showing the 30% probability displacement ellipsoids, crystalline water molecule and the atomic numbering [symmetry code: (A) −1 + *x*, *y*, *z*]. H atoms have been omitted for clarity.

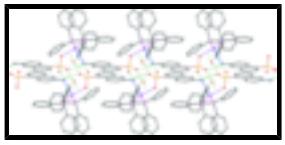


Fig. 2. The double-chain framework of (I), formed through hydrogen-bonding (dashed lines) interactions. The atoms of H not involved in hydrogen bonding interactions have been omitted.

catena-Poly[[[bis(triphenylphosphine)silver(I)]-μ-6- aminonaphthalene-1-sulfonato-κ^2*O*:*N*] monohydrate]

Crystal data

$[Ag(C_{10}H_8NO_3S)(C_{18}H_{15}P)_2]\cdot H_2O$	$Z = 2$
$M_r = 872.66$	$F_{000} = 896$
Triclinic, $P\overline{1}$	$D_x = 1.435$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.017$ (2) Å	Cell parameters from Total reflections
$b = 13.696$ (3) Å	$\theta = 1.3$–27.5º
$c = 16.792$ (3) Å	$\mu = 0.68$ mm^{-1}
$\alpha = 69.84$ (3)º	$T = 293$ (2) K
$\beta = 81.37$ (3)º	Block, colourless
$\gamma = 69.09$ (3)º	0.29 × 0.24 × 0.19 mm
$V = 2019.1$ (9) Å^3	

Data collection

Rigaku RAXIS-RAPID diffractometer	8991 independent reflections
Radiation source: fine-focus sealed tube	5525 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.006$
$T = 293$(2) K	$\theta_{max} = 27.5$º
ω scan	$\theta_{min} = 1.3$º
Absorption correction: multi-scan Abscor (Higashi, 1995)	$h = -13\rightarrow12$
$T_{min} = 0.823$, $T_{max} = 0.886$	$k = -16\rightarrow17$
9249 measured reflections	$l = -21\rightarrow21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.91$	$(\Delta/\sigma)_{max} = 0.001$
8991 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
545 parameters	$\Delta\rho_{min} = -0.71$ e Å^{-3}

5 restraints
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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ag1	0.45345 (3)	0.40427 (2)	0.73248 (2)	0.03644 (10)	
C1	0.7118 (4)	0.6796 (3)	0.6260 (2)	0.0296 (8)	
C2	0.6465 (4)	0.7797 (3)	0.6386 (3)	0.0381 (9)	
H2	0.5473	0.8091	0.6397	0.046*	
C3	0.7281 (4)	0.8386 (3)	0.6499 (3)	0.0472 (11)	
H3	0.6827	0.9063	0.6589	0.057*	
C4	0.8730 (4)	0.7966 (3)	0.6478 (3)	0.0422 (10)	
H4	0.9260	0.8356	0.6562	0.051*	
C5	0.9447 (4)	0.6948 (3)	0.6331 (2)	0.0296 (8)	
C6	1.0960 (4)	0.6543 (3)	0.6255 (2)	0.0341 (9)	
H6	1.1486	0.6959	0.6300	0.041*	
C7	1.1658 (4)	0.5561 (3)	0.6120 (2)	0.0297 (8)	
C8	1.0864 (4)	0.4922 (3)	0.6060 (2)	0.0337 (9)	
H8	1.1338	0.4237	0.5986	0.040*	
C9	0.9410 (4)	0.5301 (3)	0.6111 (2)	0.0327 (9)	
H9	0.8907	0.4870	0.6064	0.039*	
C10	0.8642 (4)	0.6328 (3)	0.6234 (2)	0.0265 (8)	
C11	0.7677 (4)	0.1897 (3)	0.6750 (2)	0.0340 (9)	
C12	0.8273 (4)	0.2726 (3)	0.6382 (3)	0.0435 (10)	
H12	0.7834	0.3407	0.6467	0.052*	
C13	0.9527 (5)	0.2544 (3)	0.5885 (3)	0.0504 (11)	
H13	0.9924	0.3103	0.5641	0.060*	
C14	1.0176 (4)	0.1542 (3)	0.5755 (3)	0.0479 (11)	
H14	1.1011	0.1422	0.5421	0.057*	
C15	0.9590 (5)	0.0715 (4)	0.6118 (3)	0.0571 (12)	
H15	1.0031	0.0035	0.6031	0.069*	
C16	0.8354 (5)	0.0891 (3)	0.6611 (3)	0.0519 (12)	
H16	0.7967	0.0326	0.6854	0.062*	
C23	0.5068 (4)	0.1420 (3)	0.7161 (3)	0.0358 (9)	
C24	0.4707 (5)	0.0553 (4)	0.7733 (3)	0.0553 (12)	

H24	0.5002	0.0290	0.8289	0.066*
C25	0.3910 (5)	0.0066 (4)	0.7495 (3)	0.0632 (14)
H25	0.3660	−0.0513	0.7894	0.076*
C26	0.3486 (5)	0.0425 (4)	0.6680 (4)	0.0645 (15)
H26	0.2956	0.0090	0.6521	0.077*
C27	0.3849 (6)	0.1289 (5)	0.6093 (4)	0.084 (2)
H27	0.3582	0.1531	0.5532	0.101*
C28	0.4616 (6)	0.1793 (4)	0.6344 (3)	0.0667 (16)
H28	0.4828	0.2394	0.5952	0.080*
C29	0.3320 (4)	0.3793 (3)	0.9567 (3)	0.0381 (9)
C30	0.4519 (5)	0.3871 (4)	0.9811 (3)	0.0657 (15)
H30	0.5061	0.4246	0.9408	0.079*
C31	0.4929 (7)	0.3404 (5)	1.0643 (4)	0.0811 (18)
H31	0.5739	0.3470	1.0797	0.097*
C32	0.4151 (7)	0.2843 (4)	1.1243 (3)	0.0765 (17)
H32	0.4425	0.2532	1.1805	0.092*
C33	0.2989 (6)	0.2744 (4)	1.1015 (3)	0.0733 (16)
H33	0.2461	0.2358	1.1420	0.088*
C34	0.2573 (5)	0.3214 (4)	1.0178 (3)	0.0562 (12)
H34	0.1769	0.3134	1.0029	0.067*
C35	0.1219 (4)	0.4181 (3)	0.8402 (2)	0.0354 (9)
C36	0.1444 (5)	0.3180 (3)	0.8278 (3)	0.0544 (12)
H36	0.2374	0.2718	0.8235	0.065*
C37	0.0321 (6)	0.2860 (4)	0.8221 (4)	0.0694 (16)
H37	0.0493	0.2184	0.8145	0.083*
C38	−0.1054 (6)	0.3539 (4)	0.8275 (3)	0.0653 (14)
H38	−0.1816	0.3319	0.8242	0.078*
C39	−0.1309 (5)	0.4541 (4)	0.8378 (3)	0.0601 (13)
H39	−0.2243	0.5005	0.8407	0.072*
C40	−0.0173 (4)	0.4862 (3)	0.8440 (3)	0.0459 (10)
H40	−0.0351	0.5544	0.8507	0.055*
C41	0.2170 (4)	0.5942 (3)	0.8473 (2)	0.0347 (9)
C42	0.1378 (5)	0.6255 (3)	0.9147 (3)	0.0503 (11)
H42	0.1126	0.5737	0.9612	0.060*
C43	0.0961 (5)	0.7344 (4)	0.9127 (4)	0.0666 (14)
H43	0.0438	0.7554	0.9581	0.080*
C44	0.1319 (5)	0.8109 (4)	0.8436 (4)	0.0623 (14)
H44	0.1016	0.8842	0.8418	0.075*
C45	0.2114 (5)	0.7804 (3)	0.7776 (3)	0.0545 (12)
H45	0.2355	0.8330	0.7312	0.065*
C46	0.2569 (4)	0.6714 (3)	0.7790 (2)	0.0387 (9)
H46	0.3135	0.6505	0.7346	0.046*
N1	1.3174 (3)	0.5159 (3)	0.6027 (2)	0.0364 (8)
H1A	1.346 (4)	0.478 (3)	0.569 (2)	0.055*
H1B	1.354 (4)	0.568 (3)	0.590 (3)	0.055*
O1	0.6144 (3)	0.5166 (2)	0.68881 (18)	0.0472 (8)
O2	0.4561 (3)	0.6885 (2)	0.60277 (19)	0.0459 (7)
O3	0.6540 (3)	0.5791 (2)	0.53629 (19)	0.0511 (8)
P1	0.60724 (10)	0.21524 (7)	0.74155 (7)	0.0341 (2)

P2	0.27970 (10)	0.45162 (8)	0.84655 (6)	0.0332 (2)	
S1	0.60112 (9)	0.61009 (7)	0.61170 (6)	0.0319 (2)	
O1W	0.2596 (5)	0.9004 (4)	0.5468 (4)	0.1303 (19)	
H1C	0.331 (6)	0.833 (3)	0.556 (6)	0.156*	
H1D	0.317 (8)	0.946 (6)	0.525 (6)	0.156*	
C17	0.6689 (4)	0.1318 (3)	0.8487 (3)	0.0400 (10)	
C18	0.8114 (8)	0.0679 (8)	0.8659 (5)	0.060 (3)	0.677 (15)
H18	0.8801	0.0646	0.8221	0.072*	0.677 (15)
C19	0.8487 (10)	0.0088 (10)	0.9501 (6)	0.081 (4)	0.677 (15)
H19	0.9434	−0.0345	0.9621	0.097*	0.677 (15)
C20	0.7492 (7)	0.0132 (5)	1.0154 (3)	0.0781 (17)	
H20	0.7749	−0.0300	1.0708	0.094*	
C21	0.6107 (12)	0.0823 (9)	0.9983 (7)	0.068 (3)	0.677 (15)
H21	0.5432	0.0895	1.0423	0.081*	0.677 (15)
C22	0.5737 (10)	0.1405 (8)	0.9153 (6)	0.052 (2)	0.677 (15)
H22	0.4803	0.1875	0.9041	0.062*	0.677 (15)
C18'	0.733 (3)	0.0155 (15)	0.8742 (13)	0.085 (9)	0.323 (15)
H18'	0.7458	−0.0213	0.8349	0.102*	0.323 (15)
C19'	0.778 (3)	−0.0452 (15)	0.9574 (12)	0.084 (8)	0.323 (15)
H19'	0.8249	−0.1209	0.9734	0.100*	0.323 (15)
C21'	0.677 (3)	0.112 (2)	0.9961 (14)	0.080 (8)	0.323 (15)
H21'	0.6507	0.1467	1.0377	0.095*	0.323 (15)
C22'	0.634 (3)	0.1745 (16)	0.9095 (13)	0.066 (6)	0.323 (15)
H22'	0.5793	0.2485	0.8973	0.079*	0.323 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03352 (17)	0.03216 (16)	0.03996 (19)	−0.00835 (11)	0.00517 (13)	−0.01209 (13)
C1	0.032 (2)	0.033 (2)	0.027 (2)	−0.0151 (15)	0.0019 (16)	−0.0101 (16)
C2	0.032 (2)	0.038 (2)	0.048 (3)	−0.0095 (16)	0.0017 (18)	−0.0198 (19)
C3	0.047 (3)	0.037 (2)	0.069 (3)	−0.0148 (18)	0.006 (2)	−0.031 (2)
C4	0.045 (2)	0.038 (2)	0.057 (3)	−0.0201 (18)	0.000 (2)	−0.025 (2)
C5	0.033 (2)	0.0323 (19)	0.028 (2)	−0.0161 (15)	−0.0009 (16)	−0.0087 (16)
C6	0.037 (2)	0.039 (2)	0.035 (2)	−0.0211 (16)	−0.0038 (17)	−0.0110 (17)
C7	0.0278 (19)	0.038 (2)	0.0248 (19)	−0.0142 (15)	−0.0039 (16)	−0.0071 (16)
C8	0.032 (2)	0.034 (2)	0.041 (2)	−0.0133 (15)	−0.0031 (17)	−0.0157 (17)
C9	0.033 (2)	0.030 (2)	0.042 (2)	−0.0174 (16)	−0.0005 (17)	−0.0134 (17)
C10	0.0290 (19)	0.0295 (18)	0.0235 (19)	−0.0138 (14)	0.0000 (15)	−0.0074 (15)
C11	0.032 (2)	0.031 (2)	0.039 (2)	−0.0097 (15)	0.0002 (17)	−0.0126 (17)
C12	0.048 (3)	0.032 (2)	0.052 (3)	−0.0156 (18)	0.007 (2)	−0.0160 (19)
C13	0.052 (3)	0.047 (3)	0.053 (3)	−0.026 (2)	0.011 (2)	−0.013 (2)
C14	0.034 (2)	0.054 (3)	0.045 (3)	−0.0109 (19)	0.004 (2)	−0.010 (2)
C15	0.048 (3)	0.049 (3)	0.076 (4)	−0.012 (2)	0.016 (2)	−0.033 (2)
C16	0.049 (3)	0.039 (2)	0.073 (3)	−0.0196 (19)	0.022 (2)	−0.028 (2)
C23	0.033 (2)	0.030 (2)	0.041 (2)	−0.0095 (15)	0.0016 (18)	−0.0087 (17)
C24	0.075 (3)	0.052 (3)	0.044 (3)	−0.034 (2)	−0.005 (2)	−0.006 (2)
C25	0.079 (4)	0.050 (3)	0.065 (3)	−0.040 (3)	−0.006 (3)	−0.003 (2)

C26	0.059 (3)	0.052 (3)	0.088 (4)	−0.028 (2)	−0.021 (3)	−0.010 (3)
C27	0.101 (5)	0.095 (4)	0.066 (4)	−0.058 (4)	−0.039 (3)	0.005 (3)
C28	0.085 (4)	0.065 (3)	0.055 (3)	−0.050 (3)	−0.024 (3)	0.009 (3)
C29	0.037 (2)	0.036 (2)	0.038 (2)	−0.0059 (17)	0.0013 (18)	−0.0143 (18)
C30	0.066 (3)	0.064 (3)	0.066 (3)	−0.030 (3)	−0.024 (3)	−0.001 (3)
C31	0.086 (4)	0.082 (4)	0.077 (4)	−0.024 (3)	−0.044 (4)	−0.014 (3)
C32	0.098 (5)	0.065 (4)	0.043 (3)	0.002 (3)	−0.026 (3)	−0.009 (3)
C33	0.074 (4)	0.077 (4)	0.043 (3)	−0.012 (3)	0.004 (3)	−0.003 (3)
C34	0.041 (3)	0.071 (3)	0.046 (3)	−0.017 (2)	0.003 (2)	−0.007 (2)
C35	0.036 (2)	0.038 (2)	0.032 (2)	−0.0130 (17)	−0.0010 (17)	−0.0092 (17)
C36	0.050 (3)	0.044 (3)	0.072 (3)	−0.013 (2)	−0.009 (2)	−0.021 (2)
C37	0.077 (4)	0.054 (3)	0.090 (4)	−0.032 (3)	−0.022 (3)	−0.020 (3)
C38	0.061 (3)	0.079 (4)	0.068 (4)	−0.043 (3)	−0.013 (3)	−0.012 (3)
C39	0.040 (3)	0.078 (3)	0.065 (3)	−0.020 (2)	−0.002 (2)	−0.025 (3)
C40	0.039 (2)	0.053 (3)	0.048 (3)	−0.019 (2)	0.004 (2)	−0.018 (2)
C41	0.030 (2)	0.040 (2)	0.037 (2)	−0.0123 (16)	0.0011 (17)	−0.0151 (18)
C42	0.055 (3)	0.047 (3)	0.052 (3)	−0.021 (2)	0.021 (2)	−0.024 (2)
C43	0.063 (3)	0.065 (3)	0.088 (4)	−0.027 (3)	0.031 (3)	−0.052 (3)
C44	0.057 (3)	0.042 (3)	0.091 (4)	−0.013 (2)	0.004 (3)	−0.032 (3)
C45	0.067 (3)	0.042 (3)	0.054 (3)	−0.025 (2)	−0.010 (3)	−0.003 (2)
C46	0.043 (2)	0.043 (2)	0.032 (2)	−0.0177 (18)	−0.0018 (18)	−0.0117 (18)
N1	0.0252 (17)	0.047 (2)	0.043 (2)	−0.0135 (14)	−0.0022 (15)	−0.0201 (16)
O1	0.0428 (16)	0.0426 (16)	0.0540 (19)	−0.0251 (13)	−0.0090 (14)	0.0022 (14)
O2	0.0262 (14)	0.0445 (16)	0.067 (2)	−0.0110 (12)	−0.0036 (14)	−0.0175 (14)
O3	0.0448 (17)	0.077 (2)	0.0529 (19)	−0.0266 (15)	0.0033 (14)	−0.0416 (16)
P1	0.0335 (5)	0.0277 (5)	0.0383 (6)	−0.0081 (4)	0.0033 (4)	−0.0109 (4)
P2	0.0310 (5)	0.0357 (5)	0.0333 (6)	−0.0111 (4)	0.0036 (4)	−0.0134 (4)
S1	0.0256 (5)	0.0350 (5)	0.0390 (6)	−0.0137 (4)	−0.0006 (4)	−0.0127 (4)
O1W	0.120 (4)	0.109 (4)	0.123 (5)	0.026 (3)	−0.021 (4)	−0.048 (4)
C17	0.047 (3)	0.030 (2)	0.040 (2)	−0.0078 (17)	−0.001 (2)	−0.0128 (18)
C18	0.043 (4)	0.072 (6)	0.050 (5)	−0.002 (4)	−0.006 (3)	−0.016 (4)
C19	0.064 (6)	0.085 (8)	0.060 (6)	0.011 (5)	−0.023 (5)	−0.011 (5)
C20	0.093 (5)	0.071 (4)	0.043 (3)	0.001 (3)	−0.016 (3)	−0.010 (3)
C21	0.068 (7)	0.071 (6)	0.046 (5)	−0.009 (5)	0.000 (5)	−0.012 (4)
C22	0.049 (5)	0.047 (5)	0.046 (5)	−0.006 (4)	0.008 (4)	−0.012 (4)
C17'	0.047 (3)	0.030 (2)	0.040 (2)	−0.0078 (17)	−0.001 (2)	−0.0128 (18)
C18'	0.12 (2)	0.052 (11)	0.075 (13)	0.003 (11)	−0.019 (12)	−0.032 (10)
C19'	0.116 (19)	0.041 (11)	0.061 (12)	0.001 (10)	−0.030 (12)	0.007 (9)
C20'	0.093 (5)	0.071 (4)	0.043 (3)	0.001 (3)	−0.016 (3)	−0.010 (3)
C21'	0.087 (19)	0.098 (18)	0.035 (10)	0.010 (13)	−0.017 (12)	−0.034 (11)
C22'	0.069 (15)	0.039 (11)	0.054 (11)	0.018 (9)	−0.008 (10)	−0.007 (9)

Geometric parameters (Å, °)

Ag1—P1	2.4598 (13)	C33—H33	0.9300
Ag1—N1^{i}	2.460 (3)	C34—H34	0.9300
Ag1—O1	2.478 (3)	C35—C40	1.380 (5)
Ag1—P2	2.4837 (14)	C35—C36	1.391 (5)
C1—C2	1.368 (5)	C35—P2	1.823 (4)

C1—C10	1.430 (5)	C36—C37	1.371 (6)
C1—S1	1.785 (3)	C36—H36	0.9300
C2—C3	1.406 (5)	C37—C38	1.370 (7)
C2—H2	0.9300	C37—H37	0.9300
C3—C4	1.357 (5)	C38—C39	1.371 (7)
C3—H3	0.9300	C38—H38	0.9300
C4—C5	1.411 (5)	C39—C40	1.387 (6)
C4—H4	0.9300	C39—H39	0.9300
C5—C6	1.418 (5)	C40—H40	0.9300
C5—C10	1.421 (5)	C41—C42	1.385 (6)
C6—C7	1.357 (5)	C41—C46	1.385 (5)
C6—H6	0.9300	C41—P2	1.829 (4)
C7—C8	1.410 (5)	C42—C43	1.387 (6)
C7—N1	1.423 (5)	C42—H42	0.9300
C8—C9	1.361 (5)	C43—C44	1.370 (7)
C8—H8	0.9300	C43—H43	0.9300
C9—C10	1.412 (5)	C44—C45	1.362 (7)
C9—H9	0.9300	C44—H44	0.9300
C11—C12	1.384 (5)	C45—C46	1.389 (6)
C11—C16	1.386 (5)	C45—H45	0.9300
C11—P1	1.812 (4)	C46—H46	0.9300
C12—C13	1.394 (6)	N1—Ag1^{ii}	2.460 (3)
C12—H12	0.9300	N1—H1A	0.85 (4)
C13—C14	1.371 (6)	N1—H1B	0.87 (4)
C13—H13	0.9300	O1—S1	1.457 (3)
C14—C15	1.375 (6)	O2—S1	1.458 (3)
C14—H14	0.9300	O3—S1	1.440 (3)
C15—C16	1.375 (6)	P1—C17	1.827 (4)
C15—H15	0.9300	O1W—H1C	0.92 (6)
C16—H16	0.9300	O1W—H1D	0.94 (9)
C23—C24	1.370 (5)	C17—C22	1.365 (10)
C23—C28	1.375 (6)	C17—C22'	1.29 (3)
C23—P1	1.829 (4)	C17—C18	1.395 (8)
C24—C25	1.380 (6)	C17—C18'	1.42 (3)
C24—H24	0.9300	C18—C19	1.396 (11)
C25—C26	1.362 (7)	C18—H18	0.9300
C25—H25	0.9300	C19—C20	1.370 (11)
C26—C27	1.378 (7)	C19'—C20	1.40 (3)
C26—H26	0.9300	C19—H19	0.9300
C27—C28	1.386 (6)	C20—C21	1.377 (13)
C27—H27	0.9300	C20—C21'	1.24 (3)
C28—H28	0.9300	C20—H20	0.9300
C29—C34	1.369 (6)	C21—C22	1.377 (14)
C29—C30	1.375 (6)	C21—H21	0.9300
C29—P2	1.826 (4)	C22—H22	0.9300
C30—C31	1.378 (7)	C18'—C19'	1.40 (2)
C30—H30	0.9300	C18'—H18'	0.9300
C31—C32	1.368 (8)	C19'—H19'	0.9300
C31—H31	0.9300	C21'—C22'	1.45 (3)

C32—C33	1.343 (7)	C21'—H21'	0.9300
C32—H32	0.9300	C22'—H22'	0.9300
C33—C34	1.387 (7)		
P1—Ag1—N1^{i}	117.56 (9)	C29—C34—C33	121.4 (5)
P1—Ag1—O1	105.72 (7)	C29—C34—H34	119.3
N1^{i}—Ag1—O1	90.32 (10)	C33—C34—H34	119.3
P1—Ag1—P2	123.55 (5)	C40—C35—C36	118.0 (4)
N1^{i}—Ag1—P2	103.02 (9)	C40—C35—P2	124.7 (3)
O1—Ag1—P2	111.83 (8)	C36—C35—P2	117.3 (3)
C2—C1—C10	120.9 (3)	C37—C36—C35	121.3 (4)
C2—C1—S1	118.0 (3)	C37—C36—H36	119.3
C10—C1—S1	121.1 (3)	C35—C36—H36	119.3
C1—C2—C3	120.6 (3)	C38—C37—C36	119.8 (5)
C1—C2—H2	119.7	C38—C37—H37	120.1
C3—C2—H2	119.7	C36—C37—H37	120.1
C4—C3—C2	120.0 (4)	C37—C38—C39	120.2 (4)
C4—C3—H3	120.0	C37—C38—H38	119.9
C2—C3—H3	120.0	C39—C38—H38	119.9
C3—C4—C5	121.2 (3)	C38—C39—C40	120.0 (5)
C3—C4—H4	119.4	C38—C39—H39	120.0
C5—C4—H4	119.4	C40—C39—H39	120.0
C4—C5—C6	121.1 (3)	C35—C40—C39	120.7 (4)
C4—C5—C10	119.6 (3)	C35—C40—H40	119.7
C6—C5—C10	119.2 (3)	C39—C40—H40	119.7
C7—C6—C5	121.5 (3)	C42—C41—C46	119.7 (4)
C7—C6—H6	119.3	C42—C41—P2	122.3 (3)
C5—C6—H6	119.3	C46—C41—P2	117.8 (3)
C6—C7—C8	119.4 (3)	C41—C42—C43	119.8 (4)
C6—C7—N1	121.8 (3)	C41—C42—H42	120.1
C8—C7—N1	118.8 (3)	C43—C42—H42	120.1
C9—C8—C7	120.4 (3)	C44—C43—C42	120.0 (5)
C9—C8—H8	119.8	C44—C43—H43	120.0
C7—C8—H8	119.8	C42—C43—H43	120.0
C8—C9—C10	122.0 (3)	C45—C44—C43	120.5 (4)
C8—C9—H9	119.0	C45—C44—H44	119.8
C10—C9—H9	119.0	C43—C44—H44	119.8
C9—C10—C5	117.4 (3)	C44—C45—C46	120.6 (4)
C9—C10—C1	125.0 (3)	C44—C45—H45	119.7
C5—C10—C1	117.6 (3)	C46—C45—H45	119.7
C12—C11—C16	118.5 (4)	C41—C46—C45	119.3 (4)
C12—C11—P1	119.0 (3)	C41—C46—H46	120.3
C16—C11—P1	122.4 (3)	C45—C46—H46	120.3
C11—C12—C13	120.3 (4)	C7—N1—Ag1^{ii}	117.3 (2)
C11—C12—H12	119.8	C7—N1—H1A	113 (3)
C13—C12—H12	119.8	Ag1^{ii}—N1—H1A	106 (3)
C14—C13—C12	120.1 (4)	C7—N1—H1B	112 (3)
C14—C13—H13	119.9	Ag1^{ii}—N1—H1B	95 (3)

C12—C13—H13	119.9	H1A—N1—H1B	113 (4)
C13—C14—C15	119.8 (4)	S1—O1—Ag1	124.79 (15)
C13—C14—H14	120.1	C11—P1—C17	103.95 (18)
C15—C14—H14	120.1	C11—P1—C23	102.81 (18)
C14—C15—C16	120.2 (4)	C17—P1—C23	104.17 (18)
C14—C15—H15	119.9	C11—P1—Ag1	120.93 (12)
C16—C15—H15	119.9	C17—P1—Ag1	112.91 (14)
C15—C16—C11	121.0 (4)	C23—P1—Ag1	110.40 (12)
C15—C16—H16	119.5	C35—P2—C29	103.94 (18)
C11—C16—H16	119.5	C35—P2—C41	106.95 (17)
C24—C23—C28	118.3 (4)	C29—P2—C41	100.11 (18)
C24—C23—P1	124.6 (3)	C35—P2—Ag1	108.18 (14)
C28—C23—P1	117.1 (3)	C29—P2—Ag1	118.33 (13)
C23—C24—C25	120.9 (4)	C41—P2—Ag1	117.98 (13)
C23—C24—H24	119.5	O3—S1—O1	113.63 (18)
C25—C24—H24	119.5	O3—S1—O2	112.24 (18)
C26—C25—C24	120.6 (4)	O1—S1—O2	111.77 (17)
C26—C25—H25	119.7	O3—S1—C1	106.98 (17)
C24—C25—H25	119.7	O1—S1—C1	105.24 (16)
C25—C26—C27	119.5 (4)	O2—S1—C1	106.32 (16)
C25—C26—H26	120.3	H1C—O1W—H1D	99 (4)
C27—C26—H26	120.3	C22—C17—C18	118.6 (6)
C26—C27—C28	119.5 (5)	C22—C17—P1	118.3 (5)
C26—C27—H27	120.2	C18—C17—P1	122.8 (4)
C28—C27—H27	120.2	C17—C18—C19	118.6 (7)
C23—C28—C27	121.1 (4)	C17—C18—H18	120.7
C23—C28—H28	119.4	C19—C18—H18	120.7
C27—C28—H28	119.4	C20—C19—C18	121.5 (7)
C34—C29—C30	117.4 (4)	C20—C19—H19	119.2
C34—C29—P2	124.8 (3)	C18—C19—H19	119.2
C30—C29—P2	117.8 (3)	C19—C20—C21	119.4 (7)
C29—C30—C31	121.1 (5)	C19—C20—H20	120.3
C29—C30—H30	119.5	C21—C20—H20	120.3
C31—C30—H30	119.5	C22—C21—C20	119.1 (9)
C32—C31—C30	120.3 (5)	C22—C21—H21	120.5
C32—C31—H31	119.9	C20—C21—H21	120.5
C30—C31—H31	119.9	C17—C22—C21	122.5 (8)
C33—C32—C31	119.6 (5)	C17—C22—H22	118.7
C33—C32—H32	120.2	C21—C22—H22	118.7
C31—C32—H32	120.2	C19'—C18'—H18'	119.3
C32—C33—C34	120.2 (5)	C18'—C19'—H19'	121.5
C32—C33—H33	119.9	C22'—C21'—H21'	119.6
C34—C33—H33	119.9	C21'—C22'—H22'	118.6
C10—C1—C2—C3	−0.5 (6)	C12—C11—P1—C23	143.0 (3)
S1—C1—C2—C3	−179.8 (3)	C16—C11—P1—C23	−38.6 (4)
C1—C2—C3—C4	0.5 (7)	C12—C11—P1—Ag1	19.4 (4)
C2—C3—C4—C5	1.0 (7)	C16—C11—P1—Ag1	−162.2 (3)
C3—C4—C5—C6	176.0 (4)	C24—C23—P1—C11	117.8 (4)
C3—C4—C5—C10	−2.3 (6)	C28—C23—P1—C11	−64.2 (4)

C4—C5—C6—C7	179.5 (4)	C24—C23—P1—C17	9.6 (4)
C10—C5—C6—C7	−2.1 (5)	C28—C23—P1—C17	−172.4 (4)
C5—C6—C7—C8	−0.6 (5)	C24—C23—P1—Ag1	−111.9 (4)
C5—C6—C7—N1	178.7 (3)	C28—C23—P1—Ag1	66.1 (4)
C6—C7—C8—C9	2.1 (6)	N1^{i}—Ag1—P1—C11	69.36 (17)
N1—C7—C8—C9	−177.3 (3)	O1—Ag1—P1—C11	−29.46 (16)
C7—C8—C9—C10	−0.7 (6)	P2—Ag1—P1—C11	−160.02 (14)
C8—C9—C10—C5	−2.0 (5)	N1^{i}—Ag1—P1—C17	−166.70 (17)
C8—C9—C10—C1	177.4 (4)	O1—Ag1—P1—C17	94.48 (16)
C4—C5—C10—C9	−178.3 (3)	P2—Ag1—P1—C17	−36.08 (15)
C6—C5—C10—C9	3.4 (5)	N1^{i}—Ag1—P1—C23	−50.55 (17)
C4—C5—C10—C1	2.3 (5)	O1—Ag1—P1—C23	−149.38 (15)
C6—C5—C10—C1	−176.1 (3)	P2—Ag1—P1—C23	80.07 (15)
C2—C1—C10—C9	179.7 (4)	C40—C35—P2—C29	99.5 (4)
S1—C1—C10—C9	−1.1 (5)	C36—C35—P2—C29	−82.6 (4)
C2—C1—C10—C5	−0.9 (5)	C40—C35—P2—C41	−5.8 (4)
S1—C1—C10—C5	178.4 (3)	C36—C35—P2—C41	172.0 (3)
C16—C11—C12—C13	−0.1 (6)	C40—C35—P2—Ag1	−133.9 (3)
P1—C11—C12—C13	178.4 (3)	C36—C35—P2—Ag1	44.0 (3)
C11—C12—C13—C14	0.2 (7)	C34—C29—P2—C35	−4.1 (4)
C12—C13—C14—C15	−0.2 (7)	C30—C29—P2—C35	178.7 (4)
C13—C14—C15—C16	0.1 (7)	C34—C29—P2—C41	106.4 (4)
C14—C15—C16—C11	0.0 (7)	C30—C29—P2—C41	−70.8 (4)
C12—C11—C16—C15	0.0 (7)	C34—C29—P2—Ag1	−124.0 (4)
P1—C11—C16—C15	−178.4 (4)	C30—C29—P2—Ag1	58.8 (4)
C28—C23—C24—C25	0.1 (7)	C42—C41—P2—C35	67.9 (4)
P1—C23—C24—C25	178.1 (4)	C46—C41—P2—C35	−115.0 (3)
C23—C24—C25—C26	1.1 (8)	C42—C41—P2—C29	−40.2 (4)
C24—C25—C26—C27	−0.5 (9)	C46—C41—P2—C29	136.9 (3)
C25—C26—C27—C28	−1.2 (9)	C42—C41—P2—Ag1	−170.0 (3)
C24—C23—C28—C27	−1.9 (8)	C46—C41—P2—Ag1	7.1 (3)
P1—C23—C28—C27	180.0 (5)	P1—Ag1—P2—C35	−78.12 (13)
C26—C27—C28—C23	2.5 (9)	N1^{i}—Ag1—P2—C35	58.20 (15)
C34—C29—C30—C31	−1.4 (7)	O1—Ag1—P2—C35	153.87 (14)
P2—C29—C30—C31	176.0 (4)	P1—Ag1—P2—C29	39.60 (15)
C29—C30—C31—C32	0.5 (9)	N1^{i}—Ag1—P2—C29	175.92 (16)
C30—C31—C32—C33	0.5 (9)	O1—Ag1—P2—C29	−88.41 (16)
C31—C32—C33—C34	−0.5 (9)	P1—Ag1—P2—C41	160.41 (13)
C30—C29—C34—C33	1.3 (7)	N1^{i}—Ag1—P2—C41	−63.27 (16)
P2—C29—C34—C33	−175.9 (4)	O1—Ag1—P2—C41	32.40 (15)
C32—C33—C34—C29	−0.4 (8)	Ag1—O1—S1—O3	−77.8 (2)
C40—C35—C36—C37	−1.8 (7)	Ag1—O1—S1—O2	50.5 (3)
P2—C35—C36—C37	−179.8 (4)	Ag1—O1—S1—C1	165.49 (19)
C35—C36—C37—C38	0.7 (8)	C2—C1—S1—O3	129.4 (3)
C36—C37—C38—C39	0.7 (8)	C10—C1—S1—O3	−49.8 (3)
C37—C38—C39—C40	−0.9 (8)	C2—C1—S1—O1	−109.4 (3)
C36—C35—C40—C39	1.6 (6)	C10—C1—S1—O1	71.3 (3)
P2—C35—C40—C39	179.4 (3)	C2—C1—S1—O2	9.3 (4)

C38—C39—C40—C35	−0.3 (7)	C10—C1—S1—O2	−169.9 (3)
C46—C41—C42—C43	1.4 (6)	C11—P1—C17—C22	174.5 (6)
P2—C41—C42—C43	178.4 (3)	C23—P1—C17—C22	−78.1 (6)
C41—C42—C43—C44	0.8 (7)	Ag1—P1—C17—C22	41.7 (6)
C42—C43—C44—C45	−1.7 (8)	C11—P1—C17—C18	0.7 (6)
C43—C44—C45—C46	0.4 (7)	C23—P1—C17—C18	108.1 (6)
C42—C41—C46—C45	−2.7 (6)	Ag1—P1—C17—C18	−132.1 (6)
P2—C41—C46—C45	−179.9 (3)	C22—C17—C18—C19	4.8 (12)
C44—C45—C46—C41	1.8 (6)	P1—C17—C18—C19	178.5 (7)
C6—C7—N1—Ag1^{ii}	89.1 (4)	C17—C18—C19—C20	−0.5 (16)
C8—C7—N1—Ag1^{ii}	−91.5 (4)	C18—C19—C20—C21	−3.8 (16)
P1—Ag1—O1—S1	120.0 (2)	C19—C20—C21—C22	3.7 (15)
N1^{i}—Ag1—O1—S1	1.2 (2)	C18—C17—C22—C21	−4.9 (12)
P2—Ag1—O1—S1	−103.0 (2)	P1—C17—C22—C21	−179.0 (7)
C12—C11—P1—C17	−108.7 (3)	C20—C21—C22—C17	0.6 (15)
C16—C11—P1—C17	69.7 (4)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1C···O2	0.92 (6)	1.88 (3)	2.789 (5)	166 (8)
N1—H1B···O2^{ii}	0.87 (4)	2.31 (2)	3.140 (4)	162 (4)
N1—H1A···O3^{iii}	0.85 (4)	2.17 (2)	2.975 (4)	159 (4)

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

Fig. 1

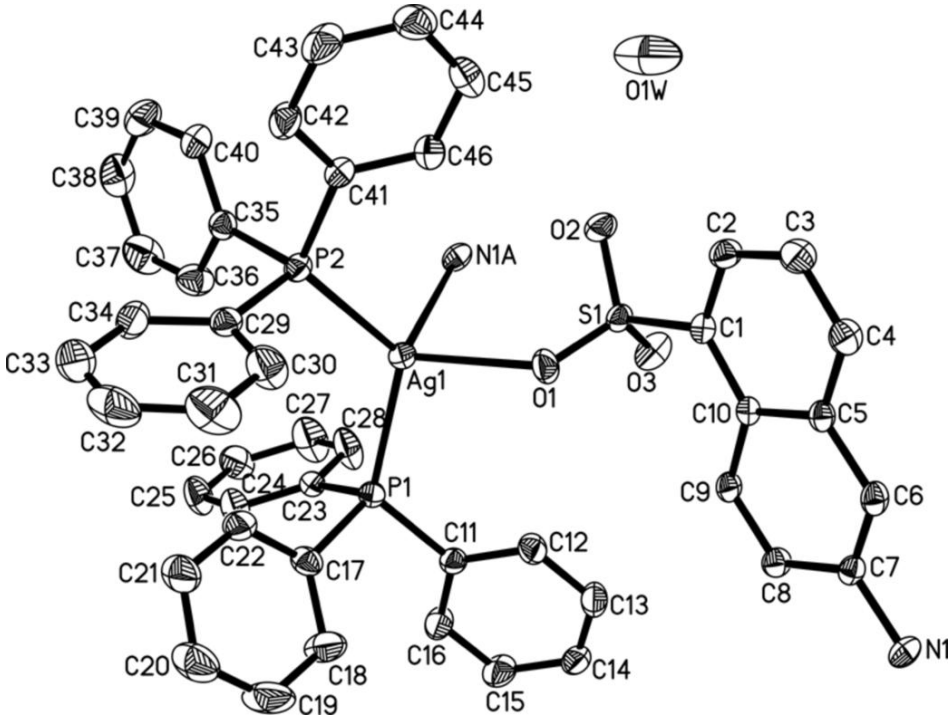

C44
C43
C45
O1W
C39
C42
C40
C46
C38
C41
C35
O2
C2
C3
C37
P2
N1A
C36
S1
C1
C34
C29
C4
C33
C31
C30
Ag1
O1
O3
C27
C28
C10
C5
C32
C26
C24
C9
C6
C25
C23
P1
C11
C12
C22
C21
C17
C8
C7
C13
C16
N1
C20
C18
C14
C19
C15

Fig. 2