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(2-Amino-4,5-dimethylbenzenesulfonato-κN)aquabis(triphenylphosphine-κP)silver(I)

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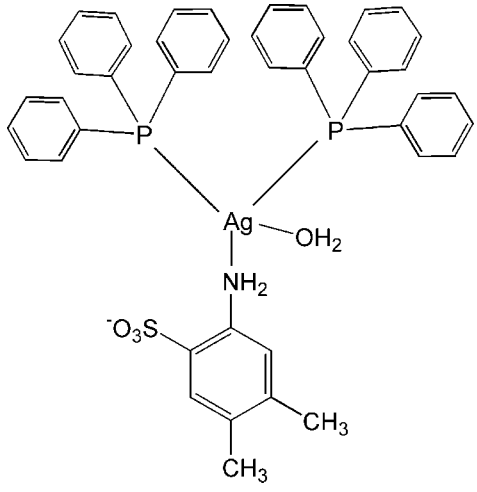
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.094; data-to-parameter ratio = 18.4.

The title compound, $[Ag(C_8H_{10}NO_3S)(C_{18}H_{15}P)_2(H_2O)]$, has a mononuclear structure, where the Ag^I cation is four-coordinated by two triphenylphosphine ligands, one water molecule and the N atom of a 2-amino-4,5-dimethylbenzenesulfonate anion in a distorted tetrahedral AgP_2NO arrangement. A network of N—H···O and O—H···O hydrogen bonds helps to consolidate the packing.

Related literature

For a study of a related silver sulfonate, see: Li *et al.* (2007).



Experimental

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_{18}H_{15}P)_2(H_2O)]$
M_r = 850.66
Monoclinic, $P2_1/c$
a = 24.872 (5) Å
b = 14.634 (3) Å
c = 11.010 (2) Å
β = 94.70 (3)°
V = 3994.0 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 292 (2) K
0.35 × 0.30 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.785, T_{max} = 0.836
37956 measured reflections
9041 independent reflections
6965 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.08
9041 reflections
492 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—P2	2.4492 (7)	Ag1—O1*W*	2.464 (2)
Ag1—P1	2.4637 (8)	Ag1—N1	2.469 (2)
P2—Ag1—P1	130.79 (2)	P2—Ag1—N1	114.57 (6)
P2—Ag1—O1*W*	105.12 (6)	P1—Ag1—N1	106.45 (5)
P1—Ag1—O1*W*	104.71 (6)	O1*W*—Ag1—N1	84.53 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*B*···O2^{i}	0.83 (3)	1.97 (3)	2.797 (3)	173 (3)
O1*W*—H1*A*···O3	0.89 (3)	2.10 (3)	2.825 (4)	137 (3)
N1—H1*C*···O1^{ii}	0.92 (3)	2.09 (3)	2.972 (3)	159 (2)
N1—H1*D*···O3	0.83 (3)	2.26 (3)	2.875 (3)	131 (3)

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

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: CF2160).

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supplementary materials

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(2-Amino-4,5-dimethylbenzenesulfonato-κN)aquabis(triphenylphosphine-κP)silver(I)

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Comment

In the title compound, (I), one water molecule, one 2-amino-4,5-dimethylbenzenesulfonate (*L*) anion and two triphenylphosphine ligands are coordinated to the metal, resulting in a distorted tetrahedral geometry for Ag (Fig. 1, Table 1). The Ag—O_{water} and Ag—N distances are different from those of a related compound (Li *et al.*, 2007).

Here, the coordination ability of the amine group of *L* is evidently stronger than that of the sulfonate group and the latter group does not coordinate to the Ag ion. In the crystal structure of (I), adjacent molecules are interconnected by strong O—H···O and N—H···O hydrogen bonds (Table 2) to form a one-dimensional supramolecular structure (Fig. 2).

Experimental

An aqueous solution (10 ml) of 2-amino-4,5-dimethylbenzenesulfonic acid (0.1005 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 over several days at room temperature.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The water H atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = 0.85 (1) Å. The amino H atoms were located in a difference Fourier map and refined with U_{iso}(H) = 1.2U_{eq}(N).

Figures

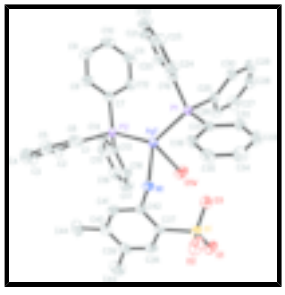


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids. All H atoms are omitted for clarity.

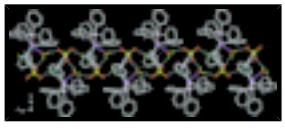


Fig. 2. One-dimensional supramolecular structure of (I), formed through hydrogen-bonding (dashed lines) interactions. The H atoms not involved in hydrogen bonding have been omitted.

(2-Amino-4,5-dimethylbenzenesulfonato-κ*N*)aquabis(triphenylphosphine- κ*P*)silver(I)

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_{18}H_{15}P)_2(H_2O)]$	F_{000} = 1752
M_r = 850.66	D_x = 1.415 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9041 reflections
a = 24.872 (5) Å	θ = 3.2–27.4º
b = 14.634 (3) Å	μ = 0.68 mm^{-1}
c = 11.010 (2) Å	T = 292 (2) K
β = 94.70 (3)º	Block, colourless
V = 3994.0 (14) Å^3	0.35 × 0.30 × 0.28 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID CCD diffractometer	9041 independent reflections
Radiation source: fine-focus sealed tube	6965 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.4º
T = 292(2) K	θ_{min} = 3.2º
ω scans	h = −32→31
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −18→18
T_{min} = 0.785, T_{max} = 0.836	l = −13→14
37956 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
$wR(F^2)$ = 0.094	$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.5293P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.001
9041 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
492 parameters	$\Delta\rho_{min}$ = −0.59 e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Ag1	0.737422 (7)	0.536786 (13)	0.982619 (17)	0.03753 (7)
C1	0.85593 (9)	0.41493 (17)	1.1156 (2)	0.0369 (5)
C2	0.90991 (10)	0.3921 (2)	1.1126 (2)	0.0555 (8)
H2	0.9238	0.3801	1.0383	0.067*
C3	0.94317 (13)	0.3872 (3)	1.2191 (3)	0.0734 (10)
H3	0.9793	0.3714	1.2167	0.088*
C4	0.92291 (13)	0.4054 (3)	1.3277 (3)	0.0674 (9)
H4	0.9455	0.4018	1.3992	0.081*
C5	0.87000 (13)	0.4288 (2)	1.3333 (3)	0.0567 (8)
H5	0.8565	0.4409	1.4080	0.068*
C6	0.83653 (11)	0.43426 (19)	1.2262 (2)	0.0432 (6)
H6	0.8006	0.4512	1.2293	0.052*
C7	0.78305 (9)	0.30617 (17)	0.9581 (2)	0.0376 (5)
C8	0.79251 (12)	0.2379 (2)	1.0447 (3)	0.0504 (7)
H8	0.8149	0.2499	1.1148	0.061*
C9	0.76929 (13)	0.1524 (2)	1.0287 (3)	0.0643 (9)
H9	0.7757	0.1077	1.0881	0.077*
C10	0.73683 (12)	0.1338 (2)	0.9248 (3)	0.0621 (8)
H10	0.7213	0.0763	0.9134	0.074*
C11	0.72722 (12)	0.2005 (2)	0.8372 (3)	0.0630 (9)
H11	0.7057	0.1875	0.7662	0.076*
C12	0.74945 (10)	0.2866 (2)	0.8547 (3)	0.0494 (7)
H12	0.7418	0.3318	0.7966	0.059*
C13	0.85297 (9)	0.43810 (19)	0.8548 (2)	0.0379 (6)
C14	0.87784 (10)	0.3656 (2)	0.7996 (2)	0.0489 (7)
H14	0.8717	0.3058	0.8235	0.059*
C15	0.91199 (12)	0.3835 (3)	0.7084 (3)	0.0665 (9)
H15	0.9286	0.3353	0.6711	0.080*
C16	0.92135 (14)	0.4717 (3)	0.6729 (3)	0.0714 (11)
H16	0.9442	0.4827	0.6117	0.086*
C17	0.89712 (14)	0.5441 (3)	0.7275 (3)	0.0691 (10)
H17	0.9037	0.6037	0.7036	0.083*
C18	0.86258 (12)	0.5271 (2)	0.8190 (3)	0.0518 (7)

H18	0.8460	0.5756	0.8558	0.062*
C19	0.61800 (9)	0.42070 (18)	1.0728 (2)	0.0386 (5)
C20	0.63163 (12)	0.3347 (2)	1.0330 (3)	0.0531 (7)
H20	0.6499	0.3288	0.9630	0.064*
C21	0.61829 (15)	0.2575 (2)	1.0960 (4)	0.0718 (10)
H21	0.6271	0.2000	1.0678	0.086*
C22	0.59193 (14)	0.2658 (3)	1.2007 (3)	0.0731 (10)
H22	0.5832	0.2139	1.2437	0.088*
C23	0.57876 (13)	0.3495 (3)	1.2410 (3)	0.0699 (10)
H23	0.5609	0.3546	1.3116	0.084*
C24	0.59156 (11)	0.4279 (2)	1.1782 (3)	0.0536 (7)
H24	0.5824	0.4851	1.2069	0.064*
C25	0.60430 (9)	0.49905 (18)	0.8353 (2)	0.0376 (5)
C26	0.63227 (12)	0.5162 (2)	0.7327 (3)	0.0518 (7)
H26	0.6674	0.5385	0.7426	0.062*
C27	0.60844 (15)	0.5006 (3)	0.6170 (3)	0.0666 (9)
H27	0.6276	0.5124	0.5496	0.080*
C28	0.55659 (14)	0.4678 (2)	0.6009 (3)	0.0663 (9)
H28	0.5406	0.4570	0.5228	0.080*
C29	0.52824 (12)	0.4509 (2)	0.7018 (3)	0.0605 (9)
H29	0.4930	0.4292	0.6912	0.073*
C30	0.55190 (11)	0.46624 (19)	0.8185 (3)	0.0491 (7)
H30	0.5326	0.4545	0.8856	0.059*
C31	0.60500 (9)	0.61544 (17)	1.0500 (2)	0.0348 (5)
C32	0.55896 (10)	0.65660 (19)	0.9950 (3)	0.0466 (6)
H32	0.5433	0.6341	0.9214	0.056*
C33	0.53621 (12)	0.7313 (2)	1.0495 (3)	0.0606 (8)
H33	0.5056	0.7589	1.0118	0.073*
C34	0.55873 (12)	0.7648 (2)	1.1591 (3)	0.0659 (9)
H34	0.5432	0.8146	1.1953	0.079*
C35	0.60383 (12)	0.7248 (2)	1.2143 (3)	0.0591 (8)
H35	0.6189	0.7475	1.2882	0.071*
C36	0.62738 (10)	0.6505 (2)	1.1611 (2)	0.0448 (6)
H36	0.6582	0.6238	1.1995	0.054*
C37	0.80874 (10)	0.79236 (17)	0.9918 (2)	0.0370 (5)
C38	0.85665 (11)	0.82206 (19)	0.9475 (2)	0.0459 (6)
H38	0.8557	0.8732	0.8972	0.055*
C39	0.90552 (11)	0.7785 (2)	0.9752 (3)	0.0511 (7)
C40	0.90660 (10)	0.7015 (2)	1.0502 (3)	0.0494 (7)
C41	0.85908 (10)	0.67250 (19)	1.0955 (2)	0.0434 (6)
H41	0.8603	0.6226	1.1480	0.052*
C42	0.80932 (10)	0.71503 (17)	1.0657 (2)	0.0350 (5)
C43	0.95591 (13)	0.8125 (3)	0.9209 (4)	0.0835 (12)
H43A	0.9864	0.8053	0.9793	0.125*
H43B	0.9516	0.8759	0.8997	0.125*
H43C	0.9616	0.7777	0.8491	0.125*
C44	0.95793 (12)	0.6482 (3)	1.0810 (3)	0.0760 (10)
H44A	0.9851	0.6882	1.1182	0.114*
H44B	0.9702	0.6228	1.0079	0.114*

H44C	0.9511	0.5998	1.1366	0.114*
N1	0.76224 (8)	0.67411 (15)	1.1049 (2)	0.0376 (5)
O1	0.75906 (9)	0.91154 (14)	0.84892 (17)	0.0573 (5)
O2	0.73943 (10)	0.91015 (17)	1.05962 (18)	0.0751 (7)
O3	0.70682 (8)	0.78944 (15)	0.9241 (2)	0.0741 (7)
O1W	0.74902 (10)	0.63686 (16)	0.80672 (19)	0.0616 (6)
S1	0.74872 (3)	0.85648 (5)	0.95299 (6)	0.04396 (16)
P1	0.63905 (2)	0.51895 (4)	0.98561 (6)	0.03284 (14)
P2	0.80913 (2)	0.42236 (4)	0.97888 (6)	0.03333 (14)
H1A	0.7255 (11)	0.683 (2)	0.806 (3)	0.050*
H1B	0.7489 (11)	0.624 (2)	0.733 (2)	0.050*
H1C	0.7682 (10)	0.6577 (19)	1.185 (2)	0.050*
H1D	0.7351 (11)	0.7059 (19)	1.090 (3)	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03204 (11)	0.03472 (11)	0.04610 (12)	0.00212 (7)	0.00494 (8)	−0.00024 (8)
C1	0.0379 (13)	0.0346 (14)	0.0382 (13)	0.0038 (10)	0.0027 (10)	−0.0028 (11)
C2	0.0441 (15)	0.081 (2)	0.0407 (15)	0.0188 (14)	−0.0007 (12)	−0.0118 (15)
C3	0.0502 (18)	0.099 (3)	0.068 (2)	0.0217 (18)	−0.0113 (15)	−0.016 (2)
C4	0.076 (2)	0.079 (3)	0.0433 (18)	0.0106 (18)	−0.0200 (15)	−0.0060 (17)
C5	0.072 (2)	0.063 (2)	0.0346 (15)	0.0018 (16)	0.0026 (13)	−0.0038 (14)
C6	0.0489 (15)	0.0417 (15)	0.0397 (14)	0.0025 (12)	0.0073 (11)	−0.0018 (12)
C7	0.0335 (12)	0.0373 (14)	0.0429 (14)	0.0049 (10)	0.0083 (10)	−0.0022 (11)
C8	0.0662 (18)	0.0432 (17)	0.0416 (15)	−0.0003 (13)	0.0030 (13)	0.0011 (13)
C9	0.087 (2)	0.0461 (19)	0.061 (2)	−0.0015 (16)	0.0143 (18)	0.0021 (16)
C10	0.0621 (19)	0.0438 (18)	0.083 (2)	−0.0082 (14)	0.0197 (16)	−0.0161 (17)
C11	0.0484 (17)	0.060 (2)	0.079 (2)	−0.0008 (14)	−0.0019 (15)	−0.0253 (18)
C12	0.0457 (15)	0.0504 (18)	0.0511 (17)	0.0022 (12)	−0.0033 (12)	−0.0030 (14)
C13	0.0360 (12)	0.0507 (16)	0.0271 (12)	0.0019 (11)	0.0029 (9)	−0.0043 (11)
C14	0.0441 (14)	0.0575 (19)	0.0460 (15)	0.0052 (13)	0.0080 (12)	−0.0099 (14)
C15	0.0505 (17)	0.089 (3)	0.063 (2)	−0.0007 (17)	0.0243 (15)	−0.0230 (19)
C16	0.064 (2)	0.110 (3)	0.0437 (18)	−0.024 (2)	0.0216 (15)	−0.0125 (19)
C17	0.072 (2)	0.078 (3)	0.060 (2)	−0.0199 (18)	0.0207 (17)	0.0101 (18)
C18	0.0610 (18)	0.0531 (19)	0.0427 (16)	−0.0041 (13)	0.0132 (13)	0.0032 (13)
C19	0.0343 (12)	0.0359 (14)	0.0456 (14)	−0.0023 (10)	0.0025 (10)	0.0039 (11)
C20	0.0633 (18)	0.0420 (17)	0.0540 (17)	−0.0009 (13)	0.0039 (14)	0.0010 (14)
C21	0.088 (2)	0.0345 (17)	0.092 (3)	−0.0097 (16)	−0.003 (2)	0.0081 (17)
C22	0.080 (2)	0.064 (2)	0.073 (2)	−0.0299 (19)	−0.0077 (18)	0.030 (2)
C23	0.071 (2)	0.077 (3)	0.064 (2)	−0.0171 (18)	0.0204 (16)	0.0200 (19)
C24	0.0536 (17)	0.0521 (18)	0.0572 (18)	−0.0026 (14)	0.0177 (14)	0.0082 (14)
C25	0.0378 (13)	0.0348 (13)	0.0396 (14)	0.0040 (10)	−0.0006 (10)	−0.0052 (11)
C26	0.0555 (17)	0.0542 (19)	0.0459 (17)	−0.0013 (14)	0.0054 (13)	−0.0024 (14)
C27	0.086 (2)	0.073 (2)	0.0409 (18)	0.0117 (19)	0.0054 (16)	−0.0024 (16)
C28	0.073 (2)	0.068 (2)	0.055 (2)	0.0264 (17)	−0.0168 (16)	−0.0166 (17)
C29	0.0470 (16)	0.059 (2)	0.072 (2)	0.0107 (13)	−0.0181 (15)	−0.0200 (17)
C30	0.0404 (14)	0.0484 (17)	0.0579 (18)	0.0030 (12)	0.0008 (12)	−0.0076 (14)

C31	0.0322 (12)	0.0338 (13)	0.0388 (13)	−0.0014 (9)	0.0059 (10)	−0.0009 (10)
C32	0.0438 (14)	0.0456 (16)	0.0498 (16)	0.0063 (12)	0.0004 (11)	−0.0014 (13)
C33	0.0543 (17)	0.055 (2)	0.071 (2)	0.0203 (14)	−0.0015 (15)	−0.0078 (16)
C34	0.0576 (18)	0.054 (2)	0.087 (2)	0.0116 (15)	0.0106 (17)	−0.0243 (18)
C35	0.0485 (16)	0.061 (2)	0.067 (2)	−0.0026 (14)	0.0052 (14)	−0.0297 (17)
C36	0.0359 (13)	0.0506 (17)	0.0475 (15)	0.0019 (11)	0.0018 (11)	−0.0094 (13)
C37	0.0465 (14)	0.0320 (14)	0.0329 (13)	−0.0073 (10)	0.0058 (10)	−0.0023 (10)
C38	0.0552 (16)	0.0417 (16)	0.0421 (15)	−0.0142 (12)	0.0119 (12)	−0.0016 (12)
C39	0.0449 (15)	0.062 (2)	0.0474 (16)	−0.0157 (13)	0.0090 (12)	−0.0057 (14)
C40	0.0406 (14)	0.062 (2)	0.0458 (16)	−0.0024 (12)	0.0022 (11)	−0.0077 (14)
C41	0.0492 (15)	0.0409 (15)	0.0401 (14)	0.0001 (12)	0.0033 (11)	0.0011 (12)
C42	0.0429 (13)	0.0342 (13)	0.0283 (12)	−0.0069 (10)	0.0053 (9)	−0.0045 (10)
C43	0.059 (2)	0.108 (3)	0.086 (3)	−0.024 (2)	0.0226 (18)	0.007 (2)
C44	0.0468 (17)	0.104 (3)	0.076 (2)	0.0129 (18)	−0.0003 (15)	0.004 (2)
N1	0.0402 (11)	0.0375 (12)	0.0358 (11)	−0.0019 (9)	0.0067 (9)	−0.0001 (9)
O1	0.0845 (14)	0.0471 (12)	0.0418 (11)	0.0087 (10)	0.0135 (10)	0.0097 (9)
O2	0.1054 (18)	0.0802 (18)	0.0420 (12)	0.0395 (14)	0.0208 (12)	−0.0009 (11)
O3	0.0522 (12)	0.0569 (15)	0.1095 (19)	−0.0024 (10)	−0.0162 (12)	0.0196 (14)
O1W	0.0907 (16)	0.0542 (14)	0.0399 (11)	−0.0020 (11)	0.0049 (11)	0.0082 (11)
S1	0.0561 (4)	0.0383 (4)	0.0383 (3)	0.0045 (3)	0.0090 (3)	0.0036 (3)
P1	0.0293 (3)	0.0332 (3)	0.0363 (3)	0.0005 (2)	0.0042 (2)	0.0002 (3)
P2	0.0323 (3)	0.0352 (3)	0.0329 (3)	0.0048 (2)	0.0053 (2)	−0.0005 (3)

Geometric parameters (Å, °)

Ag1—P2	2.4492 (7)	C24—H24	0.930
Ag1—P1	2.4637 (8)	C25—C30	1.387 (4)
Ag1—O1W	2.464 (2)	C25—C26	1.397 (4)
Ag1—N1	2.469 (2)	C25—P1	1.827 (3)
C1—C6	1.376 (3)	C26—C27	1.379 (4)
C1—C2	1.387 (3)	C26—H26	0.930
C1—P2	1.829 (3)	C27—C28	1.374 (5)
C2—C3	1.381 (4)	C27—H27	0.930
C2—H2	0.930	C28—C29	1.387 (5)
C3—C4	1.361 (4)	C28—H28	0.930
C3—H3	0.930	C29—C30	1.386 (4)
C4—C5	1.366 (4)	C29—H29	0.930
C4—H4	0.930	C30—H30	0.930
C5—C6	1.389 (4)	C31—C32	1.388 (3)
C5—H5	0.930	C31—C36	1.399 (3)
C6—H6	0.930	C31—P1	1.820 (2)
C7—C12	1.386 (4)	C32—C33	1.390 (4)
C7—C8	1.387 (4)	C32—H32	0.930
C7—P2	1.828 (3)	C33—C34	1.378 (4)
C8—C9	1.383 (4)	C33—H33	0.930
C8—H8	0.930	C34—C35	1.363 (4)
C9—C10	1.373 (4)	C34—H34	0.930
C9—H9	0.930	C35—C36	1.387 (4)
C10—C11	1.379 (5)	C35—H35	0.930

C10—H10	0.930	C36—H36	0.930
C11—C12	1.383 (4)	C37—C42	1.393 (3)
C11—H11	0.930	C37—C38	1.394 (3)
C12—H12	0.930	C37—S1	1.785 (3)
C13—C18	1.387 (4)	C38—C39	1.384 (4)
C13—C14	1.392 (4)	C38—H38	0.930
C13—P2	1.831 (2)	C39—C40	1.397 (4)
C14—C15	1.393 (4)	C39—C43	1.516 (4)
C14—H14	0.930	C40—C41	1.386 (4)
C15—C16	1.374 (5)	C40—C44	1.511 (4)
C15—H15	0.930	C41—C42	1.400 (3)
C16—C17	1.381 (5)	C41—H41	0.930
C16—H16	0.930	C42—N1	1.414 (3)
C17—C18	1.399 (4)	C43—H43A	0.960
C17—H17	0.930	C43—H43B	0.960
C18—H18	0.930	C43—H43C	0.960
C19—C24	1.383 (4)	C44—H44A	0.960
C19—C20	1.385 (4)	C44—H44B	0.960
C19—P1	1.829 (3)	C44—H44C	0.960
C20—C21	1.380 (4)	N1—H1C	0.92 (3)
C20—H20	0.930	N1—H1D	0.83 (3)
C21—C22	1.377 (5)	O1—S1	1.4411 (19)
C21—H21	0.930	O2—S1	1.447 (2)
C22—C23	1.351 (5)	O3—S1	1.448 (2)
C22—H22	0.930	O1W—H1A	0.89 (3)
C23—C24	1.391 (4)	O1W—H1B	0.83 (3)
C23—H23	0.930		
P2—Ag1—P1	130.79 (2)	C26—C27—H27	119.8
P2—Ag1—O1W	105.12 (6)	C27—C28—C29	119.5 (3)
P1—Ag1—O1W	104.71 (6)	C27—C28—H28	120.3
P2—Ag1—N1	114.57 (6)	C29—C28—H28	120.3
P1—Ag1—N1	106.45 (5)	C28—C29—C30	120.6 (3)
O1W—Ag1—N1	84.53 (8)	C28—C29—H29	119.7
C6—C1—C2	118.8 (2)	C30—C29—H29	119.7
C6—C1—P2	118.07 (19)	C29—C30—C25	120.1 (3)
C2—C1—P2	123.16 (19)	C29—C30—H30	119.9
C3—C2—C1	120.4 (3)	C25—C30—H30	119.9
C3—C2—H2	119.8	C32—C31—C36	118.5 (2)
C1—C2—H2	119.8	C32—C31—P1	124.05 (19)
C4—C3—C2	119.8 (3)	C36—C31—P1	117.43 (18)
C4—C3—H3	120.1	C31—C32—C33	120.2 (3)
C2—C3—H3	120.1	C31—C32—H32	119.9
C3—C4—C5	121.1 (3)	C33—C32—H32	119.9
C3—C4—H4	119.5	C34—C33—C32	120.5 (3)
C5—C4—H4	119.5	C34—C33—H33	119.8
C4—C5—C6	119.2 (3)	C32—C33—H33	119.8
C4—C5—H5	120.4	C35—C34—C33	119.9 (3)
C6—C5—H5	120.4	C35—C34—H34	120.1
C1—C6—C5	120.7 (3)	C33—C34—H34	120.1

C1—C6—H6	119.7	C34—C35—C36	120.6 (3)
C5—C6—H6	119.7	C34—C35—H35	119.7
C12—C7—C8	118.2 (3)	C36—C35—H35	119.7
C12—C7—P2	118.6 (2)	C35—C36—C31	120.3 (3)
C8—C7—P2	123.0 (2)	C35—C36—H36	119.8
C9—C8—C7	121.2 (3)	C31—C36—H36	119.8
C9—C8—H8	119.4	C42—C37—C38	119.3 (2)
C7—C8—H8	119.4	C42—C37—S1	122.34 (18)
C10—C9—C8	119.8 (3)	C38—C37—S1	118.3 (2)
C10—C9—H9	120.1	C39—C38—C37	122.7 (3)
C8—C9—H9	120.1	C39—C38—H38	118.7
C9—C10—C11	119.9 (3)	C37—C38—H38	118.7
C9—C10—H10	120.1	C38—C39—C40	118.4 (2)
C11—C10—H10	120.1	C38—C39—C43	120.1 (3)
C10—C11—C12	120.2 (3)	C40—C39—C43	121.4 (3)
C10—C11—H11	119.9	C41—C40—C39	119.0 (3)
C12—C11—H11	119.9	C41—C40—C44	119.4 (3)
C11—C12—C7	120.7 (3)	C39—C40—C44	121.6 (3)
C11—C12—H12	119.7	C40—C41—C42	122.9 (3)
C7—C12—H12	119.7	C40—C41—H41	118.6
C18—C13—C14	119.9 (2)	C42—C41—H41	118.6
C18—C13—P2	117.2 (2)	C37—C42—C41	117.7 (2)
C14—C13—P2	122.9 (2)	C37—C42—N1	123.6 (2)
C13—C14—C15	119.4 (3)	C41—C42—N1	118.6 (2)
C13—C14—H14	120.3	C39—C43—H43A	109.5
C15—C14—H14	120.3	C39—C43—H43B	109.5
C16—C15—C14	120.6 (3)	H43A—C43—H43B	109.5
C16—C15—H15	119.7	C39—C43—H43C	109.5
C14—C15—H15	119.7	H43A—C43—H43C	109.5
C15—C16—C17	120.5 (3)	H43B—C43—H43C	109.5
C15—C16—H16	119.8	C40—C44—H44A	109.5
C17—C16—H16	119.8	C40—C44—H44B	109.5
C16—C17—C18	119.5 (3)	H44A—C44—H44B	109.5
C16—C17—H17	120.2	C40—C44—H44C	109.5
C18—C17—H17	120.2	H44A—C44—H44C	109.5
C13—C18—C17	120.1 (3)	H44B—C44—H44C	109.5
C13—C18—H18	119.9	C42—N1—Ag1	110.78 (15)
C17—C18—H18	119.9	C42—N1—H1C	109.5 (17)
C24—C19—C20	118.8 (3)	Ag1—N1—H1C	109.1 (18)
C24—C19—P1	123.8 (2)	C42—N1—H1D	113 (2)
C20—C19—P1	117.4 (2)	Ag1—N1—H1D	101 (2)
C21—C20—C19	120.6 (3)	H1C—N1—H1D	113 (3)
C21—C20—H20	119.7	Ag1—O1W—H1A	109.5 (19)
C19—C20—H20	119.7	Ag1—O1W—H1B	130 (2)
C22—C21—C20	120.0 (3)	H1A—O1W—H1B	103 (3)
C22—C21—H21	120.0	O1—S1—O2	113.11 (14)
C20—C21—H21	120.0	O1—S1—O3	112.10 (14)
C23—C22—C21	119.9 (3)	O2—S1—O3	112.74 (16)
C23—C22—H22	120.0	O1—S1—C37	106.49 (12)

C21—C22—H22	120.0	O2—S1—C37	106.09 (13)
C22—C23—C24	120.9 (3)	O3—S1—C37	105.62 (12)
C22—C23—H23	119.5	C31—P1—C25	106.04 (11)
C24—C23—H23	119.5	C31—P1—C19	104.05 (12)
C19—C24—C23	119.8 (3)	C25—P1—C19	102.48 (12)
C19—C24—H24	120.1	C31—P1—Ag1	114.67 (8)
C23—C24—H24	120.1	C25—P1—Ag1	113.66 (8)
C30—C25—C26	118.7 (3)	C19—P1—Ag1	114.68 (8)
C30—C25—P1	123.0 (2)	C7—P2—C1	104.07 (12)
C26—C25—P1	118.3 (2)	C7—P2—C13	104.51 (11)
C27—C26—C25	120.8 (3)	C1—P2—C13	104.10 (11)
C27—C26—H26	119.6	C7—P2—Ag1	112.75 (8)
C25—C26—H26	119.6	C1—P2—Ag1	116.24 (8)
C28—C27—C26	120.3 (3)	C13—P2—Ag1	113.93 (9)
C28—C27—H27	119.8		
C6—C1—C2—C3	1.3 (5)	C41—C42—N1—Ag1	−73.9 (2)
P2—C1—C2—C3	−179.6 (3)	P2—Ag1—N1—C42	55.17 (18)
C1—C2—C3—C4	−0.4 (6)	P1—Ag1—N1—C42	−152.72 (15)
C2—C3—C4—C5	−0.1 (6)	O1W—Ag1—N1—C42	−48.97 (17)
C3—C4—C5—C6	−0.2 (6)	C42—C37—S1—O1	−162.6 (2)
C2—C1—C6—C5	−1.6 (4)	C38—C37—S1—O1	18.4 (2)
P2—C1—C6—C5	179.3 (2)	C42—C37—S1—O2	76.7 (2)
C4—C5—C6—C1	1.1 (5)	C38—C37—S1—O2	−102.4 (2)
C12—C7—C8—C9	0.2 (4)	C42—C37—S1—O3	−43.2 (2)
P2—C7—C8—C9	176.0 (2)	C38—C37—S1—O3	137.7 (2)
C7—C8—C9—C10	0.9 (5)	C32—C31—P1—C25	5.3 (3)
C8—C9—C10—C11	−0.4 (5)	C36—C31—P1—C25	−173.9 (2)
C9—C10—C11—C12	−1.1 (5)	C32—C31—P1—C19	−102.4 (2)
C10—C11—C12—C7	2.2 (4)	C36—C31—P1—C19	78.4 (2)
C8—C7—C12—C11	−1.8 (4)	C32—C31—P1—Ag1	131.5 (2)
P2—C7—C12—C11	−177.7 (2)	C36—C31—P1—Ag1	−47.6 (2)
C18—C13—C14—C15	−0.3 (4)	C30—C25—P1—C31	−68.7 (3)
P2—C13—C14—C15	−178.0 (2)	C26—C25—P1—C31	112.4 (2)
C13—C14—C15—C16	0.2 (5)	C30—C25—P1—C19	40.1 (3)
C14—C15—C16—C17	0.2 (6)	C26—C25—P1—C19	−138.8 (2)
C15—C16—C17—C18	−0.4 (6)	C30—C25—P1—Ag1	164.4 (2)
C14—C13—C18—C17	0.1 (4)	C26—C25—P1—Ag1	−14.4 (3)
P2—C13—C18—C17	177.9 (2)	C24—C19—P1—C31	−11.7 (3)
C16—C17—C18—C13	0.3 (5)	C20—C19—P1—C31	171.2 (2)
C24—C19—C20—C21	1.1 (4)	C24—C19—P1—C25	−122.0 (2)
P1—C19—C20—C21	178.4 (2)	C20—C19—P1—C25	60.9 (2)
C19—C20—C21—C22	−1.0 (5)	C24—C19—P1—Ag1	114.4 (2)
C20—C21—C22—C23	0.6 (5)	C20—C19—P1—Ag1	−62.8 (2)
C21—C22—C23—C24	−0.2 (5)	P2—Ag1—P1—C31	155.69 (9)
C20—C19—C24—C23	−0.6 (4)	O1W—Ag1—P1—C31	−78.68 (11)
P1—C19—C24—C23	−177.7 (2)	N1—Ag1—P1—C31	9.87 (11)
C22—C23—C24—C19	0.2 (5)	P2—Ag1—P1—C25	−82.10 (10)
C30—C25—C26—C27	−0.3 (4)	O1W—Ag1—P1—C25	43.53 (11)
P1—C25—C26—C27	178.6 (3)	N1—Ag1—P1—C25	132.09 (11)

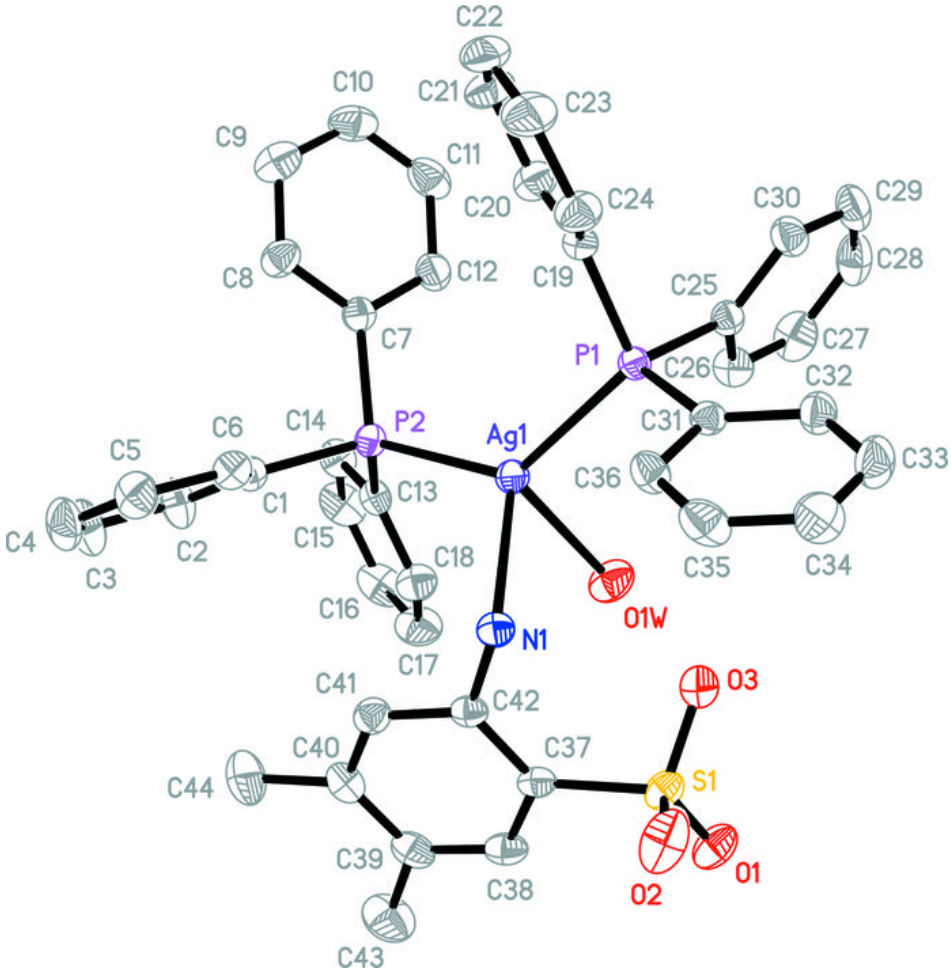
C25—C26—C27—C28	0.0 (5)	P2—Ag1—P1—C19	35.35 (10)
C26—C27—C28—C29	0.4 (5)	O1W—Ag1—P1—C19	160.98 (11)
C27—C28—C29—C30	−0.5 (5)	N1—Ag1—P1—C19	−110.47 (11)
C28—C29—C30—C25	0.3 (4)	C12—C7—P2—C1	−174.55 (19)
C26—C25—C30—C29	0.1 (4)	C8—C7—P2—C1	9.7 (2)
P1—C25—C30—C29	−178.7 (2)	C12—C7—P2—C13	−65.6 (2)
C36—C31—C32—C33	0.5 (4)	C8—C7—P2—C13	118.6 (2)
P1—C31—C32—C33	−178.7 (2)	C12—C7—P2—Ag1	58.6 (2)
C31—C32—C33—C34	−0.6 (5)	C8—C7—P2—Ag1	−117.1 (2)
C32—C33—C34—C35	0.4 (5)	C6—C1—P2—C7	−92.8 (2)
C33—C34—C35—C36	0.0 (5)	C2—C1—P2—C7	88.2 (3)
C34—C35—C36—C31	−0.1 (5)	C6—C1—P2—C13	158.0 (2)
C32—C31—C36—C35	−0.1 (4)	C2—C1—P2—C13	−21.0 (3)
P1—C31—C36—C35	179.1 (2)	C6—C1—P2—Ag1	31.9 (2)
C42—C37—C38—C39	−0.9 (4)	C2—C1—P2—Ag1	−147.2 (2)
S1—C37—C38—C39	178.2 (2)	C18—C13—P2—C7	156.7 (2)
C37—C38—C39—C40	0.3 (4)	C14—C13—P2—C7	−25.5 (2)
C37—C38—C39—C43	178.1 (3)	C18—C13—P2—C1	−94.4 (2)
C38—C39—C40—C41	−1.0 (4)	C14—C13—P2—C1	83.4 (2)
C43—C39—C40—C41	−178.8 (3)	C18—C13—P2—Ag1	33.2 (2)
C38—C39—C40—C44	177.8 (3)	C14—C13—P2—Ag1	−149.02 (19)
C43—C39—C40—C44	0.0 (5)	P1—Ag1—P2—C7	7.55 (10)
C39—C40—C41—C42	2.5 (4)	O1W—Ag1—P2—C7	−117.92 (11)
C44—C40—C41—C42	−176.3 (3)	N1—Ag1—P2—C7	151.22 (10)
C38—C37—C42—C41	2.2 (3)	P1—Ag1—P2—C1	−112.49 (9)
S1—C37—C42—C41	−176.85 (19)	O1W—Ag1—P2—C1	122.03 (11)
C38—C37—C42—N1	−173.3 (2)	N1—Ag1—P2—C1	31.18 (11)
S1—C37—C42—N1	7.6 (3)	P1—Ag1—P2—C13	126.46 (9)
C40—C41—C42—C37	−3.1 (4)	O1W—Ag1—P2—C13	0.98 (11)
C40—C41—C42—N1	172.7 (2)	N1—Ag1—P2—C13	−89.88 (11)
C37—C42—N1—Ag1	101.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1B···O2^{i}	0.83 (3)	1.97 (3)	2.797 (3)	173 (3)
O1W—H1A···O3	0.89 (3)	2.10 (3)	2.825 (4)	137 (3)
N1—H1C···O1^{ii}	0.92 (3)	2.09 (3)	2.972 (3)	159 (2)
N1—H1D···O3	0.83 (3)	2.26 (3)	2.875 (3)	131 (3)

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

Fig. 1


C22
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P1
C26
C27
C32
C6
C14
P2
Ag1
C31
C5
C33
C1
C13
C36
C4
C15
C18
C35
C34
C2
C3
C16
O1W
N1
C17
C41
C42
O3
C40
C37
S1
C44
C39
C38
O2
O1
C43
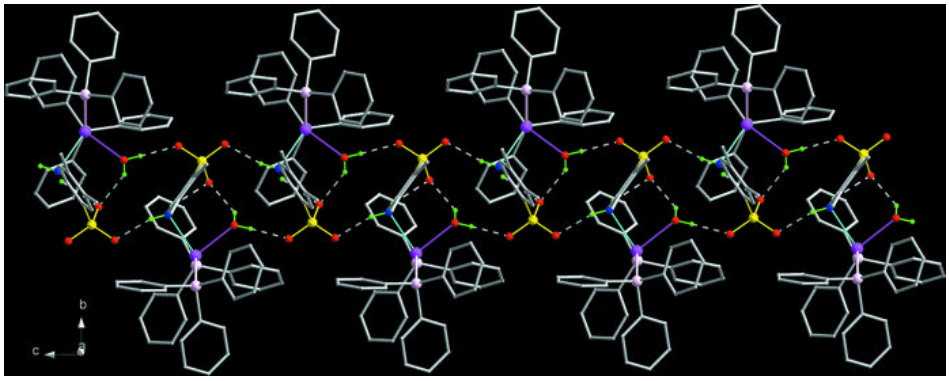
Fig. 2