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(2-Amino-3,5-dimethylbenzenesulfonato-κ*N*)bis(triphenylphosphine-κ*P*)silver(I) acetonitrile solvate

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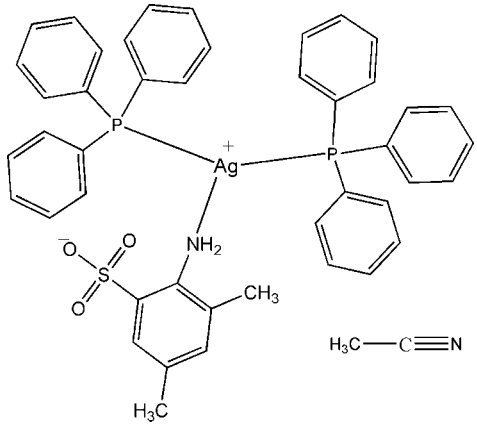
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.092; data-to-parameter ratio = 19.0.

The title compound, $[Ag(C_8H_{10}NO_3S)(C_{18}H_{15}P)_2]\cdot CH_3CN$, has a mononuclear structure, where the Ag^I cation is three-coordinated by two triphenylphosphine ligands and one N atom from the 2-amino-3,5-dimethylbenzenesulfonate anion in a distorted trigonal-planar AgP_2N arrangement. A network of N—H···O hydrogen bonds helps to consolidate the packing.

Related literature

For studies on related silver sulfonates, see: Han & Li, (2007*a*,*b*). For a review on the structural chemistry and properties of sulfonate complexes, see: Cote & Shimizu (2003).



Experimental

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_{18}H_{15}P)_2]\cdot C_2H_3N$
M_r = 873.69
Monoclinic, $P2_1/n$
a = 13.782 (3) Å
b = 12.252 (3) Å
c = 25.243 (5) Å
β = 94.32 (3)°
V = 4250.5 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 293 (2) K
0.26 × 0.21 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.841, T_{max} = 0.892
39847 measured reflections
9612 independent reflections
7595 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 0.84
9612 reflections
506 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.393 (2)	Ag1—P1	2.5005 (8)
Ag1—P2	2.4955 (9)		
N1—Ag1—P2	121.82 (6)	P2—Ag1—P1	122.09 (3)
N1—Ag1—P1	112.50 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.895 (16)	2.23 (2)	3.026 (3)	147.8 (18)
N1—H1B···O3	0.821 (17)	2.21 (2)	2.887 (3)	139 (2)

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

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: HB2567).

References

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supplementary materials

Acta Cryst. (2007). E**63**, m2650 [**doi:10.1107/S1600536807048076**]

(2-Amino-3,5-dimethylbenzenesulfonato-*κN*)bis(triphenylphosphine-*κP*)silver(I) acetonitrile solvate

J.-J. Han and N. Li

Comment

Cote & Shimizu have reviewed recent progress in the solid-state coordination and structural chemistry of sulfonates complexes as well as their properties in the gas sorption (Cote & Shimizu, 2003). However, sulfonate are generally perceived as weaker ligands regarding their coordinating ability (Han & Li, 2007*a*). Herein, we present the synthesis and structure of the title compound, (I), $[Ag(tpp)_2(L)]\cdot CNCH_3$, where tpp = triphenylphosphine and HL= 2-amino-3,5-dimethylbenzenesulfonic acid.

The Ag^I cation is three-coordinated by two P atoms from two triphenylphosphine ligands and one N atom from the *L* anion in a distorted trigonal-planar AgP_2N arrangement (Fig. 1, Table 1). The Ag—N (sulfonate) distance in (I) is similar to the equivalent value in a related compound (Han & Li, 2007*b*). Finally, the molecules are linked through N—H···O hydrogen bonds (Table 2), which help to consolidate the structure of (I).

Experimental

An aqueous solution (10 ml) of 2-amino-3,-5-dimethylbenzenesulfonic acid (0.5 mmol) was added to solid Ag_2CO_3 (0.25 mmol) and stirred for several minutes until no further CO_2 was given off; triphenylphosphine (0.5 mmol) in acetonitrile (7 ml) was then added and a solution was formed. Colourless blocks of (I) were obtained by evaporation of the solution for several days at room temperature.

Refinement

H atoms bonded to N atom were located in a difference map and refined freely, with U_{iso}(H) = 1.2U_{eq}(N). H atoms bonded to C atom were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H)=1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

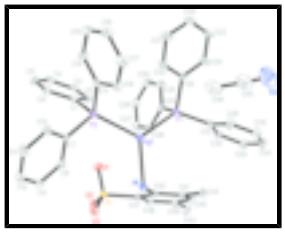


Fig. 1. The structure of (I), with displacement ellipsoids drawn at the 30% probability level (H atoms omitted for clarity).

(2-Amino-3,5-dimethylbenzenesulfonato-κ*N*)bis(triphenylphosphine-κ*P*)silver(I) acetonitrile solvate

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_{18}H_{15}P)_2]\cdot C_2H_3N$	$F_{000} = 1800$
$M_r = 873.69$	$D_x = 1.365$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 28308 reflections
$a = 13.782$ (3) Å	$\theta = 3.0$–27.5º
$b = 12.252$ (3) Å	$\mu = 0.64$ mm^{-1}
$c = 25.243$ (5) Å	$T = 293$ (2) K
$\beta = 94.32$ (3)º	Block, colorless
$V = 4250.5$ (15) Å^3	0.26 × 0.21 × 0.18 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	9612 independent reflections
Radiation source: rotating anode	7595 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.047$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 293$(2) K	$\theta_{min} = 3.2$º
ω scans	$h = -17\rightarrow17$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -15\rightarrow15$
$T_{min} = 0.841$, $T_{max} = 0.892$	$l = -32\rightarrow32$
39847 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 4.2132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.84$	$(\Delta/\sigma)_{max} = 0.003$
9612 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
506 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
3 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	0.817193 (13)	1.130397 (16)	0.175155 (7)	0.03824 (7)
C1	0.68522 (18)	0.9235 (2)	0.09214 (9)	0.0382 (5)
C2	0.76198 (19)	0.8582 (2)	0.11134 (10)	0.0450 (6)
H2	0.8141	0.8892	0.1315	0.054*
C3	0.7623 (2)	0.7471 (2)	0.10091 (12)	0.0554 (7)
H3	0.8141	0.7040	0.1141	0.067*
C4	0.6855 (3)	0.7010 (2)	0.07095 (12)	0.0610 (8)
H4	0.6863	0.6268	0.0634	0.073*
C5	0.6076 (3)	0.7635 (2)	0.05212 (11)	0.0599 (8)
H5	0.5557	0.7315	0.0322	0.072*
C6	0.6066 (2)	0.8745 (2)	0.06290 (11)	0.0510 (7)
H6	0.5534	0.9165	0.0506	0.061*
C7	0.56283 (17)	1.0923 (2)	0.12487 (9)	0.0362 (5)
C8	0.5409 (2)	1.0592 (2)	0.17539 (10)	0.0462 (6)
H8	0.5895	1.0306	0.1990	0.055*
C9	0.4474 (2)	1.0688 (3)	0.19044 (12)	0.0604 (8)
H9	0.4328	1.0458	0.2240	0.073*
C10	0.3754 (2)	1.1122 (3)	0.15611 (14)	0.0712 (10)
H10	0.3125	1.1190	0.1667	0.085*
C11	0.3960 (2)	1.1453 (3)	0.10667 (15)	0.0717 (10)
H11	0.3470	1.1748	0.0836	0.086*
C12	0.4896 (2)	1.1353 (3)	0.09050 (12)	0.0549 (7)
H12	0.5031	1.1575	0.0566	0.066*
C13	0.69171 (17)	1.1375 (2)	0.04289 (10)	0.0402 (5)
C14	0.6807 (2)	1.0852 (3)	−0.00577 (11)	0.0581 (7)
H14	0.6684	1.0105	−0.0072	0.070*
C15	0.6881 (3)	1.1437 (3)	−0.05288 (12)	0.0718 (10)
H15	0.6802	1.1078	−0.0854	0.086*
C16	0.7066 (2)	1.2523 (3)	−0.05154 (13)	0.0679 (9)
H16	0.7116	1.2906	−0.0830	0.082*
C17	0.7178 (3)	1.3057 (3)	−0.00382 (14)	0.0714 (9)
H17	0.7296	1.3804	−0.0030	0.086*
C18	0.7116 (2)	1.2486 (2)	0.04340 (12)	0.0547 (7)

H18	0.7208	1.2852	0.0757	0.066*
C19	1.02417 (18)	1.1280 (2)	0.09599 (10)	0.0417 (5)
C20	0.9506 (2)	1.1355 (4)	0.05733 (12)	0.0743 (11)
H20	0.8870	1.1249	0.0662	0.089*
C21	0.9671 (3)	1.1584 (5)	0.00530 (13)	0.1017 (17)
H21	0.9150	1.1630	−0.0203	0.122*
C22	1.0593 (2)	1.1744 (4)	−0.00861 (12)	0.0747 (10)
H22	1.0708	1.1911	−0.0435	0.090*
C23	1.1335 (3)	1.1656 (4)	0.02877 (14)	0.0954 (15)
H23	1.1970	1.1754	0.0195	0.115*
C24	1.1168 (2)	1.1423 (4)	0.08089 (13)	0.0902 (15)
H24	1.1693	1.1361	0.1061	0.108*
C25	1.01384 (17)	0.9537 (2)	0.17303 (10)	0.0408 (5)
C26	0.9726 (2)	0.9045 (3)	0.21528 (12)	0.0575 (7)
H26	0.9434	0.9473	0.2400	0.069*
C27	0.9744 (2)	0.7918 (3)	0.22113 (15)	0.0693 (9)
H27	0.9473	0.7598	0.2500	0.083*
C28	1.0161 (2)	0.7276 (3)	0.18456 (14)	0.0668 (9)
H28	1.0154	0.6520	0.1879	0.080*
C29	1.0590 (3)	0.7757 (3)	0.14282 (13)	0.0670 (9)
H29	1.0886	0.7325	0.1184	0.080*
C30	1.0580 (2)	0.8881 (2)	0.13729 (11)	0.0538 (7)
H30	1.0875	0.9200	0.1092	0.065*
C31	1.09295 (18)	1.1680 (2)	0.20333 (10)	0.0444 (6)
C32	1.1509 (2)	1.1166 (3)	0.24300 (11)	0.0517 (7)
H32	1.1424	1.0428	0.2498	0.062*
C33	1.2219 (2)	1.1761 (3)	0.27261 (13)	0.0681 (9)
H33	1.2598	1.1420	0.2999	0.082*
C34	1.2366 (3)	1.2835 (3)	0.26212 (15)	0.0785 (11)
H34	1.2856	1.3218	0.2815	0.094*
C35	1.1795 (3)	1.3353 (3)	0.22308 (17)	0.0797 (11)
H35	1.1890	1.4090	0.2162	0.096*
C36	1.1079 (2)	1.2776 (3)	0.19408 (14)	0.0671 (9)
H36	1.0690	1.3132	0.1678	0.081*
C37	0.83280 (18)	1.00119 (18)	0.32193 (9)	0.0360 (5)
C38	0.9007 (2)	0.9489 (2)	0.35648 (11)	0.0507 (7)
H38	0.8870	0.8794	0.3687	0.061*
C39	0.9880 (2)	0.9975 (3)	0.37310 (13)	0.0625 (8)
C40	1.0055 (2)	1.1013 (2)	0.35416 (12)	0.0543 (7)
H40	1.0642	1.1349	0.3649	0.065*
C41	0.93999 (19)	1.1572 (2)	0.32017 (10)	0.0403 (5)
C42	0.85182 (17)	1.10647 (18)	0.30314 (8)	0.0333 (5)
C43	1.0621 (3)	0.9410 (4)	0.4119 (2)	0.120 (2)
H43A	1.0287	0.9031	0.4384	0.180*
H43B	1.1049	0.9946	0.4288	0.180*
H43C	1.0994	0.8899	0.3930	0.180*
C44	0.9608 (2)	1.2719 (2)	0.30369 (12)	0.0501 (6)
H44A	0.9456	1.2795	0.2661	0.075*
H44B	1.0283	1.2880	0.3121	0.075*

H44C	0.9216	1.3216	0.3223	0.075*
C45	1.0471 (7)	1.4892 (5)	0.0828 (3)	0.134 (2)
C46	0.9466 (5)	1.4605 (6)	0.0753 (2)	0.152 (3)
H46A	0.9111	1.5189	0.0575	0.227*
H46B	0.9215	1.4477	0.1092	0.227*
H46C	0.9397	1.3954	0.0541	0.227*
N1	0.78530 (16)	1.15978 (16)	0.26594 (8)	0.0348 (4)
N2	1.1273 (6)	1.5132 (6)	0.0876 (4)	0.204 (3)
O1	0.73360 (15)	0.90495 (15)	0.24511 (7)	0.0498 (4)
O2	0.71669 (16)	0.83858 (15)	0.33439 (8)	0.0563 (5)
O3	0.64498 (14)	1.01177 (15)	0.30577 (8)	0.0535 (5)
S1	0.72303 (5)	0.93324 (5)	0.30021 (2)	0.03896 (14)
P1	0.99383 (4)	1.10000 (6)	0.16382 (2)	0.03733 (14)
P2	0.68730 (4)	1.06931 (5)	0.10741 (2)	0.03495 (13)
H1B	0.7286 (14)	1.142 (2)	0.2687 (11)	0.044 (8)*
H1A	0.8049 (13)	1.2294 (15)	0.2671 (11)	0.053 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03310 (10)	0.04632 (12)	0.03491 (10)	0.00240 (8)	0.00002 (7)	−0.00437 (7)
C1	0.0399 (13)	0.0437 (13)	0.0314 (12)	−0.0014 (11)	0.0040 (9)	−0.0043 (9)
C2	0.0401 (14)	0.0495 (15)	0.0460 (14)	0.0029 (11)	0.0072 (11)	−0.0005 (11)
C3	0.0609 (19)	0.0484 (16)	0.0590 (17)	0.0126 (14)	0.0167 (14)	0.0079 (13)
C4	0.089 (2)	0.0398 (15)	0.0565 (17)	−0.0039 (16)	0.0201 (16)	−0.0014 (13)
C5	0.078 (2)	0.0503 (17)	0.0503 (16)	−0.0165 (16)	−0.0018 (15)	−0.0045 (13)
C6	0.0549 (17)	0.0496 (16)	0.0466 (15)	−0.0044 (13)	−0.0089 (12)	−0.0029 (12)
C7	0.0316 (12)	0.0376 (12)	0.0391 (13)	−0.0010 (9)	0.0013 (9)	−0.0069 (9)
C8	0.0476 (15)	0.0488 (15)	0.0422 (14)	0.0012 (12)	0.0039 (11)	−0.0049 (11)
C9	0.0576 (19)	0.073 (2)	0.0532 (17)	−0.0070 (16)	0.0186 (14)	−0.0091 (14)
C10	0.0382 (16)	0.098 (3)	0.079 (2)	−0.0005 (17)	0.0159 (15)	−0.0185 (19)
C11	0.0372 (16)	0.099 (3)	0.077 (2)	0.0131 (17)	−0.0027 (15)	0.0028 (19)
C12	0.0375 (14)	0.074 (2)	0.0520 (16)	0.0047 (14)	−0.0032 (12)	0.0066 (14)
C13	0.0315 (12)	0.0511 (15)	0.0376 (13)	−0.0001 (11)	0.0003 (9)	0.0004 (10)
C14	0.071 (2)	0.0616 (18)	0.0406 (15)	−0.0094 (16)	−0.0008 (13)	−0.0016 (13)
C15	0.084 (3)	0.094 (3)	0.0366 (16)	−0.006 (2)	0.0003 (15)	0.0019 (15)
C16	0.061 (2)	0.089 (3)	0.0532 (18)	0.0060 (18)	0.0019 (14)	0.0264 (17)
C17	0.083 (2)	0.057 (2)	0.075 (2)	0.0048 (17)	0.0060 (18)	0.0206 (17)
C18	0.0634 (19)	0.0510 (16)	0.0500 (16)	0.0028 (14)	0.0056 (13)	0.0025 (12)
C19	0.0322 (12)	0.0544 (15)	0.0388 (13)	0.0037 (11)	0.0040 (10)	0.0020 (11)
C20	0.0343 (15)	0.149 (4)	0.0397 (16)	0.0009 (18)	0.0041 (12)	0.0065 (18)
C21	0.050 (2)	0.216 (5)	0.0391 (17)	0.012 (3)	0.0029 (14)	0.014 (2)
C22	0.0552 (19)	0.130 (3)	0.0398 (16)	0.003 (2)	0.0096 (14)	0.0117 (18)
C23	0.0424 (18)	0.189 (5)	0.057 (2)	−0.014 (2)	0.0133 (15)	0.020 (2)
C24	0.0335 (16)	0.187 (5)	0.0500 (18)	−0.010 (2)	0.0003 (13)	0.027 (2)
C25	0.0310 (12)	0.0510 (15)	0.0395 (13)	0.0027 (11)	−0.0025 (9)	0.0018 (10)
C26	0.0514 (17)	0.0591 (18)	0.0637 (18)	0.0077 (14)	0.0170 (14)	0.0090 (14)
C27	0.061 (2)	0.062 (2)	0.086 (2)	0.0031 (16)	0.0159 (17)	0.0233 (17)

C28	0.063 (2)	0.0486 (18)	0.085 (2)	0.0063 (15)	−0.0188 (17)	0.0062 (16)
C29	0.083 (2)	0.062 (2)	0.0531 (18)	0.0226 (17)	−0.0129 (16)	−0.0089 (15)
C30	0.0612 (18)	0.0606 (18)	0.0391 (14)	0.0126 (14)	0.0018 (12)	−0.0013 (12)
C31	0.0325 (13)	0.0571 (16)	0.0434 (14)	−0.0031 (11)	0.0015 (10)	−0.0024 (11)
C32	0.0399 (15)	0.0653 (18)	0.0490 (15)	0.0026 (13)	−0.0029 (11)	−0.0071 (13)
C33	0.0458 (17)	0.094 (3)	0.062 (2)	0.0034 (17)	−0.0155 (14)	−0.0098 (18)
C34	0.055 (2)	0.091 (3)	0.087 (3)	−0.0170 (19)	−0.0126 (18)	−0.022 (2)
C35	0.068 (2)	0.068 (2)	0.100 (3)	−0.0246 (19)	−0.008 (2)	−0.001 (2)
C36	0.0587 (19)	0.065 (2)	0.075 (2)	−0.0126 (16)	−0.0134 (16)	0.0073 (16)
C37	0.0434 (13)	0.0307 (11)	0.0336 (12)	−0.0012 (10)	0.0013 (9)	−0.0005 (9)
C38	0.0621 (18)	0.0366 (14)	0.0516 (16)	−0.0045 (12)	−0.0089 (13)	0.0096 (11)
C39	0.0626 (19)	0.0511 (17)	0.070 (2)	−0.0022 (14)	−0.0220 (15)	0.0145 (14)
C40	0.0469 (16)	0.0496 (16)	0.0642 (18)	−0.0078 (13)	−0.0104 (13)	−0.0004 (13)
C41	0.0415 (14)	0.0373 (13)	0.0423 (13)	−0.0034 (10)	0.0047 (10)	−0.0016 (10)
C42	0.0402 (13)	0.0298 (11)	0.0299 (11)	−0.0006 (9)	0.0033 (9)	−0.0030 (8)
C43	0.103 (3)	0.089 (3)	0.157 (4)	−0.014 (3)	−0.073 (3)	0.048 (3)
C44	0.0466 (15)	0.0401 (14)	0.0638 (17)	−0.0095 (12)	0.0057 (13)	−0.0008 (12)
C45	0.183 (7)	0.083 (4)	0.144 (5)	0.005 (5)	0.062 (6)	0.005 (3)
C46	0.159 (6)	0.175 (7)	0.127 (5)	−0.013 (5)	0.054 (5)	−0.004 (4)
N1	0.0385 (12)	0.0310 (10)	0.0351 (10)	−0.0014 (9)	0.0034 (8)	0.0018 (8)
N2	0.206 (8)	0.140 (6)	0.274 (9)	−0.020 (6)	0.072 (7)	0.026 (5)
O1	0.0611 (12)	0.0489 (11)	0.0392 (10)	−0.0095 (9)	0.0020 (8)	−0.0069 (8)
O2	0.0761 (14)	0.0386 (10)	0.0536 (11)	−0.0185 (10)	0.0004 (10)	0.0097 (8)
O3	0.0446 (11)	0.0458 (11)	0.0712 (13)	−0.0007 (9)	0.0112 (9)	−0.0014 (9)
S1	0.0466 (3)	0.0311 (3)	0.0392 (3)	−0.0061 (2)	0.0031 (2)	−0.0005 (2)
P1	0.0284 (3)	0.0482 (4)	0.0352 (3)	0.0018 (3)	0.0009 (2)	0.0012 (3)
P2	0.0309 (3)	0.0406 (3)	0.0328 (3)	0.0005 (2)	−0.0012 (2)	−0.0036 (2)

Geometric parameters (Å, °)

Ag1—N1	2.393 (2)	C25—C30	1.383 (4)
Ag1—P2	2.4955 (9)	C25—P1	1.826 (3)
Ag1—P1	2.5005 (8)	C26—C27	1.388 (5)
C1—C2	1.385 (4)	C26—H26	0.9300
C1—C6	1.399 (4)	C27—C28	1.372 (5)
C1—P2	1.828 (3)	C27—H27	0.9300
C2—C3	1.386 (4)	C28—C29	1.379 (5)
C2—H2	0.9300	C28—H28	0.9300
C3—C4	1.374 (5)	C29—C30	1.385 (4)
C3—H3	0.9300	C29—H29	0.9300
C4—C5	1.374 (5)	C30—H30	0.9300
C4—H4	0.9300	C31—C32	1.384 (4)
C5—C6	1.386 (4)	C31—C36	1.381 (4)
C5—H5	0.9300	C31—P1	1.830 (3)
C6—H6	0.9300	C32—C33	1.392 (4)
C7—C12	1.384 (4)	C32—H32	0.9300
C7—C8	1.393 (3)	C33—C34	1.361 (5)
C7—P2	1.825 (2)	C33—H33	0.9300
C8—C9	1.376 (4)	C34—C35	1.370 (5)

C8—H8	0.9300	C34—H34	0.9300
C9—C10	1.374 (5)	C35—C36	1.378 (4)
C9—H9	0.9300	C35—H35	0.9300
C10—C11	1.362 (5)	C36—H36	0.9300
C10—H10	0.9300	C37—C38	1.387 (3)
C11—C12	1.388 (4)	C37—C42	1.406 (3)
C11—H11	0.9300	C37—S1	1.777 (2)
C12—H12	0.9300	C38—C39	1.379 (4)
C13—C14	1.384 (4)	C38—H38	0.9300
C13—C18	1.388 (4)	C39—C40	1.386 (4)
C13—P2	1.836 (3)	C39—C43	1.528 (4)
C14—C15	1.399 (4)	C40—C41	1.380 (4)
C14—H14	0.9300	C40—H40	0.9300
C15—C16	1.354 (5)	C41—C42	1.403 (3)
C15—H15	0.9300	C41—C44	1.499 (3)
C16—C17	1.369 (5)	C42—N1	1.421 (3)
C16—H16	0.9300	C43—H43A	0.9600
C17—C18	1.390 (4)	C43—H43B	0.9600
C17—H17	0.9300	C43—H43C	0.9600
C18—H18	0.9300	C44—H44A	0.9600
C19—C20	1.356 (4)	C44—H44B	0.9600
C19—C24	1.371 (4)	C44—H44C	0.9600
C19—P1	1.825 (3)	C45—N2	1.141 (10)
C20—C21	1.378 (4)	C45—C46	1.428 (9)
C20—H20	0.9300	C46—H46A	0.9600
C21—C22	1.358 (5)	C46—H46B	0.9600
C21—H21	0.9300	C46—H46C	0.9600
C22—C23	1.343 (5)	N1—H1B	0.821 (17)
C22—H22	0.9300	N1—H1A	0.895 (16)
C23—C24	1.382 (5)	O1—S1	1.4513 (18)
C23—H23	0.9300	O2—S1	1.4522 (19)
C24—H24	0.9300	O3—S1	1.458 (2)
C25—C26	1.384 (4)		
N1—Ag1—P2	121.82 (6)	C29—C28—H28	120.2
N1—Ag1—P1	112.50 (6)	C28—C29—C30	120.1 (3)
P2—Ag1—P1	122.09 (3)	C28—C29—H29	120.0
C2—C1—C6	118.5 (2)	C30—C29—H29	120.0
C2—C1—P2	119.46 (19)	C25—C30—C29	120.9 (3)
C6—C1—P2	122.0 (2)	C25—C30—H30	119.6
C1—C2—C3	120.9 (3)	C29—C30—H30	119.6
C1—C2—H2	119.5	C32—C31—C36	118.6 (3)
C3—C2—H2	119.5	C32—C31—P1	123.6 (2)
C4—C3—C2	119.6 (3)	C36—C31—P1	117.8 (2)
C4—C3—H3	120.2	C31—C32—C33	119.6 (3)
C2—C3—H3	120.2	C31—C32—H32	120.2
C3—C4—C5	120.7 (3)	C33—C32—H32	120.2
C3—C4—H4	119.7	C34—C33—C32	120.7 (3)
C5—C4—H4	119.7	C34—C33—H33	119.6
C4—C5—C6	119.9 (3)	C32—C33—H33	119.6

C4—C5—H5	120.1	C33—C34—C35	120.2 (3)
C6—C5—H5	120.1	C33—C34—H34	119.9
C5—C6—C1	120.3 (3)	C35—C34—H34	119.9
C5—C6—H6	119.8	C36—C35—C34	119.6 (4)
C1—C6—H6	119.8	C36—C35—H35	120.2
C12—C7—C8	119.1 (2)	C34—C35—H35	120.2
C12—C7—P2	124.2 (2)	C35—C36—C31	121.3 (3)
C8—C7—P2	116.68 (19)	C35—C36—H36	119.4
C9—C8—C7	120.0 (3)	C31—C36—H36	119.4
C9—C8—H8	120.0	C38—C37—C42	120.1 (2)
C7—C8—H8	120.0	C38—C37—S1	119.73 (19)
C8—C9—C10	120.4 (3)	C42—C37—S1	120.12 (18)
C8—C9—H9	119.8	C39—C38—C37	121.6 (2)
C10—C9—H9	119.8	C39—C38—H38	119.2
C11—C10—C9	120.2 (3)	C37—C38—H38	119.2
C11—C10—H10	119.9	C38—C39—C40	117.5 (3)
C9—C10—H10	119.9	C38—C39—C43	121.7 (3)
C10—C11—C12	120.4 (3)	C40—C39—C43	120.8 (3)
C10—C11—H11	119.8	C41—C40—C39	123.2 (3)
C12—C11—H11	119.8	C41—C40—H40	118.4
C7—C12—C11	119.9 (3)	C39—C40—H40	118.4
C7—C12—H12	120.0	C40—C41—C42	118.8 (2)
C11—C12—H12	120.0	C40—C41—C44	120.6 (2)
C14—C13—C18	118.1 (3)	C42—C41—C44	120.6 (2)
C14—C13—P2	124.6 (2)	C37—C42—C41	118.8 (2)
C18—C13—P2	117.3 (2)	C37—C42—N1	121.2 (2)
C13—C14—C15	120.4 (3)	C41—C42—N1	120.0 (2)
C13—C14—H14	119.8	C39—C43—H43A	109.5
C15—C14—H14	119.8	C39—C43—H43B	109.5
C16—C15—C14	120.5 (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	120.0 (3)	H43B—C43—H43C	109.5
C15—C16—H16	120.0	C41—C44—H44A	109.5
C17—C16—H16	120.0	C41—C44—H44B	109.5
C16—C17—C18	120.3 (3)	H44A—C44—H44B	109.5
C16—C17—H17	119.9	C41—C44—H44C	109.5
C18—C17—H17	119.9	H44A—C44—H44C	109.5
C13—C18—C17	120.7 (3)	H44B—C44—H44C	109.5
C13—C18—H18	119.7	N2—C45—C46	178.5 (10)
C17—C18—H18	119.7	C45—C46—H46A	109.5
C20—C19—C24	116.9 (3)	C45—C46—H46B	109.5
C20—C19—P1	118.4 (2)	H46A—C46—H46B	109.5
C24—C19—P1	124.7 (2)	C45—C46—H46C	109.5
C19—C20—C21	122.1 (3)	H46A—C46—H46C	109.5
C19—C20—H20	118.9	H46B—C46—H46C	109.5
C21—C20—H20	118.9	C42—N1—Ag1	114.06 (14)
C22—C21—C20	120.0 (3)	C42—N1—H1B	113 (2)
C22—C21—H21	120.0	Ag1—N1—H1B	107 (2)

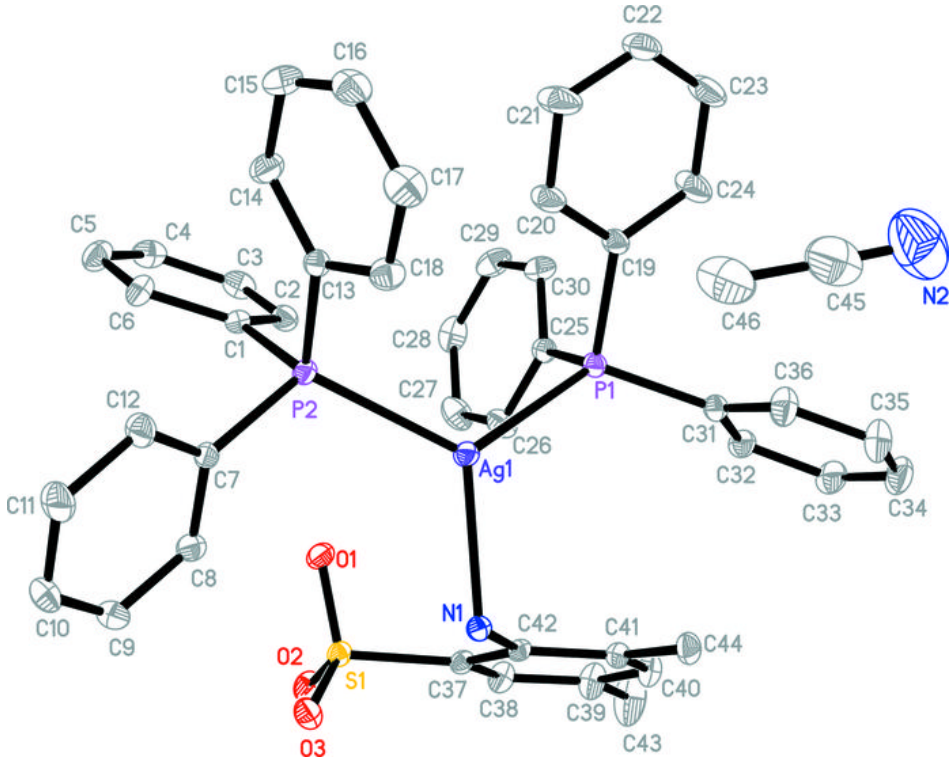
C20—C21—H21	120.0	C42—N1—H1A	103.8 (16)
C23—C22—C21	119.0 (3)	Ag1—N1—H1A	95.6 (18)
C23—C22—H22	120.5	H1B—N1—H1A	123 (2)
C21—C22—H22	120.5	O1—S1—O2	113.17 (12)
C22—C23—C24	120.9 (3)	O1—S1—O3	112.21 (12)
C22—C23—H23	119.6	O2—S1—O3	113.08 (13)
C24—C23—H23	119.6	O1—S1—C37	105.25 (11)
C19—C24—C23	121.1 (3)	O2—S1—C37	106.19 (12)
C19—C24—H24	119.5	O3—S1—C37	106.16 (11)
C23—C24—H24	119.5	C19—P1—C25	105.11 (12)
C26—C25—C30	118.4 (3)	C19—P1—C31	102.19 (12)
C26—C25—P1	117.3 (2)	C25—P1—C31	106.17 (12)
C30—C25—P1	123.9 (2)	C19—P1—Ag1	111.92 (9)
C25—C26—C27	120.7 (3)	C25—P1—Ag1	105.71 (8)
C25—C26—H26	119.7	C31—P1—Ag1	124.26 (9)
C27—C26—H26	119.7	C7—P2—C1	101.65 (11)
C28—C27—C26	120.3 (3)	C7—P2—C13	103.80 (11)
C28—C27—H27	119.9	C1—P2—C13	105.01 (11)
C26—C27—H27	119.9	C7—P2—Ag1	115.28 (8)
C27—C28—C29	119.6 (3)	C1—P2—Ag1	115.90 (8)
C27—C28—H28	120.2	C13—P2—Ag1	113.67 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.895 (16)	2.23 (2)	3.026 (3)	147.8 (18)
N1—H1B···O3	0.821 (17)	2.21 (2)	2.887 (3)	139 (2)

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

Fig. 1


C22
C16
C15
C23
C21
C17
C14
C24
C5
C4
C20
C29
C3
C19
C18
C45
N2
C2
C13
C30
C46
C6
C25
C28
C1
P1
C36
C27
P2
C12
C35
C31
C26
Ag1
C7
C32
C11
C33
C34
O1
C8
N1
C42
C41
C44
C10
C9
O2
S1
C37
C40
C38
C39
C43
O3