Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Di-μ-thiocyanato-bis[bis(tri-*p*-tolylphosphine)silver(I)] acetonitrile disolvate

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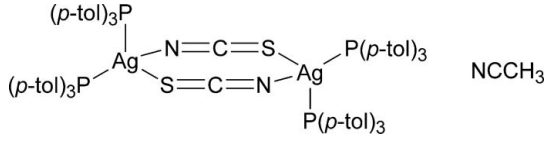
Received 12 November 2007; accepted 13 November 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.121; data-to-parameter ratio = 21.8.

In the centrosymmetric title compound, $[Ag_2(NCS)_2(C_{21}H_{21}P)_4]\cdot 2CH_3CN$, the Ag atom is coordinated by two phosphine ligands and two bridging thiocyanate ligands in a distorted tetrahedral configuration. The Ag—P bond distances are 2.4615 (7) and 2.5091 (7) Å, while the Ag—N and the Ag—S bond distances are 2.364 (2) and 2.3269 (18) Å, respectively. The crystal structure exhibits C—H···S hydrogen bonds.

Related literature

For a general introduction to the coordination chemistry of silver phosphine complexes, see: Meijboom *et al.* (2008). For the original preparation of silver phosphine complexes, see: Mann *et al.* (1937). For related silver(I) thiocyanate complexes, see: Bowmaker *et al.* (1997); Effendy *et al.* (2005). For related silver(I) tri-*p*-tolylphosphine complexes, see: Meijboom *et al.* (2006); Meijboom (2006, 2007); Meijboom & Muller (2006); Venter *et al.* (2006)7. For related literature, see: Allen (2002).



Experimental

Crystal data

$[Ag_2(NCS)_2(C_{21}H_{21}P)_4]\cdot 2C_2H_3N$
M_r = 1631.49
Triclinic, $P\overline{1}$
a = 10.8842 (5) Å
b = 13.8418 (7) Å
c = 15.4048 (8) Å
α = 75.839 (3)°
β = 69.345 (2)°
γ = 72.833 (2)°
V = 2049.11 (18) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 100 (2) K
0.43 × 0.28 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.766, T_{max} = 0.891
41388 measured reflections
10186 independent reflections
7349 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.121
S = 1.03
10186 reflections
467 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

P1—Ag	2.5091 (8)	N—C	1.149 (4)
P2—Ag	2.4612 (7)	S—C	1.653 (3)
Ag—N	2.363 (3)	S—Ag^{i}	2.5955 (9)
N—Ag—P1	95.55 (7)	P1—Ag—S^{i}	107.61 (3)
P2—Ag—P1	119.75 (3)	C—N—Ag	147.5 (2)
N—Ag—S^{i}	103.43 (7)	C—S—Ag^{i}	100.60 (11)
P2—Ag—S^{i}	112.43 (3)	N—C—S	178.2 (3)
P2—Ag—N—C	−164.1 (4)	S^{i}—Ag—N—C	−40.6 (5)
P1—Ag—N—C	69.0 (5)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C01—H01A···S^{i}	0.98	2.59	3.443 (6)	146

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Financial assistance from the South African National Research Foundation, the Research Fund of the University of the Free State and SASOL is gratefully acknowledged. Part of this material is based on work supported by the South African National Research Foundation (SA NRF, GUN 2038915). Opinions, findings, conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the NRF.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2355).

  doi:10.1107/S1600536807058837

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supplementary materials

Acta Cryst. (2007). E**63**, m3076-m3077 [**doi:10.1107/S1600536807058837**]

Di-μ-thiocyanato-bis[bis(tri-*p*-tolylphosphine)silver(I)] acetonitrile disolvate

G. J. S. Venter, R. Meijboom and A. Roodt

Comment

Silver(I) complexes of the type [AgL_nX] (L is a tertiary phosphine or arsine, n = 1–4 and X is a coordinating or noncoordinating anion) were first prepared by Mann *et al.* (1937) and were the first crystallographic examples of metal phosphine complexes. These compounds display a rich diversity of structural types due to the interplay of parameters such as the geometric flexibility of Ag(I), the bite angle, the electronic properties of the group 15 donor ligand, the coordination of the supporting ligand, *etc*. (Meijboom *et al.*, 2008).

We recently embarked on a structural research project aimed at the identification which roles the above mentioned properties play during the crystallization of simple silver(I) salts with Group 15 donor ligands. Initial focus on tri-*p*-tolylphosphine complexes (Meijboom *et al.*, 2006; Meijboom, 2006; Meijboom & Muller, 2006; Venter *et al.*, 2006; Meijboom, 2007) enable us to compare these structures with the isosteric triphenylphosphine complexes.

As part of the above mentioned series, we present here the title compound, (I), a silver(I) bis[tri(*p*-tolyl)phosphine] complex, of which only relatively few examples can be found in the literature [Cambridge Structural Database (CSD), Version 5.28, November 2006 update; Allen, 2002].

The Ag atom in compound (I) is surrounded by two phosphine ligands as well as an N and a S atom of two different thiocyanate ligands, forming a distorted tetrahedral configuration; selected geometric parameters are given in Table 1. The thiocyanate ligands form bridges to give a dimeric structure. In addition, some weak inter- and intramolecular interactions are observed (Table 2). All bond distances and angles are otherwise unremarkable.

Experimental

The title compound was synthesized by heating one equivalent of P(*p*-tol)$_3$ (0.324 g, 1.06 mmol) with AgSCN (0.176 g, 1.06 mmol) in acetonitrile (10.0 ml) under reflux. Recrystallization from acetone produced white crystals suitable for X-ray diffraction in quantitative yield (0.486 g, 97.1%).

Refinement

H atoms were positioned geometrically and refined using a riding model, with fixed C—H distances of 0.93 Å (CH) [U_{iso}(H) = 1.2U_{eq}] and 0.96 Å (CH_3) [U_{iso}(H) = 1.5U_{eq}]. The highest residual peak is 0.95 e located 0.78 Å from atom Ag and the deepest hole −0.62 e, 0.75 Å from Ag. A Hirschfield test failure appeared in the structure validation. Using a disordered model the U values of the Ag atoms were refined to an 98.6% occupancy, allowing the structure to pass the Hirschfield test.

Figures

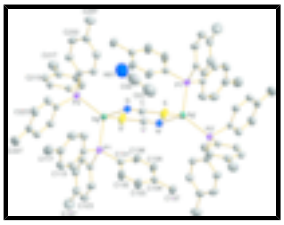

Fig. 1. The structure (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity. For the C atoms, the first digit indicates ring number and the second digit indicates the position of the atom in the ring. Primed atoms were generated by symmetry (1 − *x*, 1 − *y*, 1 − *z*).

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Crystal data

$[Ag_2(NCS)_2(C_{21}H_{21}P)_4]\cdot 2C_2H_3N$	$Z = 1$
$M_r = 1631.49$	$F_{000} = 844$
Triclinic, $P\overline{1}$	$D_x = 1.322$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.8842$ (5) Å	Cell parameters from 5879 reflections
$b = 13.8418$ (7) Å	$\theta = 2.3$–$23.8°$
$c = 15.4048$ (8) Å	$\mu = 0.65$ mm^{-1}
$\alpha = 75.839$ (3)°	$T = 100$ (2) K
$\beta = 69.345$ (2)°	Cuboid, colourless
$\gamma = 72.833$ (2)°	0.43 × 0.28 × 0.18 mm
$V = 2049.11$ (18) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	10186 independent reflections
Monochromator: graphite	7349 reflections with $I > 2\sigma(I)$
Detector resolution: 0 pixels mm^{-1}	$R_{int} = 0.037$
$T = 100$(2) K	$\theta_{max} = 28.4°$
ω and φ scans	$\theta_{min} = 1.9°$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -14\rightarrow14$
$T_{min} = 0.766$, $T_{max} = 0.891$	$k = -18\rightarrow18$
41388 measured reflections	$l = -20\rightarrow20$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 1.0074P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.121$	$\Delta\rho_{max} = 0.95$ e Å^{-3}

S = 1.03
10186 reflections
467 parameters

$\Delta\rho_{min}$ = −0.62 e Å^{-3}
Extinction correction: none

Special details

Experimental. The intensity data was collected on a Bruker X8 Apex II 4 K Kappa CCD diffractometer using an exposure time of 10 s/frame. A total of 1408 frames were collected with a frame width of 0.5° covering up to θ = 28.36° with 99.3% completeness accomplished.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N01	0.8035 (8)	0.8517 (7)	0.2119 (5)	0.181 (3)
C02	0.8093 (6)	0.7898 (6)	0.2777 (6)	0.123 (2)
C01	0.8191 (6)	0.7107 (6)	0.3612 (5)	0.139 (2)
H01A	0.8171	0.6448	0.3494	0.209*
H01B	0.7428	0.7307	0.4159	0.209*
H01C	0.9038	0.7043	0.3735	0.209*
P1	0.45861 (8)	0.33722 (6)	0.33462 (5)	0.04830 (18)
P2	0.33522 (8)	0.65463 (6)	0.22390 (5)	0.04649 (17)
Ag	0.44006 (2)	0.522764 (16)	0.332532 (15)	0.05329 (9)
N	0.3217 (3)	0.5219 (2)	0.49407 (18)	0.0596 (6)
S	0.32370 (9)	0.45764 (9)	0.68088 (6)	0.0755 (3)
C	0.3244 (3)	0.4944 (2)	0.5702 (2)	0.0517 (7)
C111	0.3066 (3)	0.3150 (2)	0.32640 (19)	0.0498 (7)
C112	0.3026 (4)	0.2392 (3)	0.2849 (2)	0.0657 (9)
H112	0.3842	0.194	0.2565	0.079*
C113	0.1803 (4)	0.2281 (3)	0.2841 (3)	0.0740 (10)
H113	0.1801	0.1748	0.2553	0.089*
C114	0.0598 (3)	0.2916 (3)	0.3235 (3)	0.0645 (9)
C115	0.0640 (4)	0.3680 (3)	0.3641 (3)	0.0715 (10)
H115	−0.0178	0.4138	0.3912	0.086*
C116	0.1839 (3)	0.3799 (3)	0.3665 (2)	0.0642 (8)
H116	0.1832	0.4329	0.3959	0.077*
C117	−0.0723 (4)	0.2789 (4)	0.3219 (3)	0.0927 (13)
H11A	−0.0546	0.2318	0.2784	0.139*
H11B	−0.1256	0.3455	0.3012	0.139*
H11C	−0.1226	0.251	0.3851	0.139*
C121	0.5996 (3)	0.2773 (2)	0.2425 (2)	0.0489 (6)
C122	0.6476 (3)	0.1721 (2)	0.2459 (2)	0.0636 (8)
H122	0.6048	0.1272	0.2975	0.076*
C123	0.7569 (4)	0.1320 (3)	0.1748 (3)	0.0730 (10)
H123	0.7876	0.0598	0.1784	0.088*

C124	0.8224 (3)	0.1942 (3)	0.0990 (3)	0.0692 (9)
C125	0.7767 (3)	0.2984 (3)	0.0961 (2)	0.0647 (8)
H125	0.8213	0.3428	0.045	0.078*
C126	0.6662 (3)	0.3398 (2)	0.1666 (2)	0.0551 (7)
H126	0.6359	0.412	0.1627	0.066*
C127	0.9419 (5)	0.1491 (4)	0.0214 (3)	0.1131 (17)
H12A	0.9629	0.0742	0.0372	0.17*
H12B	1.0203	0.1745	0.0148	0.17*
H12C	0.9198	0.1692	−0.0379	0.17*
C131	0.4852 (3)	0.2517 (2)	0.44051 (19)	0.0495 (6)
C132	0.4380 (5)	0.1640 (3)	0.4788 (3)	0.0909 (14)
H132	0.3838	0.1462	0.4512	0.109*
C133	0.4684 (5)	0.1014 (3)	0.5567 (3)	0.0928 (14)
H133	0.4356	0.0408	0.5811	0.111*
C134	0.5437 (4)	0.1239 (3)	0.5997 (2)	0.0649 (9)
C135	0.5942 (4)	0.2076 (3)	0.5603 (3)	0.0726 (10)
H135	0.651	0.2234	0.587	0.087*
C136	0.5653 (3)	0.2713 (3)	0.4818 (3)	0.0677 (9)
H136	0.6022	0.3301	0.4563	0.081*
C137	0.5763 (5)	0.0539 (3)	0.6853 (3)	0.0930 (14)
H13A	0.6359	0.0803	0.704	0.14*
H13B	0.6215	−0.0151	0.6701	0.14*
H13C	0.4927	0.0513	0.7372	0.14*
C211	0.4437 (3)	0.7267 (2)	0.12818 (19)	0.0473 (6)
C212	0.4250 (3)	0.7632 (2)	0.0403 (2)	0.0551 (7)
H212	0.3579	0.7449	0.0256	0.066*
C213	0.5037 (4)	0.8261 (3)	−0.0262 (2)	0.0642 (9)
H213	0.4895	0.8503	−0.0859	0.077*
C214	0.6017 (4)	0.8542 (3)	−0.0077 (2)	0.0619 (8)
C215	0.6228 (4)	0.8157 (3)	0.0789 (2)	0.0670 (9)
H215	0.692	0.8323	0.0926	0.08*
C216	0.5443 (3)	0.7530 (2)	0.1462 (2)	0.0591 (8)
H216	0.56	0.7279	0.2054	0.071*
C217	0.6843 (5)	0.9264 (3)	−0.0789 (3)	0.0908 (13)
H21A	0.6912	0.977	−0.0471	0.136*
H21B	0.6401	0.9616	−0.1273	0.136*
H21C	0.7748	0.8872	−0.1083	0.136*
C221	0.2629 (3)	0.5939 (2)	0.16666 (19)	0.0477 (6)
C222	0.1265 (3)	0.6102 (3)	0.1810 (2)	0.0644 (8)
H222	0.0655	0.6634	0.2143	0.077*
C223	0.0773 (4)	0.5504 (3)	0.1475 (3)	0.0724 (9)
H223	−0.0172	0.5634	0.1584	0.087*
C224	0.1611 (4)	0.4726 (3)	0.0990 (2)	0.0675 (9)
C225	0.2979 (4)	0.4586 (3)	0.0817 (3)	0.0719 (10)
H225	0.3588	0.4076	0.0457	0.086*
C226	0.3483 (4)	0.5174 (3)	0.1158 (2)	0.0636 (8)
H226	0.443	0.505	0.1041	0.076*
C227	0.1079 (6)	0.4033 (4)	0.0663 (4)	0.1025 (15)
H22A	0.1084	0.4291	0.001	0.154*

H22B	0.0154	0.4018	0.1062	0.154*
H22C	0.1653	0.3339	0.0704	0.154*
C231	0.1978 (3)	0.7558 (2)	0.27808 (19)	0.0471 (6)
C232	0.1569 (3)	0.8513 (2)	0.2292 (2)	0.0623 (8)
H232	0.1986	0.8659	0.1634	0.075*
C233	0.0550 (4)	0.9258 (3)	0.2755 (3)	0.0700 (9)
H233	0.0284	0.9908	0.2405	0.084*
C234	−0.0082 (3)	0.9086 (3)	0.3703 (2)	0.0612 (8)
C235	0.0337 (4)	0.8138 (3)	0.4184 (2)	0.0696 (9)
H235	−0.0086	0.7996	0.4841	0.084*
C236	0.1356 (4)	0.7384 (2)	0.3739 (2)	0.0625 (8)
H236	0.163	0.6741	0.4096	0.075*
C237	−0.1194 (4)	0.9897 (3)	0.4205 (3)	0.0917 (13)
H23A	−0.0812	1.0264	0.4478	0.138*
H23B	−0.1868	0.9572	0.4705	0.138*
H23C	−0.1623	1.0381	0.3756	0.138*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N01	0.176 (6)	0.208 (8)	0.162 (7)	−0.054 (6)	−0.043 (5)	−0.035 (6)
C02	0.085 (3)	0.152 (6)	0.142 (6)	−0.040 (4)	−0.012 (4)	−0.058 (5)
C01	0.119 (5)	0.161 (6)	0.135 (5)	−0.059 (4)	−0.002 (4)	−0.040 (5)
P1	0.0595 (4)	0.0380 (4)	0.0417 (4)	−0.0077 (3)	−0.0149 (3)	−0.0009 (3)
P2	0.0560 (4)	0.0399 (4)	0.0413 (4)	−0.0059 (3)	−0.0193 (3)	−0.0018 (3)
Ag	0.06801 (16)	0.04370 (13)	0.04507 (13)	−0.00633 (10)	−0.02247 (11)	−0.00144 (9)
N	0.0651 (16)	0.0592 (16)	0.0476 (15)	−0.0068 (13)	−0.0157 (12)	−0.0075 (12)
S	0.0586 (5)	0.1111 (8)	0.0462 (4)	−0.0207 (5)	−0.0171 (4)	0.0101 (5)
C	0.0435 (15)	0.0527 (17)	0.0484 (16)	−0.0051 (12)	−0.0091 (12)	−0.0039 (13)
C111	0.0601 (17)	0.0421 (15)	0.0406 (14)	−0.0082 (13)	−0.0152 (13)	0.0004 (12)
C112	0.0627 (19)	0.064 (2)	0.072 (2)	−0.0011 (16)	−0.0241 (17)	−0.0237 (17)
C113	0.076 (2)	0.074 (2)	0.083 (3)	−0.0118 (19)	−0.032 (2)	−0.026 (2)
C114	0.0611 (19)	0.061 (2)	0.066 (2)	−0.0133 (16)	−0.0229 (17)	0.0034 (16)
C115	0.0570 (19)	0.061 (2)	0.081 (2)	−0.0087 (16)	−0.0077 (17)	−0.0101 (18)
C116	0.066 (2)	0.0511 (18)	0.068 (2)	−0.0124 (15)	−0.0085 (16)	−0.0139 (16)
C117	0.074 (3)	0.093 (3)	0.114 (4)	−0.024 (2)	−0.036 (2)	−0.007 (3)
C121	0.0548 (16)	0.0432 (15)	0.0455 (15)	−0.0058 (12)	−0.0181 (13)	−0.0039 (12)
C122	0.070 (2)	0.0471 (18)	0.065 (2)	−0.0076 (15)	−0.0195 (17)	−0.0023 (15)
C123	0.073 (2)	0.055 (2)	0.085 (3)	0.0096 (17)	−0.029 (2)	−0.0220 (19)
C124	0.0568 (19)	0.084 (3)	0.061 (2)	0.0048 (18)	−0.0210 (16)	−0.0220 (19)
C125	0.0622 (19)	0.072 (2)	0.0479 (17)	−0.0096 (17)	−0.0127 (15)	−0.0012 (15)
C126	0.0617 (18)	0.0489 (17)	0.0495 (16)	−0.0082 (14)	−0.0196 (14)	−0.0002 (13)
C127	0.083 (3)	0.135 (4)	0.086 (3)	0.023 (3)	−0.008 (2)	−0.040 (3)
C131	0.0613 (17)	0.0409 (15)	0.0428 (14)	−0.0126 (13)	−0.0146 (13)	−0.0010 (12)
C132	0.143 (4)	0.090 (3)	0.073 (2)	−0.071 (3)	−0.063 (3)	0.028 (2)
C133	0.149 (4)	0.080 (3)	0.075 (2)	−0.066 (3)	−0.060 (3)	0.031 (2)
C134	0.096 (3)	0.0499 (18)	0.0531 (18)	−0.0127 (17)	−0.0352 (18)	−0.0015 (14)
C135	0.075 (2)	0.075 (2)	0.074 (2)	−0.0207 (19)	−0.0414 (19)	0.0083 (19)

C136	0.064 (2)	0.066 (2)	0.073 (2)	−0.0252 (17)	−0.0310 (18)	0.0156 (17)
C137	0.148 (4)	0.068 (2)	0.072 (2)	−0.022 (3)	−0.062 (3)	0.013 (2)
C211	0.0540 (16)	0.0425 (15)	0.0416 (14)	−0.0061 (12)	−0.0154 (12)	−0.0048 (11)
C212	0.0676 (19)	0.0540 (18)	0.0439 (15)	−0.0122 (15)	−0.0212 (14)	−0.0037 (13)
C213	0.087 (2)	0.0565 (19)	0.0389 (15)	−0.0092 (17)	−0.0183 (16)	−0.0004 (14)
C214	0.071 (2)	0.0533 (18)	0.0509 (17)	−0.0140 (16)	−0.0068 (16)	−0.0083 (14)
C215	0.068 (2)	0.070 (2)	0.065 (2)	−0.0237 (17)	−0.0210 (17)	−0.0043 (17)
C216	0.070 (2)	0.0566 (18)	0.0508 (17)	−0.0150 (15)	−0.0249 (15)	0.0020 (14)
C217	0.107 (3)	0.081 (3)	0.067 (2)	−0.038 (2)	0.000 (2)	0.001 (2)
C221	0.0601 (17)	0.0393 (14)	0.0428 (14)	−0.0066 (12)	−0.0210 (13)	−0.0024 (11)
C222	0.0615 (19)	0.070 (2)	0.063 (2)	−0.0094 (16)	−0.0188 (16)	−0.0194 (17)
C223	0.069 (2)	0.085 (3)	0.071 (2)	−0.024 (2)	−0.0254 (18)	−0.013 (2)
C224	0.098 (3)	0.0537 (19)	0.062 (2)	−0.0219 (19)	−0.042 (2)	0.0025 (16)
C225	0.094 (3)	0.0519 (19)	0.075 (2)	0.0012 (18)	−0.040 (2)	−0.0207 (17)
C226	0.0651 (19)	0.0539 (19)	0.074 (2)	0.0008 (15)	−0.0301 (17)	−0.0170 (16)
C227	0.147 (4)	0.080 (3)	0.113 (4)	−0.039 (3)	−0.073 (3)	−0.008 (3)
C231	0.0554 (16)	0.0427 (15)	0.0426 (14)	−0.0084 (12)	−0.0186 (12)	−0.0034 (11)
C232	0.068 (2)	0.0521 (18)	0.0522 (17)	−0.0075 (15)	−0.0128 (15)	0.0028 (14)
C233	0.072 (2)	0.0428 (17)	0.078 (2)	−0.0015 (15)	−0.0184 (19)	−0.0009 (16)
C234	0.0607 (18)	0.0525 (18)	0.071 (2)	−0.0077 (15)	−0.0196 (17)	−0.0173 (16)
C235	0.082 (2)	0.067 (2)	0.0473 (17)	−0.0051 (18)	−0.0132 (17)	−0.0112 (16)
C236	0.081 (2)	0.0491 (18)	0.0478 (17)	−0.0027 (16)	−0.0214 (16)	−0.0030 (14)
C237	0.084 (3)	0.071 (3)	0.103 (3)	0.002 (2)	−0.011 (2)	−0.031 (2)

Geometric parameters (Å, °)

N01—C02	1.163 (9)	C133—H133	0.95
C02—C01	1.485 (9)	C134—C135	1.345 (5)
C01—H01A	0.98	C134—C137	1.519 (4)
C01—H01B	0.98	C135—C136	1.387 (5)
C01—H01C	0.98	C135—H135	0.95
P1—C111	1.821 (3)	C136—H136	0.95
P1—C131	1.825 (3)	C137—H13A	0.98
P1—C121	1.829 (3)	C137—H13B	0.98
P1—Ag	2.5091 (8)	C137—H13C	0.98
P2—C211	1.820 (3)	C211—C216	1.381 (4)
P2—C221	1.830 (3)	C211—C212	1.389 (4)
P2—C231	1.830 (3)	C212—C213	1.388 (4)
P2—Ag	2.4612 (7)	C212—H212	0.95
Ag—N	2.363 (3)	C213—C214	1.372 (5)
Ag—S^{i}	2.5955 (10)	C213—H213	0.95
N—C	1.149 (4)	C214—C215	1.383 (5)
S—C	1.653 (3)	C214—C217	1.520 (5)
S—Ag^{i}	2.5955 (9)	C215—C216	1.389 (5)
C111—C112	1.373 (4)	C215—H215	0.95
C111—C116	1.398 (4)	C216—H216	0.95
C112—C113	1.390 (5)	C217—H21A	0.98
C112—H112	0.95	C217—H21B	0.98
C113—C114	1.371 (5)	C217—H21C	0.98

C113—H113	0.95	C221—C222	1.378 (4)
C114—C115	1.372 (5)	C221—C226	1.382 (4)
C114—C117	1.510 (5)	C222—C223	1.380 (5)
C115—C116	1.376 (5)	C222—H222	0.95
C115—H115	0.95	C223—C224	1.372 (5)
C116—H116	0.95	C223—H223	0.95
C117—H11A	0.98	C224—C225	1.379 (5)
C117—H11B	0.98	C224—C227	1.511 (5)
C117—H11C	0.98	C225—C226	1.383 (5)
C121—C126	1.385 (4)	C225—H225	0.95
C121—C122	1.390 (4)	C226—H226	0.95
C122—C123	1.381 (5)	C227—H22A	0.98
C122—H122	0.95	C227—H22B	0.98
C123—C124	1.377 (5)	C227—H22C	0.98
C123—H123	0.95	C231—C236	1.383 (4)
C124—C125	1.375 (5)	C231—C232	1.383 (4)
C124—C127	1.516 (5)	C232—C233	1.390 (5)
C125—C126	1.389 (5)	C232—H232	0.95
C125—H125	0.95	C233—C234	1.370 (5)
C126—H126	0.95	C233—H233	0.95
C127—H12A	0.98	C234—C235	1.373 (5)
C127—H12B	0.98	C234—C237	1.512 (5)
C127—H12C	0.98	C235—C236	1.386 (5)
C131—C136	1.362 (4)	C235—H235	0.95
C131—C132	1.375 (4)	C236—H236	0.95
C132—C133	1.379 (5)	C237—H23A	0.98
C132—H132	0.95	C237—H23B	0.98
C133—C134	1.357 (5)	C237—H23C	0.98
N01—C02—C01	179.1 (7)	C135—C134—C137	121.4 (3)
C02—C01—H01A	109.5	C133—C134—C137	121.3 (3)
C02—C01—H01B	109.5	C134—C135—C136	121.6 (3)
H01A—C01—H01B	109.5	C134—C135—H135	119.2
C02—C01—H01C	109.5	C136—C135—H135	119.2
H01A—C01—H01C	109.5	C131—C136—C135	121.5 (3)
H01B—C01—H01C	109.5	C131—C136—H136	119.2
C111—P1—C131	104.29 (13)	C135—C136—H136	119.2
C111—P1—C121	106.51 (13)	C134—C137—H13A	109.5
C131—P1—C121	101.71 (13)	C134—C137—H13B	109.5
C111—P1—Ag	112.36 (10)	H13A—C137—H13B	109.5
C131—P1—Ag	115.15 (10)	C134—C137—H13C	109.5
C121—P1—Ag	115.59 (10)	H13A—C137—H13C	109.5
C211—P2—C221	105.03 (13)	H13B—C137—H13C	109.5
C211—P2—C231	102.62 (13)	C216—C211—C212	118.1 (3)
C221—P2—C231	106.15 (13)	C216—C211—P2	118.0 (2)
C211—P2—Ag	117.54 (9)	C212—C211—P2	123.7 (2)
C221—P2—Ag	109.03 (9)	C213—C212—C211	120.4 (3)
C231—P2—Ag	115.44 (9)	C213—C212—H212	119.8
N—Ag—P2	115.81 (7)	C211—C212—H212	119.8
N—Ag—P1	95.55 (7)	C214—C213—C212	121.6 (3)

P2—Ag—P1	119.75 (3)	C214—C213—H213	119.2
N—Ag—S^{i}	103.43 (7)	C212—C213—H213	119.2
P2—Ag—S^{i}	112.43 (3)	C213—C214—C215	118.0 (3)
P1—Ag—S^{i}	107.61 (3)	C213—C214—C217	121.7 (3)
C—N—Ag	147.5 (2)	C215—C214—C217	120.3 (4)
C—S—Ag^{i}	100.60 (11)	C214—C215—C216	121.0 (3)
N—C—S	178.2 (3)	C214—C215—H215	119.5
C112—C111—C116	117.5 (3)	C216—C215—H215	119.5
C112—C111—P1	125.4 (2)	C211—C216—C215	120.9 (3)
C116—C111—P1	117.2 (2)	C211—C216—H216	119.5
C111—C112—C113	120.5 (3)	C215—C216—H216	119.5
C111—C112—H112	119.7	C214—C217—H21A	109.5
C113—C112—H112	119.7	C214—C217—H21B	109.5
C114—C113—C112	122.0 (3)	H21A—C217—H21B	109.5
C114—C113—H113	119	C214—C217—H21C	109.5
C112—C113—H113	119	H21A—C217—H21C	109.5
C113—C114—C115	117.4 (3)	H21B—C217—H21C	109.5
C113—C114—C117	121.5 (4)	C222—C221—C226	117.7 (3)
C115—C114—C117	121.1 (3)	C222—C221—P2	123.9 (2)
C114—C115—C116	121.6 (3)	C226—C221—P2	117.9 (2)
C114—C115—H115	119.2	C221—C222—C223	120.9 (3)
C116—C115—H115	119.2	C221—C222—H222	119.5
C115—C116—C111	121.0 (3)	C223—C222—H222	119.5
C115—C116—H116	119.5	C224—C223—C222	121.8 (4)
C111—C116—H116	119.5	C224—C223—H223	119.1
C114—C117—H11A	109.5	C222—C223—H223	119.1
C114—C117—H11B	109.5	C223—C224—C225	117.3 (3)
H11A—C117—H11B	109.5	C223—C224—C227	122.3 (4)
C114—C117—H11C	109.5	C225—C224—C227	120.4 (4)
H11A—C117—H11C	109.5	C224—C225—C226	121.4 (3)
H11B—C117—H11C	109.5	C224—C225—H225	119.3
C126—C121—C122	117.7 (3)	C226—C225—H225	119.3
C126—C121—P1	118.6 (2)	C221—C226—C225	120.9 (3)
C122—C121—P1	123.7 (2)	C221—C226—H226	119.5
C123—C122—C121	120.6 (3)	C225—C226—H226	119.5
C123—C122—H122	119.7	C224—C227—H22A	109.5
C121—C122—H122	119.7	C224—C227—H22B	109.5
C124—C123—C122	121.6 (3)	H22A—C227—H22B	109.5
C124—C123—H123	119.2	C224—C227—H22C	109.5
C122—C123—H123	119.2	H22A—C227—H22C	109.5
C125—C124—C123	118.0 (3)	H22B—C227—H22C	109.5
C125—C124—C127	121.0 (4)	C236—C231—C232	117.8 (3)
C123—C124—C127	121.0 (4)	C236—C231—P2	118.6 (2)
C124—C125—C126	121.0 (3)	C232—C231—P2	123.5 (2)
C124—C125—H125	119.5	C231—C232—C233	120.5 (3)
C126—C125—H125	119.5	C231—C232—H232	119.8
C121—C126—C125	121.0 (3)	C233—C232—H232	119.8
C121—C126—H126	119.5	C234—C233—C232	122.0 (3)

C125—C126—H126	119.5	C234—C233—H233	119
C124—C127—H12A	109.5	C232—C233—H233	119
C124—C127—H12B	109.5	C233—C234—C235	117.1 (3)
H12A—C127—H12B	109.5	C233—C234—C237	121.9 (3)
C124—C127—H12C	109.5	C235—C234—C237	121.0 (3)
H12A—C127—H12C	109.5	C234—C235—C236	122.0 (3)
H12B—C127—H12C	109.5	C234—C235—H235	119
C136—C131—C132	116.7 (3)	C236—C235—H235	119
C136—C131—P1	118.3 (2)	C231—C236—C235	120.6 (3)
C132—C131—P1	124.9 (2)	C231—C236—H236	119.7
C131—C132—C133	120.8 (3)	C235—C236—H236	119.7
C131—C132—H132	119.6	C234—C237—H23A	109.5
C133—C132—H132	119.6	C234—C237—H23B	109.5
C134—C133—C132	122.1 (3)	H23A—C237—H23B	109.5
C134—C133—H133	119	C234—C237—H23C	109.5
C132—C133—H133	119	H23A—C237—H23C	109.5
C135—C134—C133	117.2 (3)	H23B—C237—H23C	109.5
C211—P2—Ag—N	134.40 (13)	C136—C131—C132—C133	1.7 (7)
C221—P2—Ag—N	−106.31 (13)	P1—C131—C132—C133	177.0 (4)
C231—P2—Ag—N	13.01 (13)	C131—C132—C133—C134	1.0 (8)
C211—P2—Ag—P1	−112.01 (11)	C132—C133—C134—C135	−3.4 (7)
C221—P2—Ag—P1	7.28 (11)	C132—C133—C134—C137	−179.9 (5)
C231—P2—Ag—P1	126.61 (11)	C133—C134—C135—C136	3.1 (6)
C211—P2—Ag—S^i	15.79 (11)	C137—C134—C135—C136	179.6 (4)
C221—P2—Ag—S^i	135.08 (10)	C132—C131—C136—C135	−1.9 (6)
C231—P2—Ag—S^i	−105.59 (11)	P1—C131—C136—C135	−177.6 (3)
C111—P1—Ag—N	82.47 (12)	C134—C135—C136—C131	−0.5 (6)
C131—P1—Ag—N	−36.74 (13)	C221—P2—C211—C216	−159.2 (2)
C121—P1—Ag—N	−155.00 (12)	C231—P2—C211—C216	90.0 (3)
C111—P1—Ag—P2	−41.54 (10)	Ag—P2—C211—C216	−37.8 (3)
C131—P1—Ag—P2	−160.75 (11)	C221—P2—C211—C212	25.7 (3)
C121—P1—Ag—P2	80.99 (11)	C231—P2—C211—C212	−85.1 (3)
C111—P1—Ag—S^i	−171.52 (10)	Ag—P2—C211—C212	147.1 (2)
C131—P1—Ag—S^i	69.27 (11)	C216—C211—C212—C213	−1.4 (5)
C121—P1—Ag—S^i	−48.99 (10)	P2—C211—C212—C213	173.6 (2)
P2—Ag—N—C	−164.1 (4)	C211—C212—C213—C214	0.0 (5)
P1—Ag—N—C	69.0 (5)	C212—C213—C214—C215	1.7 (5)
S^i—Ag—N—C	−40.6 (5)	C212—C213—C214—C217	−177.5 (3)
C131—P1—C111—C112	−85.8 (3)	C213—C214—C215—C216	−2.0 (5)
C121—P1—C111—C112	21.3 (3)	C217—C214—C215—C216	177.3 (4)
Ag—P1—C111—C112	148.9 (3)	C212—C211—C216—C215	1.2 (5)
C131—P1—C111—C116	93.6 (3)	P2—C211—C216—C215	−174.2 (3)
C121—P1—C111—C116	−159.3 (2)	C214—C215—C216—C211	0.6 (5)
Ag—P1—C111—C116	−31.8 (3)	C211—P2—C221—C222	−120.2 (3)
C116—C111—C112—C113	−0.4 (5)	C231—P2—C221—C222	−12.0 (3)
P1—C111—C112—C113	178.9 (3)	Ag—P2—C221—C222	113.0 (3)
C111—C112—C113—C114	0.4 (6)	C211—P2—C221—C226	68.5 (3)

C112—C113—C114—C115	0.3 (6)	C231—P2—C221—C226	176.7 (2)
C112—C113—C114—C117	179.8 (4)	Ag—P2—C221—C226	−58.3 (3)
C113—C114—C115—C116	−0.9 (5)	C226—C221—C222—C223	1.6 (5)
C117—C114—C115—C116	179.5 (4)	P2—C221—C222—C223	−169.7 (3)
C114—C115—C116—C111	0.8 (5)	C221—C222—C223—C224	0.1 (6)
C112—C111—C116—C115	−0.2 (5)	C222—C223—C224—C225	−2.3 (5)
P1—C111—C116—C115	−179.5 (3)	C222—C223—C224—C227	176.9 (4)
C111—P1—C121—C126	110.7 (2)	C223—C224—C225—C226	3.0 (5)
C131—P1—C121—C126	−140.3 (2)	C227—C224—C225—C226	−176.2 (3)
Ag—P1—C121—C126	−14.9 (3)	C222—C221—C226—C225	−0.9 (5)
C111—P1—C121—C122	−71.8 (3)	P2—C221—C226—C225	171.0 (3)
C131—P1—C121—C122	37.1 (3)	C224—C225—C226—C221	−1.5 (5)
Ag—P1—C121—C122	162.6 (2)	C211—P2—C231—C236	−147.7 (3)
C126—C121—C122—C123	−0.9 (5)	C221—P2—C231—C236	102.3 (3)
P1—C121—C122—C123	−178.3 (3)	Ag—P2—C231—C236	−18.6 (3)
C121—C122—C123—C124	0.4 (6)	C211—P2—C231—C232	28.9 (3)
C122—C123—C124—C125	0.6 (6)	C221—P2—C231—C232	−81.1 (3)
C122—C123—C124—C127	−179.8 (4)	Ag—P2—C231—C232	158.0 (2)
C123—C124—C125—C126	−1.2 (5)	C236—C231—C232—C233	−1.0 (5)
C127—C124—C125—C126	179.3 (4)	P2—C231—C232—C233	−177.6 (3)
C122—C121—C126—C125	0.4 (5)	C231—C232—C233—C234	0.1 (6)
P1—C121—C126—C125	178.0 (2)	C232—C233—C234—C235	0.3 (6)
C124—C125—C126—C121	0.7 (5)	C232—C233—C234—C237	−179.7 (4)
C111—P1—C131—C136	−160.5 (3)	C233—C234—C235—C236	0.2 (6)
C121—P1—C131—C136	88.9 (3)	C237—C234—C235—C236	−179.8 (4)
Ag—P1—C131—C136	−36.9 (3)	C232—C231—C236—C235	1.4 (5)
C111—P1—C131—C132	24.2 (4)	P2—C231—C236—C235	178.2 (3)
C121—P1—C131—C132	−86.4 (4)	C234—C235—C236—C231	−1.1 (6)
Ag—P1—C131—C132	147.8 (3)		

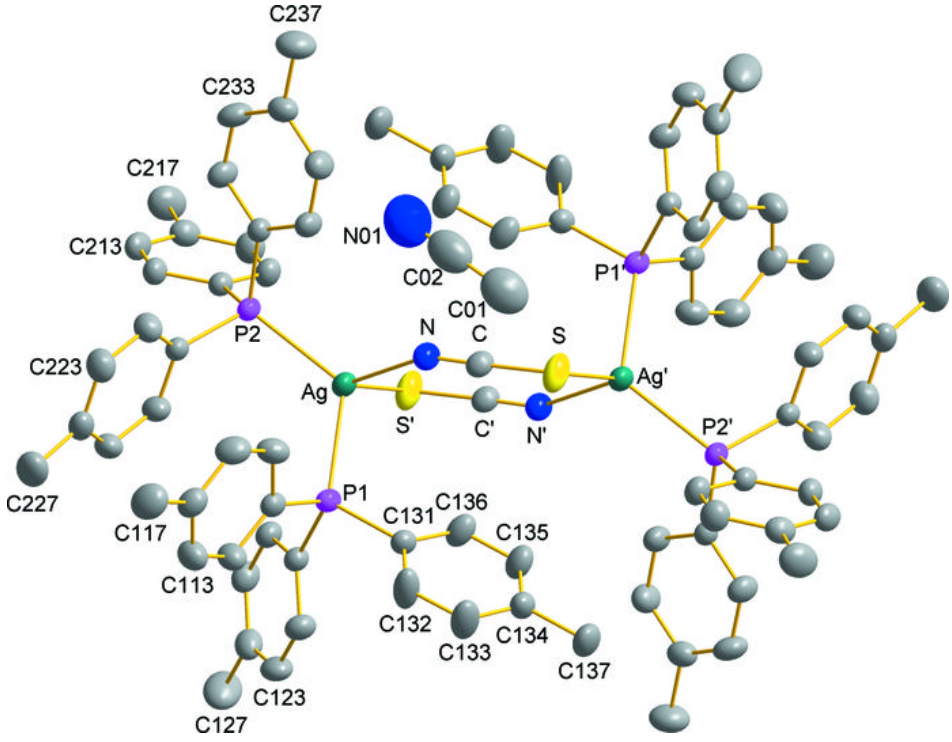
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C01—H01A···S^{i}	0.98	2.59	3.443 (6)	146

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

Fig. 1


C237
C233
C217
C213
N01
C02
C01
P1'
P2
N
C
S
C223
Ag
Ag'
S'
C'
N'
P2'
C227
P1
C131
C136
C135
C117
C113
C132
C133
C134
C137
C123
C127